

Delocalization and quantum diffusion of random band matrices in high dimensions II: T -expansion

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We consider Green's functions $G(z) := (H - z)^{-1}$ of Hermitian random band matrices H on the d -dimensional lattice $(\mathbb{Z}/L\mathbb{Z})^d$. The entries $h_{xy} = \bar{h}_{yx}$ of H are independent centered complex Gaussian random variables with variances $s_{xy} = \mathbb{E}|h_{xy}|^2$, which satisfy a banded profile so that s_{xy} is negligible if $|x - y|$ exceeds the band width W . For any fixed $n \in \mathbb{N}$, we construct an expansion of the T -variable, $T_{xy} = |m|^2 \sum_{\alpha} s_{x\alpha} |G_{\alpha y}|^2$, with an error $\mathcal{O}(W^{-nd/2})$, and use it to prove a local law on the Green's function. This T -expansion was the main tool to prove the delocalization and quantum diffusion of random band matrices for dimensions $d \geq 8$ in part I [32] of this series.

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1 INTRODUCTION

Random band matrices $H = (h_{xy})$ model interacting quantum systems on a lattice of scale L with random transition amplitudes effective up to a short scale $W \ll L$. In this paper, we consider a general Hermitian random band matrix ensemble on the d -dimensional integer lattice $\mathbb{Z}_L^d := \{1, 2, \dots, L\}^d$ with $N := L^d$ many lattice sites. The entries of H are independent centered random variables up to the Hermitian condition $h_{xy} = \overline{h_{yx}}$. The variance $s_{xy} := \mathbb{E}|h_{xy}|^2$ typically decays with the distance between x and y on a characteristic length scale W , called the *band width* of H , and is negligible when $|x - y| \gg W$. We require that s_{xy} satisfy the normalization condition

$$\sum_x s_{xy} = \sum_y s_{xy} = 1. \quad (1.1)$$

It is well-known that under the condition (1.1), the global eigenvalue distribution of H converges weakly to the Wigner's semicircle law supported in $[-2, 2]$.

As W varies, random band matrices naturally interpolate between the random Schrödinger operator [1] and mean-field (generalized) Wigner matrix ensembles [30]. One important conjecture about random band matrices is that a sharp *localization-delocalization transition* occurs at some critical band width W_c . An eigenvector is said to be *localized* if most of its weight resides in a region of scale $\ell \ll L$, and *delocalized* if $\ell \sim L$. In physics, this length scale ℓ is called the *localization length*, which generally depends on the energy level of the eigenvector. We restrict ourselves to the bulk eigenvectors with eigenvalues in $(-2 + \kappa, 2 - \kappa)$ for a small constant $\kappa > 0$. It is conjectured that there exists $W_c \in [1, L]$ such that if $W \ll W_c$, the bulk eigenvectors of H are localized, while if $W \gg W_c$, the bulk eigenvectors of H are delocalized. Based on simulations [7, 8, 15, 31] and non-rigorous supersymmetric arguments [16], the critical band width of one-dimensional random band matrices is conjectured to be of order $W_c \sim \sqrt{L}$. In higher dimensions, the critical band width is conjectured to be $W_c \sim \sqrt{\log L}$ when $d = 2$ and $W_c \sim 1$ when $d \geq 3$; see [3, 27–29] for more details about these conjectures.

Many partial results have been proved rigorously concerning the localization-delocalization conjecture of random band matrices in dimension $d = 1$ [2, 4–6, 9, 10, 12, 13, 17–26, 33] and dimensions $d \geq 2$ [9, 10, 12, 17, 33]. We refer the reader to the introduction of [32] for a brief review. In this series (i.e. part I [32] and the current paper), we prove that, as long as $W \geq L^\varepsilon$ for a small constant $\varepsilon > 0$, most bulk eigenvectors of H have localization lengths comparable to L . This gives a positive answer to the delocalization conjecture (in the weak delocalization sense) for dimensions $d \geq 8$ under the slightly stronger assumption $W \geq L^\varepsilon$ (vs. $W \geq C$).

In part I [32], we described the main structure of the proof of the delocalization conjecture and quantum diffusion of random band matrices. This paper will provide some key results used in [32]. Our proof is based on the resolvent (or Green's function) of H defined by

$$G(z) = (H - z)^{-1}, \quad z \in \mathbb{C}_+ := \{x \in \mathbb{C} : \text{Im } z > 0\},$$

and the T -matrix defined by [12]

$$T_{xy}(z) := |m|^2 \sum_\alpha s_{x\alpha} |G_{\alpha y}(z)|^2, \quad x, y \in \mathbb{Z}_L^d. \quad (1.2)$$

An important tool is an expansion of the T -matrix, called the *T -expansion*, with errors of order $W^{-nd/2}$ for $n \in \mathbb{N}$. In [32], we defined basic graph operations in constructing the T -expansion (see Section 4), studied the local expansion strategy, and explored a key self-energy renormalization property. In this paper, we will describe the subtle global expansion strategy (see Sections 5 and 6) and complete the construction of the T -expansion up to any fixed order. The T -expansion thus obtained gives a precise description of the fluctuation of the T -matrix by decomposing it into a sum of terms with sophisticated but sufficiently nice structures. Furthermore, given an n -th order T -expansion for any fixed $n \in \mathbb{N}$, we will use it to prove an almost sharp local law on $G(z)$ (cf. Theorem 3.6), which is also a key input for [32]. For the convenience of the reader, we will repeat some notations and definitions of [32] in Sections 2–4 so that this paper is relatively self-contained.

1.1 The model and T -expansion

We will consider d -dimensional random band matrices indexed by a cube of linear size L in \mathbb{Z}^d , i.e.,

$$\mathbb{Z}_L^d := (\mathbb{Z} \cap (-L/2, L/2))^d. \quad (1.3)$$

We will view \mathbb{Z}_L^d as a torus and denote by $[x - y]_L$ the representative of $x - y$ in \mathbb{Z}_L^d , i.e.,

$$[x - y]_L := [(x - y) + LZ^d] \cap \mathbb{Z}_L^d. \quad (1.4)$$

Clearly, $\|x - y\|_L := \|[x - y]_L\|$ is a periodic distance on \mathbb{Z}_L^d for any norm $\|\cdot\|$ on \mathbb{Z}^d . For definiteness, we use ℓ^∞ -norm in this paper, i.e. $\|x - y\|_L := \|[x - y]_L\|_\infty$. In this paper, we consider the following class of d -dimensional random band matrices.

Assumption 1.1 (Random band matrix). *Fix any $d \in \mathbb{N}$. For $L \gg W \gg 1$ and $N := L^d$, we assume that $H \equiv H_{d,f,W,L}$ is an $N \times N$ complex Hermitian random matrix whose entries $(\operatorname{Re} h_{xy}, \operatorname{Im} h_{xy} : x, y \in \mathbb{Z}_L^d)$ are independent Gaussian random variables (up to symmetry $H = H^\dagger$) such that*

$$\mathbb{E}h_{xy} = 0, \quad \mathbb{E}(\operatorname{Re} h_{xy})^2 = \mathbb{E}(\operatorname{Im} h_{xy})^2 = s_{xy}/2, \quad x, y \in \mathbb{Z}_L^d, \quad (1.5)$$

where the variances s_{xy} satisfy that

$$s_{xy} = f_{W,L}([x - y]_L) \quad (1.6)$$

for a positive symmetric function $f_{W,L}$ satisfying Assumption 1.2 below. Then we say that H is a d -dimensional random band matrix with linear size L , band width W and variance profile $f_{W,L}$. Denote the variance matrix by $S := (s_{xy})_{x,y \in \mathbb{Z}_L^d}$, which is a doubly stochastic symmetric $N \times N$ matrix.

Assumption 1.2 (Variance profile). *We assume that $f_{W,L} : \mathbb{Z}_L^d \rightarrow \mathbb{R}_+$ is a positive symmetric function on \mathbb{Z}_L^d that can be expressed by the Fourier transform*

$$f_{W,L}(x) := \frac{1}{(2\pi)^d Z_{W,L}} \int \psi(Wp) e^{ip \cdot x} dp. \quad (1.7)$$

Here $Z_{W,L}$ is the normalization constant so that $\sum_{x \in \mathbb{Z}_L^d} f_{W,L}(x) = 1$, and $\psi \in C^\infty(\mathbb{R}^d)$ is a symmetric smooth function independent of W and L and satisfies the following properties:

- (i) $\psi(0) = 1$ and $\|\psi\|_\infty \leq 1$;
- (ii) $\psi(p) \leq \max\{1 - c_\psi |p|^2, 1 - c_\psi\}$ for a constant $c_\psi > 0$;
- (iii) ψ is in the Schwartz space, i.e.,

$$\lim_{|p| \rightarrow \infty} (1 + |p|)^k |\psi^{(l)}(p)| = 0, \quad \text{for any } k, l \in \mathbb{N}. \quad (1.8)$$

Clearly, $f_{W,L}$ is of order $O(W^{-d})$ and decays faster than any polynomial, that is, for any fixed $k \in \mathbb{N}$, there exists a constant $C_k > 0$ so that

$$|f_{W,L}(x)| \leq C_k W^{-d} (\|x\|_L/W)^{-k}. \quad (1.9)$$

Hence the variance profile S defined in (1.6) has a banded structure, namely, for any constants $\tau, D > 0$,

$$\mathbf{1}_{|x-y| \geq W^{1+\tau}} |s_{xy}| \leq W^{-D}. \quad (1.10)$$

Combining (1.8) and (1.9) with the Poisson summation formula, we obtain that

$$Z_{W,L} = \psi(0) + O(W^{-D}) = 1 + O(W^{-D}), \quad (1.11)$$

for any large constant $D > 0$ as long as $L \geq W^{1+\varepsilon}$ for a constant $\varepsilon > 0$.

The diagonal resolvent entries of $G(z)$ are expected to be given by the Stieltjes transform of Wigner's semicircle law,

$$m(z) := \frac{-z + \sqrt{z^2 - 4}}{2} = \frac{1}{2\pi} \int_{-2}^2 \frac{\sqrt{4 - \xi^2}}{\xi - z} d\xi, \quad z \in \mathbb{C}_+. \quad (1.12)$$

On the other hand, it was proved in [32] that off-diagonal resolvent entries can be approximated by a *diffusive kernel* Θ defined by

$$\Theta(z) := \frac{|m(z)|^2 S}{1 - |m(z)|^2 S}, \quad (1.13)$$

for $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $\eta \geq W^{2+\varepsilon}/L^2$ for a constant $\varepsilon > 0$. In this case, it is well-known that (see, e.g., [12, 33] for a proof of (1.14))

$$\Theta_{xy}(z) \leq \frac{W^\tau \mathbf{1}_{|x-y| \leq \eta^{-1/2} W^{1+\tau}}}{W^2 (\|x-y\|_L + W)^{d-2}} + \frac{1}{(\|x-y\|_L + W)^D} \leq W^\tau B_{xy}, \quad (1.14)$$

for any small constant $\tau > 0$ and large constant $D > 0$, where we have abbreviated that

$$B_{xy} := W^{-2} (\|x-y\|_L + W)^{-d+2}. \quad (1.15)$$

In part I of this series [32], we proved the following local law in Theorem 1.3 and quantum diffusion in Theorem 1.4. In addition, Theorem 1.3 was used in [32] to prove the delocalization of random band matrices in dimensions $d \geq 8$. We remark that all results in this paper hold only for large enough W and L , and, for simplicity, we do not repeat it in our statements.

Theorem 1.3 (Theorem 1.4 of [32]). *Fix $d \geq 8$ and any small constants $c_w, \varepsilon, \kappa > 0$. Suppose that $L^{c_w} \leq W \leq L$, and H is a d -dimensional random band matrix satisfying Assumptions 1.1 and 1.2. Then for any small constant $\tau > 0$ and large constant $D > 0$, we have the following estimate for $z = E + i\eta$ and all $x, y \in \mathbb{Z}_L^d$:*

$$\mathbb{P} \left(\sup_{E \in (-2+\kappa, 2-\kappa)} \sup_{W^{2+\varepsilon}/L^2 \leq \eta \leq 1} |G_{xy}(z) - m(z)\delta_{xy}|^2 \leq W^\tau B_{xy} \right) \geq 1 - L^{-D}. \quad (1.16)$$

Theorem 1.4 (Theorem 1.5 of [32]). *Suppose the assumptions of Theorem 1.3 hold. Fix any small constant $\varepsilon > 0$ and large constant $M \in \mathbb{N}$. Then for all $x, y \in \mathbb{Z}_L^d$ and $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $W^{2+\varepsilon}/L^2 \leq \eta \leq 1$, we have that*

$$\mathbb{E} T_{xy} = \left[\Theta^{(M)} \left(|m|^2 + \mathcal{G}^{(M)} \right) \right]_{xy} + O(W^{-Md/2}). \quad (1.17)$$

Here $\Theta^{(M)}$ is the M -th order renormalized diffusive matrix

$$\Theta^{(M)} := \frac{1}{1 - |m|^2 S (1 + \Sigma^{(M)})} |m|^2 S, \quad (1.18)$$

and it satisfies the bound

$$|\Theta_{xy}^{(M)}| \leq W^\tau B_{xy}, \quad (1.19)$$

for any constant $\tau > 0$. Furthermore, the self-energy correction $\Sigma^{(M)}$ is given by $\Sigma^{(M)}(z) := \sum_{l=4}^M \mathcal{E}_l(z)$ where $\{\mathcal{E}_l\}_{l=4}^M$ is a sequence of deterministic matrices satisfying the following properties:

$$\mathcal{E}_l(x, x+a) = \mathcal{E}_l(0, a), \quad \mathcal{E}_l(0, a) = \mathcal{E}_l(0, -a), \quad \forall x, a \in \mathbb{Z}_L^d, \quad (1.20)$$

and for any constant $\tau > 0$,

$$|(\mathcal{E}_l)_{0x}(z)| \leq W^{-(l-4)d/2+\tau} B_{0x}^2, \quad \forall x \in \mathbb{Z}_L^d, \eta \in [W^{2+\varepsilon}/L^2, 1], \quad (1.21)$$

$$\left| \sum_{x \in \mathbb{Z}_L^d} (\mathcal{E}_l)_{0x}(z) \right| \leq \eta W^{-(l-2)d/2+\tau}, \quad \forall \eta \in [W^{2+\varepsilon}/L^2, 1]. \quad (1.22)$$

Here in (1.20) and throughout the rest of this paper, we use \mathcal{A}_{xy} and $\mathcal{A}(x, y)$ interchangeably for any matrix \mathcal{A} . The M -th order local correction $\mathcal{G}^{(M)}$ satisfies that

$$|\mathcal{G}_{xy}^{(M)}| \leq W^\tau B_{xy}^{3/2}, \quad (1.23)$$

for any constant $\tau > 0$.

As remarked in [32], the proof in this paper can be adapted to non-Gaussian band matrices after some technical modifications. The proof for the real symmetric Gaussian case is similar to the complex case except that the number of terms will double in every expansion step (which is due to the fact that $\mathbb{E} h_{xy}^2 = 0$ in the complex case but not in the real case). The condition $d \geq 8$ can also be improved, but it seems to require

substantial improvements in estimating the terms in the T -expansion to reach the physical dimension $d = 3$. We will deal with these improvements in forthcoming papers.

The proofs of Theorem 1.3 and Theorem 1.4 in [32] depend on main results of this paper. More precisely, we will prove Lemmas 5.2, 5.4, 5.6 and 5.7 of [32]. We summarize our main results in Section 3.3: in Theorem 3.7, we will construct the T -equation defined in Definition 3.3; as a corollary of Theorem 3.7, in Corollary 3.8, we will construct the T -expansion defined in Definition 3.2; in Theorem 3.6, we will prove a local law on $G(z)$ using the T -expansion.

Define T -variables with three subscripts by

$$T_{x,yy'} := |m|^2 \sum_{\alpha} s_{x\alpha} G_{\alpha y} \bar{G}_{\alpha y'}, \quad \text{and} \quad T_{yy',x} := |m|^2 \sum_{\alpha} G_{y\alpha} \bar{G}_{y'\alpha} s_{\alpha x}. \quad (1.24)$$

By definition, the T -variable in (1.2) can be written as $T_{xy} \equiv T_{x,yy}$. For any $x \in \mathbb{Z}_L^d$, we define \mathbb{E}_x as the partial expectation with respect to the x -th row and column of H , i.e., $\mathbb{E}_x(\cdot) := \mathbb{E}(\cdot | H^{(x)})$, where $H^{(x)}$ denotes the $(N-1) \times (N-1)$ minor of H obtained by removing the x -th row and column. For simplicity, in this paper we will use the notations

$$P_x := \mathbb{E}_x, \quad Q_x := 1 - \mathbb{E}_x.$$

Then we write

$$T_{x,yy'} = |m|^2 \sum_{\alpha} s_{x\alpha} P_{\alpha} (G_{\alpha y} \bar{G}_{\alpha y'}) + |m|^2 \sum_{\alpha} s_{x\alpha} Q_{\alpha} (G_{\alpha y} \bar{G}_{\alpha y'}).$$

The Q_{α} term is a fluctuation term. We will calculate the P_{α} term using Gaussian integration by parts to derive an expression of the form

$$T_{x,yy'} = m \bar{G}_{yy'} \Theta_{xy} + (\text{higher order term}) + (\text{fluctuation term}),$$

where the higher order term is a sum of expressions of order $O(W^{-3d/2})$ (see (3.8) for the explicit form). We call this expansion a second order T -expansion. However, this expansion is useful only when L is not too large compared to W , because the error is bounded in terms of a power of W instead of L .

In order to handle the case $L \geq W^C$ for any large constant $C > 0$, we need to obtain much finer expansions of the T -matrix with arbitrarily high order errors. In this paper, we will construct a sequence of n -th order T -expansions with leading terms $\Theta^{(n)}$ and errors of order $O(W^{-(n+1)d/2})$. Roughly speaking, we will construct an expansion of the form

$$T_{x,yy'} = m \bar{G}_{yy'} \Theta_{xy}^{(n)} + (\text{recollision term}) + (\text{higher order term}) + (\text{fluctuation term}) + (\text{error term}), \quad (1.25)$$

where the recollision term is a sum of expressions with coincidences in the summation indices, the higher order term is a sum of expressions of order $O(W^{-(n+1)d/2})$, the fluctuation term is a sum of expressions that can be written into the form $\sum_{\alpha} Q_{\alpha}(\cdot)$, and the error term is negligible for all of our proofs. In the expansion process, we need to give a precise construction of the self-energies \mathcal{E}_l , and show that they lead to the renormalized diffusive matrix $\Theta^{(n)}$ defined in (1.18). In addition, we also need to track the recollision, higher order and fluctuation terms very carefully, so that they satisfy a key structural property—*doubly connected property* in Definition 2.12—which we will explain now.

In this paper, we represent all expressions using graphs with edge labels G , Θ and S as in the standard graphic language in quantum physics. These graphs naturally have *two-level structures*: a pair of atoms are at most $O(W)$ apart from each other if they are connected by a path of S edges; otherwise the distance between them can vary up to L . We define quotient graphs with the equivalence relation that two vertices are equivalent if they are connected by a path of S edges. Following notations in [32, 33], we call equivalence classes of vertices *molecules* (cf. Definition 2.10) and corresponding quotient graphs *molecular graphs* (cf. Definition 2.11). The (original) subgraph inside a molecule is called the *local structure* of this molecule, and the structure of a molecular graph is said to be *global*. Local structures are easy to track while global structures are our main focus. In particular, the *doubly connected property* defined in Definition 2.12 is the most important global structural property of this paper. Roughly speaking, a doubly connected graph contains a spanning tree of Θ edges and a spanning tree of G edges that connect all molecules together. This property is needed to derive effective estimates on the terms in (1.25). By (1.14) and (1.16), the typical sizes of Θ_{xy} and G_{xy} are of order B_{xy} and $B_{xy}^{1/2}$, respectively. The doubly connected property of a graph ensures

that in each sum of an index, we have at least a product of a Θ factor and a G factor, so that the sum can be controlled by the row sums of $B_{xy}^{3/2}$, which are bounded by $O(W^{-d/2})$ independently of L . This is one of the reasons why we can treat random band matrices with large $L \geq W^C$.

The main difficulty in constructing the T -expansion is that the doubly connectedness is not necessarily preserved in arbitrary graph expansions. With terminologies that will be introduced in Section 4, *local expansions* in Section 4.2 will always preserve the doubly connectedness and have been discussed in details in part I [32]. On the other hand, global expansions in Section 4.3 may break the doubly connected structure of a graph. Roughly speaking, a global expansion involves a substitution of a T -variable with a lower order T -expansion. We will see that a global expansion does not break the doubly connected property if and only if it involves a substitution of a *redundant* T -variable, where a T -variable is said to be redundant in a graph if after removing it, the remaining graph is still doubly connected (cf. Definition 5.5). In this paper, we find a sophisticated global expansion strategy such that we only need to expand a redundant T -variable in every global expansion until getting the expansion (1.25). Hence doubly connected structures of the graphs in (1.25) will follow immediately from our construction. The global expansion strategy is based on a deeper study of subtle structures of the molecular graphs, where we identify two key graphical properties: the sequentially pre-deterministic property (cf. Definition 5.9) and the globally standard property (cf. Definition 6.2). We refer the reader to Section 3.4 for a more detailed discussion of some key ideas.

The rest of this paper is organized as follows. In Section 2, we introduce some graphical notations that will be used in the definition of the T -expansion. In Section 3, we define two main concepts of this paper—the T -expansion and T -equation. Then we will state main results of this paper, that is, Theorem 3.7 and Corollary 3.8 regarding the construction of the T -equation and T -expansion up to arbitrarily high order, and, Theorem 3.6 giving a sharp local law on $G(z)$ as a consequence of the n -th order T -expansion for any fixed $n \in \mathbb{N}$. In Section 4, we introduce basic graph operations that are used to construct the T -equation and T -expansion, and in Section 5, we explore the *pre-deterministic property* of graphs appearing in our expansions. With the tools in Sections 4 and 5, we prove Theorem 3.7 and Corollary 3.8 in Section 6. In Section 7, we give the proof of Theorem 3.6 based on three lemmas, Lemma 7.2, Lemma 7.3 and Lemma 7.4. Lemma 7.2 and Lemma 7.4 will be proved in Section 8, and Lemma 7.3 will be proved in Section 9.

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2 GRAPHICAL TOOLS

To be prepared for the definition of the T -equation and T -expansion, we introduce the concept of atomic and molecular graphs, and some important graphical properties that will be satisfied by our graphs. The graphical notations in this section have been defined in [32], and we repeat them in this section for completeness of this paper.

We introduce the following two deterministic matrices that will appear in expansions:

$$S^+(z) := \frac{m^2(z)S}{1 - m^2(z)S}, \quad S^-(z) := \overline{S}^+(z). \quad (2.1)$$

For the reason of defining these two matrices, we refer the reader to Definitions 4.3 and 4.5 below. The matrix $S^+(z)$ satisfies the following Lemma 2.1, which is a folklore result. A formal proof is given in equation (4.21) of [5]. For simplicity of notations, throughout the rest of this paper, we abbreviate

$$|x - y| \equiv \|x - y\|_L, \quad \langle x - y \rangle := \|x - y\|_L + W. \quad (2.2)$$

Lemma 2.1. *Suppose the assumptions of Theorem 1.3 hold and $\eta \geq W^{2+\varepsilon}/L^2$ for a small constant $\varepsilon > 0$. Then for any small constant $\tau > 0$ and large constant $D > 0$, we have that*

$$|S_{xy}^\pm(z)| \lesssim W^{-d} \mathbf{1}_{|x-y| \leq W^{1+\tau}} + O(\langle x - y \rangle^{-D}). \quad (2.3)$$

2.1 Atomic graphs

In an n -th order T -expansion, the number of terms will grow super-exponentially with respect to n (there are about n^{Cn} many terms). Moreover, each term has a complicated structure, which is represented by a

graph in this paper. Our goal is to expand the T -variable $T_{\mathbf{a}, \mathbf{b}_1, \mathbf{b}_2}$ for some fixed indices $\mathbf{a}, \mathbf{b}_1, \mathbf{b}_2 \in \mathbb{Z}_L^d$. We represent these three indices by special vertices

$$\mathbf{a} \equiv \otimes, \quad \mathbf{b}_1 \equiv \oplus, \quad \mathbf{b}_2 \equiv \ominus, \quad (2.4)$$

in graphs. In other words, we use $\mathbf{a}, \mathbf{b}_1, \mathbf{b}_2$ in expressions, and draw them as \otimes, \oplus, \ominus in graphs. Some of these indices can be equal to each other. For example, if $\mathbf{b}_1 = \mathbf{b}_2$, then we only have two special vertices \otimes and \oplus . We first introduce atomic graphs, and the concept of subgraphs.

Definition 2.2 (Atomic graphs). *Given a standard oriented graph with vertices and edges, we assign the following structures and call the resulting graph an atomic graph.*

- **Atoms:** *We will call the vertices atoms (vs. molecules in Definition 2.10 below). Each graph has some external atoms and internal atoms. The external atoms represent external indices whose values are fixed, while internal atoms represent summation indices that will be summed over. In particular, each graph in expansions of $T_{\mathbf{a}, \mathbf{b}_1, \mathbf{b}_2}$ has \otimes, \oplus and \ominus atoms. By fixing the value of an internal atom, it will become an external atom; by summing over an external atom, it will become an internal atom.*
- **Regular weights:** *A regular weight on an atom x represents a G_{xx} or \overline{G}_{xx} factor. Each regular weight has a charge, where “+” charge indicates that the weight is a G factor, represented by a blue solid Δ , and “−” charge indicates that the weight is a \overline{G} factor, represented by a red solid Δ .*
- **Light weights:** *Corresponding to regular weights defined above, we define the light weights on atom x representing $G_{xx} - m$ and $\overline{G}_{xx} - \overline{m}$ factors. They are drawn as blue or red hollow Δ in graphs depending on their charges.*
- **Edges:** *The edges are divided into the following types.*
 - (i) **Solid edges:** *A solid edge represents a G factor. More precisely,*
 - each oriented edge from atom α to atom β with + charge represents a $G_{\alpha\beta}$ factor;
 - each oriented edge from atom α to atom β with − charge represents a $\overline{G}_{\alpha\beta}$ factor.*Plus G edges will be drawn as blue solid edges, while minus G edges will be drawn as red solid edges. In this paper, whenever we say “ G edges”, we mean both the plus and minus G edges.*
 - (ii) **Waved edges:** *We have neutral black, positive blue and negative red waved edges:*
 - a neutral waved edge connecting atoms x and y represents an s_{xy} factor;
 - a blue waved edge of positive charge between atoms x and y represents an S_{xy}^+ factor;
 - a red waved edge of negative charge between atoms x and y represents an S_{xy}^- factor.
 - (iii) **Diffusive edges:** *A diffusive edge connecting atoms x and y represents a Θ_{xy} factor; we draw it as a double-line edge between atoms x and y .*
 - (iv) **Dotted edges:** *A dotted line connecting atoms α and β represents the factor $\mathbf{1}_{\alpha=\beta} \equiv \delta_{\alpha\beta}$; a dotted line with a cross (\times) represents the factor $\mathbf{1}_{\alpha \neq \beta} \equiv 1 - \delta_{\alpha\beta}$. There is at most one dotted or \times -dotted edge between each pair of atoms. By definition, a \times -dotted edge between the two ending atoms of a G edge indicates that this G edge is off-diagonal. We also allow for dotted edges between external atoms.*

The orientations of non-solid edges do not matter. Edges between internal atoms are called internal edges, while edges with at least one end at an external atom are called external edges.

- **P and Q labels:** *Some solid edges and weights may have a label P_x or Q_x for an atom x in the graph. Moreover, every edge or weight can have at most one P or Q label.*
- **Coefficients:** *There is a coefficient (which is a polynomial of $m, m^{-1}, (1 - m^2)^{-1}$ and their complex conjugates) associated with each graph.*

Along the proof, we will introduce some other types of weights and edges.

Definition 2.3 (Sugraphs). A graph \mathcal{G}_1 is said to be a subgraph of \mathcal{G}_2 , denoted by $\mathcal{G}_1 \subset \mathcal{G}_2$, if every graphical component of \mathcal{G}_1 is also in \mathcal{G}_2 . Moreover, \mathcal{G}_1 is a proper subgraph of \mathcal{G}_2 if $\mathcal{G}_1 \subset \mathcal{G}_2$ and $\mathcal{G}_1 \neq \mathcal{G}_2$. Given a subset \mathcal{S} of atoms in a graph \mathcal{G} , the subgraph $\mathcal{G}|_{\mathcal{S}}$ induced on \mathcal{S} refers to the subgraph of \mathcal{G} with atoms in \mathcal{S} as vertices, the edges between these atoms, and the weights on these atoms.

We assign a *value* to each graph as follows.

Definition 2.4 (Values of graphs). Given an atomic graph \mathcal{G} , we define its value, denoted by $\llbracket \mathcal{G} \rrbracket$, as an expression obtained as follows. We first take the product of all the edges, all the weights and the coefficient of the graph \mathcal{G} . Then for the edges and weights with the same P_x or Q_x label, we take the product of them and apply P_x or Q_x to them. Finally, we sum over all the internal indices represented by the internal atoms. The values of the external indices are fixed by their given values. For a linear combination of graphs $\sum_i c_i \mathcal{G}_i$, where $\{c_i\}$ is a sequence of coefficients and $\{\mathcal{G}_i\}$ is a sequence of graphs, we naturally define its value by

$$\llbracket \sum_i c_i \mathcal{G}_i \rrbracket = \sum_i c_i \llbracket \mathcal{G}_i \rrbracket.$$

For simplicity, we will abuse the notation by identifying a graph (which is a geometric object) with its value (which is an analytic expression).

Next, we introduce the concepts of *regular* and *normal regular* graphs.

Definition 2.5 (Normal regular graphs). We say an atomic graph \mathcal{G} is regular if it satisfies the following properties:

- (i) it is a connected graph that contains at most $O(1)$ many atoms and edges;
- (ii) all internal atoms are connected together through paths of wavy and diffusive edges;
- (iii) there are no dotted edges between internal atoms.

Moreover, we say a regular graph is normal if it satisfies the following additional property:

- (iv) any pair of atoms α and β in the graph are connected by a \times -dotted edge if and only if they are connected by a G edge.

By this definition, every G edge in a normal regular graph is off-diagonal, while all diagonal G factors will be represented by weights. Given a normal regular graph, we define its scaling order as follows.

Definition 2.6 (Scaling order). Given a normal regular graph \mathcal{G} , we define its scaling order as

$$\begin{aligned} \text{ord}(\mathcal{G}) := & \#\{\text{off-diagonal } G \text{ edges}\} + \#\{\text{light weights}\} + 2\#\{\text{wavy edges}\} + 2\#\{\text{diffusive edges}\} \\ & - 2[\#\{\text{internal atoms}\} - \#\{\text{dotted edges}\}]. \end{aligned} \quad (2.5)$$

Here every dotted edge in a normal regular graph means that an internal atom is equal to an external atom, so we lose one free summation index. The concept of scaling order can be also defined for subgraphs.

In the following proof, whenever we say the order of a graph, we are referring to its scaling order. We emphasize that in general the scaling order does not imply the real size of the graph value directly. In order to establish such a connection, we need to introduce the *doubly connected property* in Definition 2.12 below.

2.2 Self-energies and labelled diffusive edges

One of the most important concepts in the T -expansion is the self-energy introduced in [32]. More precisely, an l -th order self-energy is a linear combination of deterministic graphs satisfying the following definition.

Definition 2.7 (Self-energies). Fix any $l \in \mathbb{N}$. $\mathcal{E}_l(z)$ is a deterministic matrix depending on $m(z)$, S , $S^\pm(z)$ and $\Theta(z)$ only, and satisfying the following properties for $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $\eta \in [W^{2+\varepsilon}/L^2, 1]$.

- (i) For any $x, y \in \mathbb{Z}_L^d$, $(\mathcal{E}_l)_{xy}$ is a sum of at most C_l many deterministic graphs of scaling order l and with external atoms x and y . Here C_l is a large constant depending on l . Some graphs, say \mathcal{G} , in \mathcal{E}_l can be diagonal matrices satisfying $\mathcal{G}_{xy} = \mathcal{G}_{xx} \delta_{xy}$, i.e. there is a dotted edge between the atoms x and y .

(ii) $\mathcal{E}_l(z)$ satisfies the properties (1.20)–(1.22).

Then we call \mathcal{E}_l the l -th order self-energy and graphically we will use a square, \square , with a label l and between x and y to represent $(\mathcal{E}_l)_{xy}$.

By Definition 2.6, the scaling order of a deterministic graph can only be even. Moreover, every nontrivial self-energy \mathcal{E}_l in this paper has scaling order ≥ 4 . Hence we always have

$$\mathcal{E}_1 = \mathcal{E}_2 = \mathcal{E}_3 = 0, \quad \text{and} \quad \mathcal{E}_{2l+1} := 0, \quad l \in \mathbb{N}. \quad (2.6)$$

Using the properties (1.20)–(1.22), we have proved the following crucial estimates in [32]. These estimates are necessary for bounding the graphs in the T -expansion and T -equation.

Lemma 2.8 (Lemma 6.2 of [32]). *Fix $d \geq 6$. Let \mathcal{E}_{2l} be a self-energy satisfying Definition 2.7. We have that for any constant $\tau > 0$ and $x, y \in \mathbb{Z}_L^d$,*

$$\left| \sum_{\alpha} \Theta_{x\alpha} (\mathcal{E}_{2l})_{\alpha y} \right| \leq \frac{W^{\tau}}{W^{(l-1)d} \langle x-y \rangle^d}. \quad (2.7)$$

Let $\mathcal{E}_{2k_1}, \mathcal{E}_{2k_2}, \dots, \mathcal{E}_{2k_l}$ be a sequence of self-energies satisfying Definition 2.7. We have that for any constant $\tau > 0$ and $x, y \in \mathbb{Z}_L^d$,

$$\left| (\Theta \mathcal{E}_{2k_1} \Theta \mathcal{E}_{2k_2} \Theta \cdots \Theta \mathcal{E}_{2k_l} \Theta)_{xy} \right| \leq W^{-(k-2)d/2+\tau} B_{xy}, \quad (2.8)$$

where $k := \sum_{i=1}^l 2k_i - 2(l-1)$ is the scaling order of $(\Theta \mathcal{E}_{2k_1} \Theta \mathcal{E}_{2k_2} \Theta \cdots \Theta \mathcal{E}_{2k_l} \Theta)_{xy}$.

By (2.8), $(\Theta \mathcal{E}_{2k_1} \Theta \mathcal{E}_{2k_2} \Theta \cdots \Theta \mathcal{E}_{2k_l} \Theta)_{xy}$ has the same decay with respect to $|x-y|$ as Θ_{xy} except for an extra $W^{-(k-2)d/2}$ factor. Hence we will regard it as another type of diffusive edge. The proof of Lemma 2.8 uses a summation by parts argument. In particular, the η factor in (1.22) plays an essential role in the sense that it will cancel the following factor from a row sum of Θ :

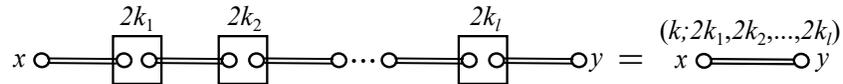
$$\sum_y \Theta_{xy}(z) = \frac{|m(z)|^2}{1 - |m(z)|^2} \sim \eta^{-1}. \quad (2.9)$$

In [32], we refer to (1.22) as a *sum zero property*.

Definition 2.9 (Labelled diffusive edges). *Given l self-energies \mathcal{E}_{2k_i} , $i = 1, 2, \dots, l$, we represent the entry*

$$(\Theta \mathcal{E}_{2k_1} \Theta \mathcal{E}_{2k_2} \Theta \cdots \Theta \mathcal{E}_{2k_l} \Theta)_{xy} \quad (2.10)$$

by a labelled diffusive edge between atoms x and y with label $(k; 2k_1, \dots, 2k_l)$, where $k := \sum_{i=1}^l 2k_i - 2(l-1)$ is the scaling order of this edge. In graphs, every labelled diffusive edge is drawn as one single double-line edge with a label but without any internal structure as in the following figure:



In this paper, whenever we refer to diffusive edges, we mean both the diffusive and labelled diffusive edges. The scaling order of a normal regular graph with labelled diffusive edges can be equivalently calculated as

$$\begin{aligned} \text{ord}(\mathcal{G}) := & \#\{\text{off-diagonal } G \text{ edges}\} + \#\{\text{light weights}\} + 2\#\{\text{waved edges}\} + 2\#\{\text{diffusive edges}\} \\ & + \sum_k k \cdot \#\{k\text{-th order labelled diffusive edges}\} - 2[\#\{\text{internal atoms}\} - \#\{\text{dotted edges}\}]. \end{aligned} \quad (2.11)$$

In other words, a k -th order labelled diffusive edge is simply counted as an edge of scaling order k , and there is no need to count its internal structures using Definition 2.6.

2.3 Molecular graphs and doubly connected property

Each of our graphs has a two-level structure, that is, a local structure varying on scales of order W , and a global structure varying on scales up to L . To explain this, we introduce the following concept of molecules.

Definition 2.10 (Molecules). *We partition the set of all atoms into a union of disjoint sets $\{\text{all atoms}\} = \cup_j \mathcal{M}_j$, where every \mathcal{M}_j is called a molecule. Two internal atoms belong to the same molecule if and only if they are connected by a path of neutral/plus/minus wavy edges and dotted edges. Every external atom will be by definition called an external molecule (such as \otimes , \oplus and \ominus molecules). An edge is said to be inside a molecule if its ending atoms belong to this molecule.*

By (1.9) and (2.3), if two atoms x and y are in the same molecule, then we essentially have $|x - y| \leq W^{1+\tau}$ up to a negligible error $O(W^{-D})$. Given an atomic graph, we will call the subgraph inside a molecule the *local structure* of this molecule. On the other hand, the *global structure* of an atomic graph refers to its *molecular graph*, which is the quotient graph with each molecule regarded as a vertex.

Definition 2.11 (Molecular graphs). *Molecular graphs are graphs consisting of*

- *external molecules which represent the external atoms (such as the \otimes , \oplus and \ominus molecules);*
- *internal molecules;*
- *blue and red solid edges, which represent the plus and minus G edges between molecules;*
- *diffusive edges between molecules;*
- *dotted edges between external and internal molecules.*

Given any atomic graph \mathcal{G} , we define its molecular version, called $\mathcal{G}_{\mathcal{M}}$, in the following way:

- *every molecule of \mathcal{G} is represented by a vertex in $\mathcal{G}_{\mathcal{M}}$;*
- *every blue or red solid edge of \mathcal{G} between atoms in different molecules is represented by a blue or red solid edge between these two molecules in $\mathcal{G}_{\mathcal{M}}$;*
- *every diffusive edge of \mathcal{G} between atoms in different molecules is represented by a diffusive edge between these two molecules in $\mathcal{G}_{\mathcal{M}}$;*
- *every dotted edge of \mathcal{G} between an external atom and an internal atom is represented by a dotted edge between the corresponding external and internal molecules;*
- *we discard all the other components in \mathcal{G} (including weights, \times -dotted edges, and edges inside molecules).*

In this paper, molecular graphs are used solely to help with the analysis of graph structures, while all graph expansions are applied to atomic graphs only. In the proof, we assume that there is automatically a molecular graph associated with each atomic graph. In general, local structures are almost trivial to bound, while global structures are much harder to analyze. This is one of the main reasons why we want to introduce the concept of molecular graphs—we want to get rid of all local structures and focus on the more intricate global structures instead.

The following *doubly connected property* is crucial for our proof, because it allows us to establish a direct connection between the scaling order of a graph and a bound on its value. All graphs in the T -expansion and T -equation will satisfy this property (cf. Definitions 3.2 and 3.3).

Definition 2.12 (Doubly connected property). *A subgraph \mathcal{G} without external molecules is said to be doubly connected if its molecular graph $\mathcal{G}_{\mathcal{M}}$ satisfies the following property. There exists a collection, say $\mathcal{B}_{\text{black}}$, of diffusive edges, and another collection, say $\mathcal{B}_{\text{blue}}$, of either blue solid or diffusive edges such that (a) $\mathcal{B}_{\text{black}} \cap \mathcal{B}_{\text{blue}} = \emptyset$, and (b) both $\mathcal{B}_{\text{black}}$ and $\mathcal{B}_{\text{blue}}$ contain a spanning tree that connects all molecules in the graph. For simplicity of notations, we call the diffusive edges in $\mathcal{B}_{\text{black}}$ as black edges, and the blue solid and diffusive edges in $\mathcal{B}_{\text{blue}}$ as blue edges. Correspondingly, $\mathcal{B}_{\text{black}}$ and $\mathcal{B}_{\text{blue}}$ are referred to as black net and blue net, respectively, where a “net” refers to a subset of edges that contains a spanning tree.*

A graph \mathcal{G} with external molecules is called doubly connected if its subgraph with all external molecules removed is doubly connected, i.e. the spanning trees in the two nets are not required to contain the external molecules.

Note that red solid edges are not tracked in the doubly connected property. In fact, the connectivity of red solid edges will be broken in our expansion procedures. Hence we will often consider molecular graphs with all red solid edges removed. Doubly connected graphs satisfy some important bounds that depend explicitly on their scaling orders; see Lemma 8.4 below.

3 MAIN RESULTS

In this section, we define the concepts of T -expansion and T -equation, which were introduced in [32, Section 2]. Then we will state our main results in Section 3.3. In this paper, we will focus on expansions of the T -variable $T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, while expansions of $T_{\mathbf{b}_1 \mathbf{b}_2, \mathbf{a}}$ can be obtained immediately by considering the transposition of $T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$.

3.1 T -expansion

In this subsection, we define the T -expansion using the notations introduced in Section 2. In addition, we also introduce the following two types of graphs.

Definition 3.1 (Recollision graphs and Q -graphs). (i) We say a graph is a \oplus/\ominus -recollision graph, if there is at least one dotted edge connecting \oplus or \ominus to an internal atom. In other words, a recollision graph represents an expression where we set at least one summation index to be equal to \mathbf{b}_1 or \mathbf{b}_2 .

(ii) We say a graph is a Q -graph if all G edges and G weights in the graph have the same Q_x label with a specific atom x , i.e., all Q labels in the graph are the same Q_x for some atom x . In other words, the value of a Q -graph can be written as $Q_x(\Gamma)$ for an external atom x or $\sum_x Q_x(\Gamma)$ for an internal atom x , where Γ is a graph without Q labels.

For any $n \in \mathbb{N}$, we now define the n -th order T -expansion. Its graphs actually satisfy several more delicate properties to be stated later in Definition 6.3.

Definition 3.2 (n -th order T -expansion). Fix any $n \in \mathbb{N}$ and a large constant $D > n$. For $\mathbf{a}, \mathbf{b}_1, \mathbf{b}_2 \in \mathbb{Z}_L^d$, an n -th order T -expansion of $T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ with D -th order error is an expression of the following form:

$$\begin{aligned} T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} &= m\Theta_{\mathbf{a}\mathbf{b}_1} \overline{G}_{\mathbf{b}_1 \mathbf{b}_2} + m(\Theta_{\Sigma_T^{(n)}} \Theta)_{\mathbf{a}\mathbf{b}_1} \overline{G}_{\mathbf{b}_1 \mathbf{b}_2} \\ &+ (\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{Err}_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}. \end{aligned} \quad (3.1)$$

The graphs on the right side depend only on n , D , $m(z)$, S , $S^\pm(z)$, $\Theta(z)$ and $G(z)$, but do not depend on W , L and d explicitly. Moreover, they satisfy the following properties with C_n and C_D denoting large constants depending on n and D , respectively.

- (i) The graphs on the right side are normal regular graphs (recall Definition 2.5) with external atoms $\otimes \equiv \mathbf{a}$, $\oplus \equiv \mathbf{b}_1$ and $\ominus \equiv \mathbf{b}_2$, and with at most C_D many atoms.
- (ii) A diffusive edge in any graph on the right-hand side of (3.1) is either a diffusive edge or a labelled diffusive edge of the form (2.10) with $4 \leq 2k_i \leq n$.
- (iii) $\Sigma_T^{(n)}$ is a sum of at most C_n many deterministic normal regular graphs. We decompose it according to the scaling order as

$$\Sigma_T^{(n)} = \sum_{k \leq n} \Sigma_{T,k}. \quad (3.2)$$

Moreover, we have a sequence of self-energies \mathcal{E}_k satisfying Definition 2.7 for $4 \leq k \leq n$ such that $\Sigma_{T,k}$ can be written into the form

$$\Sigma_{T,k} = \mathcal{E}_k + \sum_{l=2}^k \sum_{\mathbf{k}=(k_1, \dots, k_l) \in \Omega_k^{(l)}} \mathcal{E}_{k_1} \Theta \mathcal{E}_{k_2} \Theta \cdots \Theta \mathcal{E}_{k_l}. \quad (3.3)$$

Here all deterministic graphs with $l = 1$ are included into \mathcal{E}_k so that the summation starts with $l = 2$. Moreover, $\Omega_k^{(l)} \subset \mathbb{N}^l$ is the subset of vectors \mathbf{k} satisfying that

$$4 \leq k_i \leq k - 1, \quad \text{and} \quad \sum_{i=1}^l k_i - 2(l - 1) = k. \quad (3.4)$$

The second condition of (3.4) guarantees that the subgraph $(\mathcal{E}_{k_1} \Theta \mathcal{E}_{k_2} \Theta \cdots \Theta \mathcal{E}_{k_l})_{xy}$ has scaling order k .

(iv) $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of at most C_n many \oplus/\ominus -recollision graphs of scaling order $\leq n$ and without any P/Q labels. Moreover, it can be decomposed as

$$(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_{k=3}^n (\mathcal{R}_{T,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}, \quad (3.5)$$

where each $(\mathcal{R}_{T,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of the \oplus/\ominus -recollision graphs of scaling order k in $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$.

(v) $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of at most C_D many graphs of scaling order $> n$ and without any P/Q labels.

(vi) $(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of at most C_D many Q -graphs. Moreover, it can be decomposed as

$$(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_{k=2}^n (\mathcal{Q}_{T,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{Q}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}, \quad (3.6)$$

where $(\mathcal{Q}_{T,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of the Q -graphs in $(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ of scaling order k , and $(\mathcal{Q}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of all the Q -graphs in $(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ of scaling order $> n$.

(vii) $\Sigma_{T,k}$, $\mathcal{R}_{T,k}$ and $\mathcal{Q}_{T,k}$ are independent of n .

(viii) $(\mathcal{E}rr_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of at most C_D many graphs, each of which has scaling order $> D$ and may contain some P/Q labels in it.

(ix) In every graph of $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{E}rr_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, there is a unique diffusive edge connected to \otimes . Furthermore, there is at least an edge, which is either blue solid or diffusive or dotted, connected to \oplus , and there is at least an edge, which is either red solid or diffusive or dotted, connected to \ominus .

(x) Every graph in $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{E}rr_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is doubly connected in the sense of Definition 2.12.

The graphs on the right-hand side of (3.1) satisfy some additional properties given in Definition 6.3 below.

By (2.8), the term $(\Theta \Sigma_{T,k} \Theta)_{\mathbf{a} \mathbf{b}_1}$ can be bounded as

$$|(\Theta \Sigma_{T,k} \Theta)_{\mathbf{a} \mathbf{b}_1}| \leq W^{-(k-2)d/2+\tau} B_{\mathbf{a} \mathbf{b}_1} \quad (3.7)$$

for any constant $\tau > 0$. This bound shows that when $\mathbf{b}_1 = \mathbf{b}_2 = \mathbf{b}$, the second term on the right-hand side of (3.1) can be bounded by $m \bar{G}_{\mathbf{b} \mathbf{b}} (\Theta \Sigma_T^{(n)} \Theta)_{\mathbf{a} \mathbf{b}} = O(W^\tau B_{\mathbf{a} \mathbf{b}})$, which is necessary for the local law (1.16) to hold.

In [32], the following second order T -expansion is given explicitly in Lemma 2.5:

$$T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = m \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} \Theta_{\mathbf{a} \mathbf{b}_1} + (\mathcal{A}_T^{(>2)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{Q}_T^{(2)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}, \quad (3.8)$$

where

$$(\mathcal{A}_T^{(>2)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} := m \sum_{x,y} \Theta_{\mathbf{a} x} s_{xy} (G_{yy} - m) G_{x \mathbf{b}_1} \bar{G}_{x \mathbf{b}_2} + m \sum_{x,y} \Theta_{\mathbf{a} x} s_{xy} (\bar{G}_{xx} - \bar{m}) G_{y \mathbf{b}_1} \bar{G}_{y \mathbf{b}_2}, \quad (3.9)$$

$$\begin{aligned} (\mathcal{Q}_T^{(2)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} &:= \sum_x Q_x (\Theta_{\mathbf{a} x} G_{x \mathbf{b}_1} \bar{G}_{x \mathbf{b}_2}) - m Q_{\mathbf{b}_1} (\Theta_{\mathbf{a} \mathbf{b}_1} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2}) \\ &\quad - m \sum_{x,y} Q_x [\Theta_{\mathbf{a} x} s_{xy} (G_{yy} - m) G_{x \mathbf{b}_1} \bar{G}_{x \mathbf{b}_2}] - m \sum_{x,y} Q_x [\Theta_{\mathbf{a} x} s_{xy} \bar{G}_{xx} G_{y \mathbf{b}_1} \bar{G}_{y \mathbf{b}_2}]. \end{aligned} \quad (3.10)$$

We still need to expand $(\mathcal{A}_T^{(>2)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{Q}_T^{(2)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ into sums of normal regular graphs using the operation in Definition 4.2 below, but we omit this minor issue here.

3.2 T -equation

In this subsection, we define the n -th order T -equation for any fixed $n \in \mathbb{N}$.

Definition 3.3 (n -th order T -equation). *Fix any $n \in \mathbb{N}$ and a large constant $D > n$. For $\mathbf{a}, \mathbf{b}_1, \mathbf{b}_2 \in \mathbb{Z}_L^d$, an n -th order T -equation of $T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ with D -th order error is an expression of the following form:*

$$\begin{aligned} T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} &= m\Theta_{\mathbf{a}\mathbf{b}_1} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} + \sum_x (\Theta \Sigma^{(n)})_{\mathbf{a}x} T_{x, \mathbf{b}_1 \mathbf{b}_2} \\ &+ (\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{A}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{E}rr'_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}, \end{aligned} \quad (3.11)$$

where the graphs on the right-hand side depend only on n , D , $m(z)$, S , $S^\pm(z)$, $\Theta(z)$ and $G(z)$, but do not depend on W , L and d explicitly. Moreover, they satisfy the following properties.

- (i) $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{A}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{E}rr'_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ respectively satisfy the same properties as $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{E}rr_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ in Definition 3.2. Furthermore, $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be decomposed as

$$(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_{k=3}^n (\mathcal{R}_{IT,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}, \quad (3.12)$$

and

$$(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_{k=2}^n (\mathcal{Q}_{IT,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{Q}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}, \quad (3.13)$$

where $(\mathcal{R}_{IT,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of the \oplus/\ominus -recollision graphs in $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ of scaling order k , $(\mathcal{Q}_{IT,k})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of the Q -graphs in $(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ of scaling order k , and $(\mathcal{Q}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of the Q -graphs in $(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ of scaling order $> n$. Moreover, $\mathcal{R}_{IT,k}$ and $\mathcal{Q}_{IT,k}$ are independent of n .

- (ii) $\Sigma^{(n)}$ can be decomposed according to the scaling order as

$$\Sigma^{(n)} = \mathcal{E}_n + \sum_{l=4}^{n-1} \mathcal{E}_l, \quad (3.14)$$

where \mathcal{E}_l (which is the same as that appeared in (3.3)), $1 \leq l \leq n-1$, is a sequence of self-energies satisfying Definition 2.7. For any $x, y \in \mathbb{Z}_L^d$, $(\mathcal{E}_n)_{xy}$ is a sum of at most C_n many deterministic graphs of scaling order n and with external atoms x and y .

- (iii) A diffusive edge in \mathcal{E}_n , $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{A}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{E}rr'_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is either a diffusive edge or a labelled diffusive edge of the form (2.10) with $4 \leq 2k_i \leq n-1$.

- (iv) Every graph in $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{A}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{E}rr'_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be written as

$$\sum_x \Theta_{\mathbf{a}x} \mathcal{G}_{x, \mathbf{b}_1 \mathbf{b}_2},$$

where $\mathcal{G}_{x, \mathbf{b}_1 \mathbf{b}_2}$ is a normal regular graph with external atoms x , \mathbf{b}_1 and \mathbf{b}_2 . Moreover, $\mathcal{G}_{x, \mathbf{b}_1 \mathbf{b}_2}$ has at least an edge, which is either blue solid or diffusive or dotted, connected to \oplus , and at least an edge, which is either red solid or diffusive or dotted, connected to \ominus .

- (v) Every graph in \mathcal{E}_n , $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{A}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, $(\mathcal{Q}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{E}rr'_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is doubly connected in the sense of Definition 2.12.

The graphs on the right side of (3.11) satisfy some additional properties given in Definition 6.3 below.

Remark 3.4. The form of (3.11) is different from (3.1) only in the second term on the right-hand side. It can be regarded as a linear equation of the T -variable $T_{x, \mathbf{b}_1 \mathbf{b}_2}$. If we move the second term on the right-hand side of (3.11) to the left-hand side and multiply both sides with $(1 - \Theta \Sigma^{(n)})^{-1}$, we can get the n -th order

T -equation (see Section 6.1 for more details). Furthermore, taking expectation and choosing $\mathfrak{b}_1 = \mathfrak{b}_2$ and $n = M$, we will get (1.17) as discussed in [32]. We remark that using the language of Feynman diagrams, Σ_n in (3.14) is a sum of *one-particle irreducible graphs*, while $\Sigma_T^{(n)}$ in (3.2) is a sum of *one-particle reducible graphs*. We also remark that $\Theta \Sigma_T^{(n)} \Theta$ is exactly the sum of scaling order $\leq n$ graphs in the Taylor expansion of $\Theta^{(n)} = (1 - \Theta \Sigma^{(n)})^{-1} \Theta$.

We will construct a sequence of T -equations inductively. In particular, before constructing the n -th order T -equation, we have obtained the k -th order T -expansion and proved the properties (1.20)–(1.22) for \mathcal{E}_k for all $4 \leq k \leq n - 1$. On the other hand, \mathcal{E}_n is a new sum of deterministic graphs obtained in the n -th order T -equation, whose properties (1.20)–(1.22) are yet to be shown. Moreover, we perform the expansions in a careful way so that the doubly connected property of the graphs in \mathcal{E}_n will follow easily from the construction.

3.3 Main results

We are ready to state the main results of this paper. First, given an n -th order T -expansion, we can get a local law in Theorem 3.6 for random band matrices satisfying (3.15). For simplicity of presentation, we will adopt the following convention of stochastic domination introduced in [11].

Definition 3.5 (Stochastic domination and high probability event). *(i) Let*

$$\xi = (\xi^{(W)}(u) : W \in \mathbb{N}, u \in U^{(W)}), \quad \zeta = (\zeta^{(W)}(u) : W \in \mathbb{N}, u \in U^{(W)}),$$

be two families of non-negative random variables, where $U^{(W)}$ is a possibly W -dependent parameter set. We say ξ is stochastically dominated by ζ , uniformly in u , if for any fixed (small) $\tau > 0$ and (large) $D > 0$,

$$\mathbb{P} \left[\bigcup_{u \in U^{(W)}} \{ \xi^{(W)}(u) > W^\tau \zeta^{(W)}(u) \} \right] \leq W^{-D},$$

for large enough $W \geq W_0(\tau, D)$, and we will use the notation $\xi \prec \zeta$. If some complex family ξ satisfies $|\xi| \prec \zeta$, then we will also write $\xi \prec \zeta$ or $\xi = O_\prec(\zeta)$.

(ii) As a convention, for two deterministic non-negative quantities ξ and ζ , we will write $\xi \prec \zeta$ if and only if $\xi \leq W^\tau \zeta$ for any constant $\tau > 0$.

(iii) We say that an event Ξ holds with high probability (w.h.p.) if for any constant $D > 0$, $\mathbb{P}(\Xi) \geq 1 - W^{-D}$ for large enough W . More generally, we say that an event Ω holds w.h.p. in Ξ if for any constant $D > 0$, $\mathbb{P}(\Xi \setminus \Omega) \leq W^{-D}$ for large enough W .

Theorem 3.6 (Local law). *Fix any $n \in \mathbb{N}$. Under the assumptions of Theorem 1.3, suppose we have an n -th order T -expansion satisfying Definition 3.2. Assume that L satisfies*

$$L^2/W^2 \leq W^{(n-1)d/2 - c_0} \tag{3.15}$$

for some constant $c_0 > 0$. Then for any constant $\varepsilon > 0$, the local law

$$|G_{xy}(z) - m(z)\delta_{xy}|^2 \prec B_{xy} \tag{3.16}$$

holds uniformly in all $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $\eta \in [W^{2+\varepsilon}/L^2, 1]$.

Next we show that we can construct the T -equation and T -expansion up to any fixed order $M \in \mathbb{N}$.

Theorem 3.7 (Construction of the T -equation). *Given any $M \in \mathbb{N}$, we can construct a sequence of n -th order T -equations satisfying Definition 3.3 for all $2 \leq n \leq M$.*

Solving the n -th order T -equation, we can get an n -th order T -expansion.

Corollary 3.8 (Construction of the T -expansion). *Assume that Theorem 3.7 holds. Then we can construct a sequence of n -th order T -expansions satisfying Definition 3.2 for all $2 \leq n \leq M - 1$. If we further assume that \mathcal{E}_M satisfies (1.20)–(1.22), then we can also construct the M -th order T -expansion.*

In the proof of Theorem 3.7, we will construct a sequence of T -equations inductively. Suppose we have constructed the T -equation up to order n . Then by Corollary 3.8, we have an $(n - 1)$ -th order T -expansion.

Using this T -expansion, we obtain from Theorem 3.6 that the local law (3.16) holds when L satisfies the condition (with n in (3.15) replaced by $n - 1$)

$$L^2/W^2 \leq W^{(n-2)d/2-c_0}.$$

Using the local law (3.16), it was proved in [32] that \mathcal{E}_n constructed in the n -th order T -equation in Theorem 3.7 is actually an n -th order self-energy.

Lemma 3.9 (Lemma 5.8 of [32]). *The deterministic matrix \mathcal{E}_n constructed in the n -th order T -equation in Theorem 3.7 satisfies the properties (1.20)–(1.22) with $l = n$.*

After showing that \mathcal{E}_n is a self-energy satisfying Definition 2.7, we can use Corollary 3.8 again to get the n -th order T -expansion. Then we use the n -th order T -expansion to construct the $(n + 1)$ -th order T -equation and prove the properties (1.20)–(1.22) for \mathcal{E}_{n+1} . Continuing this process, we can construct the T -equation up to any fixed order. One contribution of this paper is that we develop a sophisticated strategy to construct the n -th order T -equation by using the $(n - 1)$ -th order T -expansion. The reader can refer to Section 3.4 for a discussion of some key ideas in the proof.

3.4 Main ideas

In this subsection, we briefly discuss some key ideas for the proof of Theorem 3.7 in Sections 4–6. Similar ideas will also be used in the proof of Theorem 3.6 in Sections 7–9. We remark that the following discussions are only for heuristic purposes, and they are not completely rigorous regarding some technical details.

3.4.1 Basic strategy

As discussed above, we will construct a sequence of T -equations (3.11) inductively. We start with the second order T -expansion in (3.8). As an induction hypothesis, suppose we have obtained the $(n - 1)$ -th order T -expansion. We then construct the n -th order T -equation by repeating the following two steps: *local expansions* and *global expansions*. Roughly speaking, given (3.8), we first apply local expansions in Section 4.2 to expand $\mathcal{A}_T^{(>2)}$ into a sum of *locally standard* graphs in which every blue solid edge (G entry) is paired with a red solid edge (\bar{G} entry) to form a T -variable. Then in every locally standard graph, we choose a T -variable and substitute it with the $(n - 1)$ -th order T -expansion. This process is called a global expansion. If a resulting graph can be included into one of the terms on the right-hand side of (3.11), then we will not expand it anymore. Otherwise, we will further expand it using local and global expansions. Our basic strategy is to repeat the above process until we get (3.11). The main difficulty with this strategy is to maintain the doubly connectedness of graphs throughout the expansions, which will be discussed in next few subsections.

The above expansion strategy involves inserting the $(n - 1)$ -th order T -expansion into the second order T -equation and then repeating local and global expansions to obtain the n -th order T -equation. This is different from the following “naturally inductive” strategy: given an $(n - 1)$ -th order T -equation, we further expand the n -th order graphs in $\mathcal{A}_{IT}^{(>n-1)}$ into graphs satisfying Definitions 3.3 plus higher order graphs of scaling order $> n$. However, this procedure fails because there may be some non-expandable graphs in $\mathcal{A}_{IT}^{(>n-1)}$, i.e. graphs that cannot be expanded without breaking the doubly connected property. The existence of such graphs does not indicate that the concept of T -equation fails, because there may be other graphs that cancel this graph up to a small error (although it is almost impossible to know what these graphs are). On the other hand, our global expansion strategy explicitly maintains the self-energies (especially their delicate cancellations given by the sum zero property (1.22)) by replacing each T -variable with a lower order T -expansion. In particular, this allows us to plug into terms $(\Theta_{\Sigma_{T,k}\Theta})_{xy}$ as a whole, which are well-behaved by (3.7).

3.4.2 Redundant edges and pre-deterministic property

Local expansions preserve the doubly connected property (cf. Lemma 4.10), and they were dealt with in [32]. On the other hand, global expansions may break doubly connected structures of our graphs, and hence are much harder to deal with. We will see that a global expansion will preserve the doubly connected property if and only if we expand a *redundant* blue solid edge. (Here an expansion of a blue solid edge refers to an expansion of a T -variable containing this edge.) As will be defined in Definition 5.5, a blue solid edge is

redundant if after removing it, the remaining graph is still doubly connected. A non-redundant blue solid edge is called *pivotal*. To preserve the doubly connected structure of every graph, we will follow the strict rule that we only *expand a redundant blue solid edge in a global expansion*.

Under the above rule, if we expand blue solid edges in an arbitrary order, then we may get graphs that are locally standard and only contain pivotal blue solid edges, namely, *non-expandable* graphs. These graphs may not be included into one of the six terms on the right-hand side of (3.11). To avoid such “bad” graphs, we need to impose structural properties that are stronger than the doubly connected property.

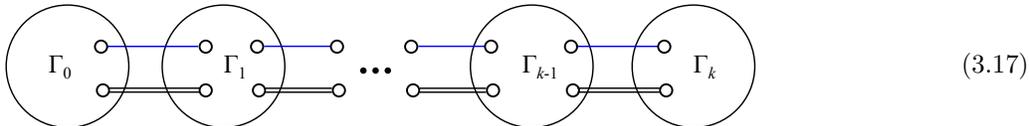
The leading term of a global expansion corresponds to replacing a blue solid edge with a diffusive edge (i.e. the first term on the right-hand side of (3.1)). Due to this observation, we see that in order to expand a graph, say \mathcal{G} , into deterministic graphs (together with some recollision, Q , higher order or error graphs) using global expansions under the above rule about redundant edges, we need the following property. All the blue solid edges in \mathcal{G} can be replaced by diffusive edges one by one according to an order, such that at each step we are dealing with a redundant edge. We call this property a *pre-deterministic property* (cf. Definition 5.8), and the corresponding order of blue solid edges a *pre-deterministic order*. The term “pre-deterministic” refers to that pre-deterministic graphs will finally contribute to deterministic graphs (i.e. graphs in the second term on the right-hand side of (3.11)) after the prescribed expansion procedure. Since there is at least one redundant edge in a pre-deterministic graph, that is, the first edge in the pre-deterministic order, a pre-deterministic graph is always expandable unless it is deterministic.

We remark that the pre-deterministic property is defined by only looking at leading terms of global expansions (i.e. replacing a T -variable with a graph in the first two terms on the right-hand side of (3.1) with n replaced by $n - 1$). If we consider subleading graphs obtained by inserting recollision, Q or higher order graphs, the pre-deterministic property may be broken in a global expansion. These subleading graphs actually satisfy a slightly weaker sequentially pre-deterministic property, which we introduce now.

3.4.3 Isolated subgraphs and sequentially pre-deterministic property

In a doubly connected molecular graph (by convention, blue and black nets are selected), every subset of molecules are connected to other molecules through at least an edge in the blue net and an edge in the black net. We define an isolated subgraph to be a subgraph induced on a subset of molecules that are connected to other molecules exactly by two edges in the molecular graph with all red solid edges removed (because red solid edges are not used in the definition of doubly connected property). It is easy to see that if a graph contains a proper isolated subgraph, then this graph cannot be pre-deterministic because of the pivotal external blue solid edge connected with this isolated subgraph. In general, global expansions may create isolated subgraphs, and hence break the pre-deterministic property. Hence we need to introduce a weaker property, called the *sequentially pre-deterministic* (SPD) property.

A SPD graph is a doubly connected graph satisfying Definition 5.9 below. Roughly speaking, the term “sequentially” refers to that a SPD graph contains a *sequence of isolated subgraphs*, say $\mathcal{I}_k \subset \mathcal{I}_{k-1} \subset \dots \subset \mathcal{I}_1$, as shown in the following figure:



Here we draw a molecular graph without red solid edges, and inside the black circles are some subgraphs. Γ_k is the minimal isolated subgraph (MIS) \mathcal{I}_k , $\Gamma_k \cup \Gamma_{k-1}$ plus the two edges between them form the isolated subgraph \mathcal{I}_{k-1} , and $\Gamma_k \cup \Gamma_{k-1} \cup \dots \cup \Gamma_{k-i}$ plus the edges between these components form the isolated subgraph \mathcal{I}_{k-i} . Γ_0 is a subgraph containing internal molecules that are connected with external edges, and we do not treat it as an isolated subgraph. The term “pre-deterministic” refers to that the MIS of a SPD graph is pre-deterministic.

As a key step of our proof, we will show that the SPD property will be preserved both in local expansions (cf. Lemma 5.10) and global expansions (cf. Lemma 6.5) if we always expand the *first blue solid edge* in a pre-deterministic order of the MIS of every SPD graph. Hence continuing expansions, we can finally expand T_{α, b_1, b_2} into a sum of SPD graphs, which, by definition, imply the doubly property of them. However, unlike pre-deterministic graphs, a SPD graph is not always expandable. For example, if (3.17) corresponds to a locally standard atomic graph and all its components Γ_i do not contain any blue solid edges, then the atomic

graph only contains pivotal blue solid edges and cannot be expanded without breaking the doubly connected property.

3.4.4 Globally standard property

Our goal is thus to find a graphical property as a compromise between the pre-deterministic and SPD properties, so that it is preserved in both local and global expansions and also guarantees that we will not get non-expandable graphs. We will identify such a property in Definition 6.2, called the *globally standard property*. Roughly speaking, a globally standard graph is a SPD graph such that its MIS is connected with at least two external red solid edges. First, using the fact that the SPD property is preserved by local and global expansions, it is not hard to show that the globally standard property is also preserved by both local and global expansions (as long as we always expand the first blue solid edge in a pre-deterministic order of the MIS). Second, a globally standard graph is always expandable. To see why, we consider the setting (3.17). If Γ_k contains at least one blue solid edge, then it contains a redundant edge due to its pre-deterministic property. Otherwise, Γ_k is connected with at least two external red solid edges and at most one blue solid edge. This shows that we cannot have a perfect pairing between blue and red solid edges, so the graph is not locally standard. Then we can apply local expansions to the graph.

Now our expansion strategy roughly proceeds as follows. We first apply local expansions to (3.8) to get locally and globally standard graphs. Then we expand the first blue solid edge in a pre-deterministic order of the MIS in every graph using the $(n - 1)$ -th order T -expansion. Next we apply local expansions to the resulting graphs and get some new locally and globally standard graphs. In every such graph, we further expand the first blue solid edge in a pre-deterministic order of the MIS. Repeating this process for sufficiently many times, we finally obtain a linear combination of graphs that can be written into the form (3.11). Throughout the expansion process, the doubly connected property is preserved, so all the graphs in (3.11) are also doubly connected.

4 BASIC GRAPH OPERATIONS

A graph operation $\mathcal{O}[\mathcal{G}]$ on a graph \mathcal{G} is a linear combination of new graphs such that the graph value of \mathcal{G} is *unchanged*, i.e. $\llbracket \mathcal{O}[\mathcal{G}] \rrbracket = \llbracket \mathcal{G} \rrbracket$. All graph operations are linear, that is,

$$\mathcal{O}\left[\sum_i c_i \mathcal{G}_i\right] = \sum_i c_i \mathcal{O}[\mathcal{G}_i]. \quad (4.1)$$

The graphs operations in Sections 4.1–4.3 have been defined in [32, Section 3], while the Q -expansions in Section 4.4 are new.

4.1 Dotted edges operations

Recall that a dotted edge between atoms α and β represents a $\delta_{\alpha\beta}$ factor. We will identify internal atoms connected by dotted edges, but we will *not* identify an external and an internal atom due to their different roles in graphs. We define the following simple merging operation regarding dotted edges.

Definition 4.1 (Merging operation). *Given a graph \mathcal{G} that contains dotted edges between different atoms, we define an operator \mathcal{O}_{merge} in the following way: $\mathcal{O}_{merge}[\mathcal{G}]$ is a graph obtained by merging every pair of internal atoms, say α and β , that are connected by a path of dotted edges into a single internal atom, say γ . Moreover, the weights and edges attached to α and β are now attached to the atom γ in $\mathcal{O}_{merge}[\mathcal{G}]$. In particular, the G edges between α and β become weights on γ , and the wavy and diffusive edges between α and β become self-loops on γ .*

Given any regular graph, we can rewrite it into a linear combination of normal regular graphs using the following *dotted edge partition* operation.

Definition 4.2 (Dotted edge partition). *Given a regular graph \mathcal{G} , for any pair of atoms α and β , if there is at least one G edge but no \times -dotted edge between them, then we write*

$$1 = \mathbf{1}_{\alpha=\beta} + \mathbf{1}_{\alpha\neq\beta};$$

if there is a \times -dotted edge but no G edge between them, then we write

$$\mathbf{1}_{\alpha \neq \beta} = 1 - \mathbf{1}_{\alpha = \beta}.$$

Expanding the product of all these sums on the right-hand sides, we can expand \mathcal{G} as

$$\mathcal{O}_{dot}[\mathcal{G}] := \sum \mathcal{O}_{merge}[\mathbf{Dot} \cdot \mathcal{G}], \quad (4.2)$$

where each \mathbf{Dot} is a product of dotted and \times -dotted edges together with a $+$ or $-$ sign. In $\mathbf{Dot} \cdot \mathcal{G}$, if there is a \times -dotted edge between α and β , then the G edges between them are off-diagonal; otherwise, the G edges between them become weights after the merging operation. If \mathbf{Dot} is “inconsistent” (i.e., two atoms are connected by a \times -dotted edge and a path of dotted edges), then we trivially have $[\mathbf{Dot} \cdot \mathcal{G}] = 0$. Thus we will drop all inconsistent graphs. Finally, if the graph \mathcal{G} is already normal, then \mathcal{O}_{dot} acting on \mathcal{G} is a null operation and we let $\mathcal{O}_{dot}[\mathcal{G}] := \mathcal{G}$.

From this definition, we see that $\mathcal{O}_{dot}[\mathcal{G}]$ of a regular graph \mathcal{G} is a sum of normal regular graphs.

4.2 Local expansions

In this section, we define the basic local expansions. We call them “local” because these expansions do not create new molecules, that is, every molecule in a new graph is obtained by adding new atoms to existing molecules or merging some molecules in the original graph. It is easy to see that \mathcal{O}_{dot} is a local expansion. We emphasize that local expansions can change the global structure, but they will preserve the doubly connected property as we will show in Lemma 4.10.

As introduced in [32], there are four basic local expansions, including one weight expansion and three edge expansions. We now define them one by one.

Definition 4.3 (Weight expansion operator). *Given a normal regular graph \mathcal{G} containing an atom x , if there is no weight or light weight on x , then we trivially define $\mathcal{O}_{weight}^{(x)}[\mathcal{G}] := \mathcal{G}$. Otherwise, we define $\mathcal{O}_{weight}^{(x)}[\mathcal{G}]$ in the following way.*

(i) Removing regular weights: *Suppose there are regular G_{xx} or \bar{G}_{xx} weights on x . Then we rewrite*

$$G_{xx} = m + (G_{xx} - m), \quad \text{or} \quad \bar{G}_{xx} = \bar{m} + (\bar{G}_{xx} - \bar{m}).$$

Expanding the product of all these sums, we can rewrite \mathcal{G} into a linear combination of normal regular graphs containing only light weights on x . We denote this graph expansion operator as $\mathcal{O}_{weight}^{(x),1}$.

(ii) Expanding light weight: *If \mathcal{G} has a light weight $G_{xx} - m$ of positive charge on x and is of the form $\mathcal{G} = (G_{xx} - m)f(G)$, then we define the light weight expansion on x by*

$$\begin{aligned} \mathcal{O}_{weight}^{(x),2}[\mathcal{G}] &:= m \sum_{\alpha} s_{x\alpha} (G_{xx} - m) (G_{\alpha\alpha} - m) f(G) + m \sum_{\alpha, \beta} S_{x\alpha}^+ s_{\alpha\beta} (G_{\alpha\alpha} - m) (G_{\beta\beta} - m) f(G) \\ &\quad - m \sum_{\alpha} s_{x\alpha} G_{\alpha x} \partial_{h_{\alpha x}} f(G) - m \sum_{\alpha, \beta} S_{x\alpha}^+ s_{\alpha\beta} G_{\beta\alpha} \partial_{h_{\beta\alpha}} f(G) + \mathcal{Q}_w, \end{aligned} \quad (4.3)$$

where \mathcal{Q}_w is a sum of Q -graphs,

$$\begin{aligned} \mathcal{Q}_w &:= Q_x [(G_{xx} - m)f(G)] + \sum_{\alpha} Q_{\alpha} [S_{x\alpha}^+ (G_{\alpha\alpha} - m)f(G)] \\ &\quad - m Q_x \left[\sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) G_{xx} f(G) \right] - m \sum_{\alpha} Q_{\alpha} \left[\sum_{\beta} S_{x\alpha}^+ s_{\alpha\beta} (G_{\beta\beta} - m) G_{\alpha\alpha} f(G) \right] \\ &\quad + m Q_x \left[\sum_{\alpha} s_{x\alpha} G_{\alpha x} \partial_{h_{\alpha x}} f(G) \right] + m \sum_{\alpha} Q_{\alpha} \left[\sum_{\beta} S_{x\alpha}^+ s_{\alpha\beta} G_{\beta\alpha} \partial_{h_{\beta\alpha}} f(G) \right]. \end{aligned}$$

If $\mathcal{G} = (\bar{G}_{xx} - \bar{m})f(G)$, then we define

$$\mathcal{O}_{weight}^{(x),2}[\mathcal{G}] := \overline{\mathcal{O}_{weight}^{(x),2}[(G_{xx} - m)f(G)]}, \quad (4.4)$$

where the right-hand side is defined using (4.3). When there are more than one light weights on x , we pick any one of them and apply (4.3) or (4.4).

Combining the above two graph operators, we define

$$\mathcal{O}_{weight}^{(x)}[\mathcal{G}] := \mathcal{O}_{weight}^{(x),1} \circ \mathcal{O}_{dot} \circ \mathcal{O}_{weight}^{(x),2} \circ \mathcal{O}_{weight}^{(x),1}[\mathcal{G}], \quad (4.5)$$

where \mathcal{O}_{dot} is applied to ensure that the resulting graphs after applying $\mathcal{O}_{weight}^{(x)}$ are normal regular.

We introduce the following notion of degree of atoms:

$$\deg(x) := \#\{\text{solid edges connected with } x\}. \quad (4.6)$$

In other words, we only count the plus and minus G edges connected with an atom regarding its ‘‘degree’’. We define the following three edge expansions on atoms of nonzero degrees.

Definition 4.4 (Multi-edge expansion operator). *Given a normal regular graph \mathcal{G} , if there are no solid edges connected with the atom x , then we trivially define $\mathcal{O}_{multi-e}^{(x)}[\mathcal{G}] := \mathcal{G}$. Otherwise, we define $\mathcal{O}_{multi-e}^{(x)}$ in the following way. Suppose the graph takes the form*

$$\mathcal{G} := \prod_{i=1}^{k_1} G_{xy_i} \cdot \prod_{i=1}^{k_2} \bar{G}_{xy'_i} \cdot \prod_{i=1}^{k_3} G_{w_i x} \cdot \prod_{i=1}^{k_4} \bar{G}_{w'_i x} \cdot f(G), \quad (4.7)$$

where $f(G)$ does not contain G edges attached to x , and the atoms y_i, y'_i, w_i and w'_i are all not equal to x .

(i) If $k_1 \geq 1$, then we define the multi-edge expansion on x as

$$\begin{aligned} \widehat{\mathcal{O}}_{multi-e}^{(x)}[\mathcal{G}] &:= \sum_{i=1}^{k_2} |m|^2 \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha y'_i} \right) \frac{\mathcal{G}}{G_{xy_1} \bar{G}_{xy'_i}} + \sum_{i=1}^{k_3} m^2 \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} G_{w_i \alpha} \right) \frac{\mathcal{G}}{G_{xy_1} G_{w_i x}} \\ &+ \sum_{i=1}^{k_2} m(\bar{G}_{xx} - \bar{m}) \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha y'_i} \right) \frac{\mathcal{G}}{G_{xy_1} \bar{G}_{xy'_i}} + \sum_{i=1}^{k_3} m(G_{xx} - m) \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} G_{w_i \alpha} \right) \frac{\mathcal{G}}{G_{xy_1} G_{w_i x}} \\ &+ m \sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} + (k_1 - 1)m \sum_{\alpha} s_{x\alpha} G_{x\alpha} G_{\alpha y_1} \frac{\mathcal{G}}{G_{xy_1}} + k_4 m \sum_{\alpha} s_{x\alpha} \bar{G}_{\alpha x} G_{\alpha y_1} \frac{\mathcal{G}}{G_{xy_1}} \\ &- m \sum_{\alpha} s_{x\alpha} \frac{\mathcal{G}}{G_{xy_1} f(G)} G_{\alpha y_1} \partial_{h_{\alpha x}} f(G) + \mathcal{Q}_{multi-e}. \end{aligned} \quad (4.8)$$

On the right-hand side of (4.8), the first two terms are main terms with the same scaling order as \mathcal{G} , but the degree of atom x is reduced by 2 and a new atom α of degree 2 is created; the third to fifth terms contain one more light weight and hence are of strictly higher scaling order than \mathcal{G} ; the sixth to eighth terms contain at least one more off-diagonal G edge and hence are of strictly higher scaling order than \mathcal{G} . The last term $\mathcal{Q}_{multi-e}$ is a sum of Q -graphs defined by

$$\begin{aligned} \mathcal{Q}_{multi-e} &:= Q_x(\mathcal{G}) - \sum_{i=1}^{k_2} m Q_x \left[\bar{G}_{xx} \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha y'_i} \right) \frac{\mathcal{G}}{G_{xy_1} \bar{G}_{xy'_i}} \right] \\ &- \sum_{i=1}^{k_3} m Q_x \left[G_{xx} \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} G_{w_i \alpha} \right) \frac{\mathcal{G}}{G_{xy_1} G_{w_i x}} \right] - m Q_x \left[\sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} \right] \\ &- (k_1 - 1)m Q_x \left[\sum_{\alpha} s_{x\alpha} G_{x\alpha} G_{\alpha y_1} \frac{\mathcal{G}}{G_{xy_1}} \right] - k_4 m Q_x \left[\sum_{\alpha} s_{x\alpha} \bar{G}_{\alpha x} G_{\alpha y_1} \frac{\mathcal{G}}{G_{xy_1}} \right] \\ &+ m Q_x \left[\sum_{\alpha} s_{x\alpha} \frac{\mathcal{G}}{G_{xy_1} f(G)} G_{\alpha y_1} \partial_{h_{\alpha x}} f(G) \right]. \end{aligned}$$

(ii) If $k_1 = 0$ and $k_2 \geq 1$, then we define

$$\widehat{\mathcal{O}}_{multi-e}^{(x)}[\mathcal{G}] := \widehat{\mathcal{O}}_{multi-e}^{(x)} \left[\prod_{i=1}^{k_2} G_{xy'_i} \cdot \prod_{i=1}^{k_3} \bar{G}_{w_i x} \cdot \prod_{i=1}^{k_4} \bar{G}_{w'_i x} \cdot f(\bar{G}) \right],$$

where the right-hand side can be defined using (i).

(iii) If $k_1 = k_2 = 0$ and $k_3 \geq 1$, then we can define $\widehat{\mathcal{O}}_{multi-e}^{(x)}[\mathcal{G}]$ by exchanging the order of matrix indices in (i). More precisely, we define

$$\begin{aligned} \widehat{\mathcal{O}}_{multi-e}^{(x)}[\mathcal{G}] &:= \sum_{i=1}^{k_4} |m|^2 \left(\sum_{\alpha} s_{x\alpha} G_{w_1\alpha} \overline{G}_{w'_i\alpha} \right) \frac{\mathcal{G}}{G_{w_1x} \overline{G}_{w'_ix}} + \sum_{i=1}^{k_4} m(\overline{G}_{xx} - \overline{m}) \left(\sum_{\alpha} s_{x\alpha} G_{w_1\alpha} \overline{G}_{w'_i\alpha} \right) \frac{\mathcal{G}}{G_{w_1x} \overline{G}_{w'_ix}} \\ &+ m \sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} + (k_3 - 1)m \sum_{\alpha} s_{x\alpha} G_{w_1\alpha} G_{\alpha x} \frac{\mathcal{G}}{G_{w_1x}} \\ &- m \sum_{\alpha} s_{x\alpha} \frac{\mathcal{G}}{G_{w_1x} f(G)} G_{w_1\alpha} \partial_{h_{x\alpha}} f(G) + \mathcal{Q}_{multi-e}, \end{aligned} \quad (4.9)$$

where

$$\begin{aligned} \mathcal{Q}_{multi-e} &:= Q_x(\mathcal{G}) - \sum_{i=1}^{k_4} m Q_x \left[\overline{G}_{xx} \left(\sum_{\alpha} s_{x\alpha} G_{w_1\alpha} \overline{G}_{w'_i\alpha} \right) \frac{\mathcal{G}}{G_{w_1x} \overline{G}_{w'_ix}} \right] - m Q_x \left[\sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} \right] \\ &- (k_3 - 1)m Q_x \left[\sum_{\alpha} s_{x\alpha} G_{w_1\alpha} G_{\alpha x} \frac{\mathcal{G}}{G_{w_1x}} \right] + m Q_x \left[\sum_{\alpha} s_{x\alpha} \frac{\mathcal{G}}{G_{w_1x} f(G)} G_{w_1\alpha} \partial_{h_{x\alpha}} f(G) \right]. \end{aligned}$$

(iv) If $k_1 = k_2 = k_3 = 0$ and $k_4 \geq 1$, then we define

$$\widehat{\mathcal{O}}_{multi-e}^{(x)}[\mathcal{G}] := \overline{\widehat{\mathcal{O}}_{multi-e}^{(x)} \left[\prod_{i=1}^{k_4} G_{w'_ix} \cdot f(G) \right]},$$

where the right-hand side can be defined using (iii).

Finally, applying the \mathcal{O}_{dot} in Definition 4.2, we define

$$\mathcal{O}_{multi-e}^{(x)}[\mathcal{G}] := \mathcal{O}_{dot} \circ \widehat{\mathcal{O}}_{multi-e}^{(x)}[\mathcal{G}].$$

Definition 4.5 (*GG expansion operator*). Suppose a normal regular graph \mathcal{G} takes the form $\mathcal{G} = G_{xy} G_{y'x} f(G)$ with $y, y' \neq x$, where $f(G)$ does not contain G edges attached to x . Then we define

$$\begin{aligned} \widehat{\mathcal{O}}_{GG}^{(x)}[\mathcal{G}] &:= m S_{xy}^+ G_{y'y} f(G) + m \sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} + m \sum_{\alpha, \beta} S_{x\alpha}^+ s_{\alpha\beta} (G_{\beta\beta} - m) G_{\alpha y} G_{y'\alpha} f(G) \\ &+ m (G_{xx} - m) \sum_{\alpha} s_{x\alpha} G_{\alpha y} G_{y'\alpha} f(G) + m \sum_{\alpha, \beta} S_{x\alpha}^+ s_{\alpha\beta} (G_{\alpha\alpha} - m) G_{\beta y} G_{y'\beta} f(G) \\ &- m \sum_{\alpha} s_{x\alpha} G_{\alpha y} G_{y'x} \partial_{h_{\alpha x}} f(G) - m \sum_{\alpha, \beta} S_{x\alpha}^+ s_{\alpha\beta} G_{\beta y} G_{y'\alpha} \partial_{h_{\beta\alpha}} f(G) + \mathcal{Q}_{GG}. \end{aligned} \quad (4.10)$$

On the right hand side of (4.10), the first term is the main term which is either of the same scaling order as \mathcal{G} if $y = y'$ or of strictly higher scaling order if $y \neq y'$; the second to fifth terms contain one more light weight and hence are of strictly higher scaling order than \mathcal{G} ; the sixth and seventh terms contain at least one more off-diagonal G edge and hence are of strictly higher scaling order than \mathcal{G} ; \mathcal{Q}_{GG} is a sum of Q -graphs defined by

$$\begin{aligned} \mathcal{Q}_{GG} &:= Q_x(\mathcal{G}) + \sum_{\alpha} Q_{\alpha} \left[S_{x\alpha}^+ G_{\alpha y} G_{y'\alpha} f(G) \right] - m Q_y \left[S_{xy}^+ G_{y'y} f(G) \right] - m Q_x \left[\sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} \right] \\ &- m \sum_{\alpha} Q_{\alpha} \left[\sum_{\beta} S_{x\alpha}^+ s_{\alpha\beta} (G_{\beta\beta} - m) G_{\alpha y} G_{y'\alpha} f(G) \right] - m Q_x \left[G_{xx} \sum_{\alpha} s_{x\alpha} G_{\alpha y} G_{y'\alpha} f(G) \right] \\ &- m \sum_{\alpha} Q_{\alpha} \left[\sum_{\beta} S_{x\alpha}^+ s_{\alpha\beta} G_{\alpha\alpha} G_{\beta y} G_{y'\beta} f(G) \right] + m Q_x \left[\sum_{\alpha} s_{x\alpha} G_{\alpha y} G_{y'x} \partial_{h_{\alpha x}} f(G) \right] \\ &+ m \sum_{\alpha} Q_{\alpha} \left[\sum_{\beta} S_{x\alpha}^+ s_{\alpha\beta} G_{\beta y} G_{y'\alpha} \partial_{h_{\beta\alpha}} f(G) \right]. \end{aligned} \quad (4.11)$$

If \mathcal{G} takes the form $\mathcal{G} = \overline{G}_{xy}\overline{G}_{y'x}f(G)$, then we define

$$\widehat{\mathcal{O}}_{GG}^{(x)}[\mathcal{G}] := \overline{\widehat{\mathcal{O}}_{GG}^{(x)}[G_{xy}G_{y'x}f(G)]},$$

where the right-hand side is defined using (4.10). Finally, applying the \mathcal{O}_{dot} in Definition 4.2, we define

$$\mathcal{O}_{GG}^{(x)}[\mathcal{G}] := \mathcal{O}_{dot} \circ \widehat{\mathcal{O}}_{GG}^{(x)}[\mathcal{G}].$$

Definition 4.6 ($G\overline{G}$ expansion operator). *Suppose a normal regular graph \mathcal{G} takes the form $\mathcal{G} = G_{xy}\overline{G}_{xy'}f(G)$ with $y, y' \neq x$, where $f(G)$ does not contain G edges attached to x . Then by taking $k_1 = k_2 = 1$ and $k_3 = k_4 = 0$ in Definition 4.4, we define*

$$\begin{aligned} \widehat{\mathcal{O}}_{G\overline{G}}^{(x)}[\mathcal{G}] := & |m|^2 \sum_{\alpha} s_{x\alpha} G_{\alpha y} \overline{G}_{\alpha y'} f(G) + m \sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} \\ & + m(\overline{G}_{xx} - \overline{m}) \sum_{\alpha} s_{x\alpha} G_{\alpha y} \overline{G}_{\alpha y'} f(G) - m \sum_{\alpha} s_{x\alpha} G_{\alpha y} \overline{G}_{xy'} \partial_{h_{\alpha x}} f(G) + \mathcal{Q}_{G\overline{G}}, \end{aligned} \quad (4.12)$$

where $\mathcal{Q}_{G\overline{G}}$ is defined by

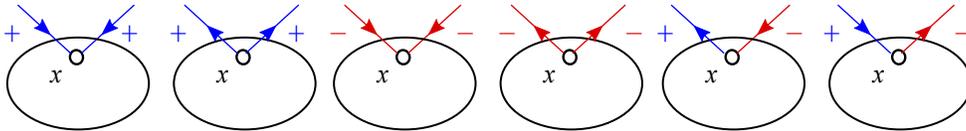
$$\begin{aligned} \mathcal{Q}_{G\overline{G}} := & Q_x(\mathcal{G}) - mQ_x \left[\sum_{\alpha} s_{x\alpha} \overline{G}_{xx} G_{\alpha y} \overline{G}_{\alpha y'} f(G) \right] - mQ_x \left[\sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} \right] \\ & + mQ_x \left[\sum_{\alpha} s_{x\alpha} G_{\alpha y} \overline{G}_{xy'} \partial_{h_{\alpha x}} f(G) \right]. \end{aligned}$$

If \mathcal{G} takes the form $\mathcal{G} = G_{yx}\overline{G}_{y'x}f(G)$, we define $\mathcal{O}_{G\overline{G}}^{(x)}[\mathcal{G}]$ by taking $k_1 = k_2 = 0$ and $k_3 = k_4 = 1$ in Definition 4.4, and we omit the explicit expression. Finally, applying the \mathcal{O}_{dot} in Definition 4.2, we define

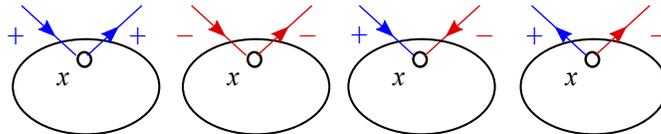
$$\mathcal{O}_{G\overline{G}}^{(x)}[\mathcal{G}] := \mathcal{O}_{dot} \circ \widehat{\mathcal{O}}_{G\overline{G}}^{(x)}[\mathcal{G}].$$

As shown in [32], the operations $\mathcal{O}_{weight}^{(x)}$, $\mathcal{O}_{multi-e}^{(x)}$, $\mathcal{O}_{GG}^{(x)}$ and $\mathcal{O}_{G\overline{G}}^{(x)}$ are all obtained from Gaussian integration by parts. Their basic properties have been summarized in Section 3 of [32]. In particular, it is easy to see that the new atoms α and β appearing in these expansions are connected to atom x through a path of waved edges, so they are included into the existing molecule containing atom x . Hence Definitions 4.3–4.6 all give local expansions. Applying these expansions repeatedly, we can expand any regular graph into a linear combination of *locally standard graphs*, Q -graphs and higher order graphs. To define locally standard graphs, we first introduce the following concept of *standard neutral atoms*.

Definition 4.7 (Standard neutral atoms). *Consider an internal atom x of degree 2 in a graph. We say the two edges connected with x are mismatched if they are of following forms:*



Otherwise the two edges are matched and of the following forms:



An atom is said to be standard neutral if it is only connected to three edges besides possible \times -dotted edges: two matched G edges of opposite charges and one waved S edge.

The edges connected with a standard neutral atom almost form a T -variable (but not an exact T -variable because of \times -dotted edges; see Section 4.3 for more details).

Definition 4.8 (Locally standard graphs). *A graph \mathcal{G} is locally standard if*

- (i) *it is a normal regular graph without P/Q labels;*
- (ii) *it has no weights or light weights;*
- (iii) *the degree of any internal atom is 0 or 2;*
- (iv) *all degree 2 internal atoms are standard neutral.*

Given a regular graph \mathcal{G} , we first apply \mathcal{O}_{dot} to expand it into a linear combination of normal regular graphs, then apply the weight expansion to remove all weights, and then apply the multi-edge, GG and $G\bar{G}$ expansions one by one to remove all atoms that are not standard neutral. In the end, we can expand \mathcal{G} into a sum of locally standard graphs, recollision graphs, Q -graphs and higher order graphs. The following basic lemma on local expansions has been proved in [32].

Lemma 4.9 (Lemma 3.22 of [32]). *Let $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ be a normal regular graph without solid edges connected with \mathbf{a} . Then for any fixed $n \in \mathbb{N}$, we have that*

$$\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = (\mathcal{G}_{local})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + \mathcal{R}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(n)} + (\mathcal{A}_{ho}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + \mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(n)}, \quad (4.13)$$

where $(\mathcal{G}_{local})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of $O(1)$ many locally standard graphs, $\mathcal{R}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(n)}$ is a sum of $O(1)$ many \oplus/\ominus -recollision graphs, $(\mathcal{A}_{ho}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of $O(1)$ many graphs of scaling order $> n$, and $(\mathcal{Q}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of $O(1)$ many Q -graphs. Every molecule in a graph on the right-hand side is obtained by merging some molecules in the original graph $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$.

If there are no dotted or wavy edges added between different molecules, then the molecules in a new graph are the same as those in $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$. In general, there may be newly added dotted edges (due to the dotted edge partition \mathcal{O}_{dot}) or wavy edges (due to the first term on the right-hand side of (4.10)), so the molecules in a new graph are obtained from merging the molecules connected by dotted or wavy edges. Now we show that local expansions do not break the doubly-connected property.

Lemma 4.10. *Suppose a normal regular graph \mathcal{G} is doubly-connected in the sense of Definition 2.12. Then applying any expansion in Definitions 4.2, 4.3, 4.4, 4.5 or 4.6 to \mathcal{G} , the new graphs (including the Q -graphs) are all doubly connected normal regular graphs.*

Proof. First, all blue solid and (labelled) diffusive edges between molecules are all unchanged in a dotted edge partition. The only changes are that in new molecular graphs, some molecules are merged into one molecule due to newly added dotted edges between different molecules. It is obvious that such merging operations will not break the doubly connected property.

Then we consider the weight expansion in Definition 4.3. It is trivial to see that $\mathcal{O}_{weight}^{(x),1}$ does not change molecular graphs at all. Hence it remains to show that $\mathcal{O}_{weight}^{(x),2}[\mathcal{G}]$ of a doubly connected graph \mathcal{G} is still a sum of doubly connected graphs. Let \mathcal{G}_1 be one of the new graphs. Since new atoms are all included into the molecule containing x , the molecules in the molecular graph of \mathcal{G}_1 are the same as those in the original molecular graph of \mathcal{G} . Moreover, (labelled) diffusive edges between molecules are also not affected, i.e. the black net does not change. It remains to consider the plus G edges between molecules in \mathcal{G}_1 . From (4.3), it is easy to see that any plus G edge in the molecular graph of \mathcal{G} between two different molecules, say \mathcal{M}_1 and \mathcal{M}_2 , either is not affected or becomes a connected path of two plus G edges between \mathcal{M}_1 and \mathcal{M}_2 due to the partial derivatives $\partial_{h_{\alpha x}}$ or $\partial_{h_{\beta \alpha}}$. (For example, if the atoms x , α and β are in molecule \mathcal{M}_3 , then the edge between \mathcal{M}_1 and \mathcal{M}_2 becomes two plus G edges from \mathcal{M}_1 to \mathcal{M}_3 and from \mathcal{M}_3 to \mathcal{M}_2 .) In either case, the path connectivity of the blue net is not affected, and hence the doubly connected property preserves in \mathcal{G}_1 .

For the edge expansions in Definitions 4.4, 4.5 and 4.6, the argument is exactly the same. \square

4.3 Global expansions

In this section, we define global expansions. As an induction hypothesis, suppose we have obtained the $(n-1)$ -th order T -expansion. Then a global expansion of a locally standard graph, say \mathcal{G} , consists of the following three steps:

- (i) we choose a standard neutral atom in \mathcal{G} ;

- (ii) we replace the T -variable containing the atom in (i) by the $(n - 1)$ -th order T -expansion;
- (iii) we apply Q -expansions to every resulting graph with Q -labels from (ii).

We call this procedure “global” because it may create new molecules in our graphs. Unlike local expansions, a global expansion may break the doubly connectedness of graphs. To avoid this issue, we need to follow a specific criterion in choosing the standard neutral atom in (i). This will be discussed in Section 5. In this subsection, we define step (ii) in the above procedure, and postpone the definition of Q -expansions in step (iii) to the next subsection.

Picking a standard neutral atom, say α , in a locally standard graph, the edges connected to it take one of the following forms:

$$t_{x,y_1y_2} := |m|^2 \sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha y_2} \mathbf{1}_{\alpha \neq y_1} \mathbf{1}_{\alpha \neq y_2}, \quad \text{or} \quad t_{y_1y_2,x} := |m|^2 \sum_{\alpha} G_{y_1\alpha} \bar{G}_{y_2\alpha} s_{\alpha x} \mathbf{1}_{\alpha \neq y_1} \mathbf{1}_{\alpha \neq y_2}. \quad (4.14)$$

Then we apply the $(n - 1)$ -th order T -expansion in (3.1) to these variables in the following way:

$$\begin{aligned} t_{x,y_1y_2} &= m\Theta_{xy_1} \bar{G}_{y_1y_2} + m(\Theta \Sigma_T^{(n-1)} \Theta)_{xy_1} \bar{G}_{y_1y_2} + (\mathcal{R}_T^{(n-1)})_{x,y_1y_2} + (\mathcal{A}_T^{(>n-1)})_{x,y_1y_2} + (\mathcal{Q}_T^{(n-1)})_{x,y_1y_2} \\ &\quad + (\mathcal{E}rr_{n-1,D})_{x,y_1y_2} - \sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha y_2} (\mathbf{1}_{\alpha \neq y_1} \mathbf{1}_{\alpha = y_2} + \mathbf{1}_{\alpha = y_1} \mathbf{1}_{\alpha \neq y_2} + \mathbf{1}_{\alpha = y_1} \mathbf{1}_{\alpha = y_2}). \end{aligned}$$

The last term on the right-hand side gives one (since $\mathbf{1}_{\alpha \neq y_1} \mathbf{1}_{\alpha = y_2} = \mathbf{1}_{\alpha = y_1} \mathbf{1}_{\alpha \neq y_2} = 0$ if $y_1 = y_2$) or two (since $\mathbf{1}_{\alpha = y_1} \mathbf{1}_{\alpha = y_2} = 0$ if $y_1 \neq y_2$) recollision graphs, so we combine it with $(\mathcal{R}_T^{(n-1)})_{x,y_1y_2}$ and denote the resulting term by $(\tilde{\mathcal{R}}_T^{(n-1)})_{x,y_1y_2}$. Hence we get the following expansion formula of the t -variable t_{x,y_1y_2} :

$$\begin{aligned} t_{x,y_1y_2} &= m\Theta_{xy_1} \bar{G}_{y_1y_2} + m(\Theta \Sigma_T^{(n-1)} \Theta)_{xy_1} \bar{G}_{y_1y_2} + (\tilde{\mathcal{R}}_T^{(n-1)})_{x,y_1y_2} + (\mathcal{A}_T^{(>n-1)})_{x,y_1y_2} \\ &\quad + (\mathcal{Q}_T^{(n-1)})_{x,y_1y_2} + (\mathcal{E}rr_{n-1,D})_{x,y_1y_2}. \end{aligned} \quad (4.15)$$

The expansion of $t_{y_1y_2,x}$ can be obtained by exchanging the order of every pair of matrix indices in the above equation.

4.4 Q -expansions

If we replace a t -variable with a graph in $\mathcal{Q}_T^{(n-1)}$, then we will get a graph of the form

$$\mathcal{G}_0 = \sum_x \Gamma_0 Q_x(\tilde{\Gamma}_0), \quad (4.16)$$

where both the graphs Γ_0 and $\tilde{\Gamma}_0$ do not contain P/Q labels. The Q -expansions defined in this subsection aim to expand the above graph into a sum of Q -graphs and graphs without P/Q labels. By Definition 3.1, Q -graphs refer to graphs where all edges and weights have the same Q -label. The graph \mathcal{G}_0 does not satisfy this property, so we will not call it a Q -graph to avoid confusion.

Step 1: First, we apply $\mathcal{O}_{weight}^{(x),1} \circ \mathcal{O}_{dot}$ to \mathcal{G}_0 in (4.16) and get a sum of normal regular graphs without regular weights on atom x . Now for any new graph, say $\mathcal{G} = \sum_x \Gamma Q_x(\tilde{\Gamma})$, if Γ does not contain any light weight or edges attached to x , then we apply the following operations.

Let $H^{(x)}$ be the $(N - 1) \times (N - 1)$ minor of H obtained by removing the x -th row and column of H , and define the resolvent minor $G^{(x)}(z) := (H^{(x)} - z)^{-1}$. The following resolvent identity is well-known:

$$G_{x_1x_2} = G_{x_1x_2}^{(x)} + \frac{G_{x_1x} G_{xx_2}}{G_{xx}}, \quad x_1, x_2 \in \mathbb{Z}_L^d, \quad (4.17)$$

which follows from the Schur complement formula. Correspondingly, we introduce a new type of weights, $(G_{xx})^{-1}$ and $(\bar{G}_{xx})^{-1}$, and a new label (x) to solid edges and weights. More precisely, if a weight on x has a label “ (-1) ”, then this weight represents a $(G_{xx})^{-1}$ or $(\bar{G}_{xx})^{-1}$ factor depending on its charge; if an edge or a weight has a label (x) , then it represents a $G^{(x)}$ entry.

Applying (4.17) to expand the resolvent entries in Γ one by one, we can get that

$$\Gamma = \Gamma^{(x)} + \sum_{\omega} \Gamma_{\omega}, \quad (4.18)$$

where $\Gamma^{(x)}$ is a graph whose weights and solid edges all have the (x) label, and hence is independent of the x -th row and column of H . The second term on the right-hand side of (4.18) is a sum of $O(1)$ many graphs. Moreover, every Γ_ω has a strictly higher scaling order than Γ , at least two new solid edges connected with x , and some weights with label (-1) on x . Using (4.18), we can expand \mathcal{G} as

$$\mathcal{G} = \sum_x \Gamma Q_x(\tilde{\Gamma}) = \sum_\omega \sum_x \Gamma_\omega Q_x(\tilde{\Gamma}) + \sum_x Q_x(\Gamma\tilde{\Gamma}) - \sum_\omega \sum_x Q_x(\Gamma_\omega\tilde{\Gamma}), \quad (4.19)$$

where the second and third terms are sums of Q -graphs.

Next, we expand graphs Γ_ω in (4.19) into graphs without $G^{(x)}$, $(G_{xx})^{-1}$ or $(\bar{G}_{xx})^{-1}$ entries. First, we apply the following expansion to the $G^{(x)}$ entries in Γ_ω :

$$G_{x_1x_2}^{(x)} = G_{x_1x_2} - \frac{G_{x_1x}G_{xx_2}}{G_{xx}}. \quad (4.20)$$

In this way, we can write Γ_ω as a sum of graphs $\sum_\zeta \Gamma_{\omega,\zeta}$, where $\Gamma_{\omega,\zeta}$ does not contain any $G^{(x)}$ entries. Second, we expand the $(G_{xx})^{-1}$ and $(\bar{G}_{xx})^{-1}$ weights in $\Gamma_{\omega,\zeta}$ using the Taylor expansion

$$\frac{1}{G_{xx}} = \frac{1}{m} + \sum_{k=1}^D \frac{1}{m} \left(-\frac{G_{xx} - m}{m} \right)^k + \mathcal{W}_D^{(x)}, \quad \mathcal{W}_D^{(x)} := \sum_{k>D} \left(-\frac{G_{xx} - m}{m} \right)^k. \quad (4.21)$$

We will regard $\mathcal{W}_D^{(x)}$ and $\bar{\mathcal{W}}_D^{(x)}$ as a new type of weights of scaling order $D+1$. Expanding the product of all Taylor expansions of the $(G_{xx})^{-1}$ and $(\bar{G}_{xx})^{-1}$ weights, we can write every $\Gamma_{\omega,\zeta}$ into a sum of graphs that do not contain weights with label (-1) . Finally, applying $\mathcal{O}_{weight}^{(x),1} \circ \mathcal{O}_{dot}$ again, we will get a sum of normal regular graphs without regular weights on x .

Now we summarize Step 1 in the following lemma.

Lemma 4.11. *Given a normal regular graph taking the form (4.16), we can expand it into a sum of $O(1)$ many graphs:*

$$\mathcal{G}_0 = \sum_\omega \Gamma_\omega Q_x(\tilde{\Gamma}_\omega) + \sum_\zeta Q_x(\mathcal{G}_\zeta) + \mathcal{G}_{err}, \quad (4.22)$$

where Γ_ω , $\tilde{\Gamma}_\omega$ and \mathcal{G}_ζ are normal regular graphs without P/Q , (x) or (-1) labels, and \mathcal{G}_{err} is a sum of normal regular graphs of scaling order $> D$. If Γ_0 does not contain any weights or edges attached to x , then every Γ_ω has a strictly higher scaling order than Γ_0 and contains at least one atom which either is connected to x through a solid edge or has been merged with x .

Proof. We only need to prove the second statement. Suppose Γ_0 does not contain any weights or edges attached to x . Then there exists at least one $G_{x_1x_2}$ or $\bar{G}_{x_1x_2}$ entry in Γ_0 that has been replaced by two solid edges $G_{x_1x}G_{xx_2}$ or $\bar{G}_{x_1x}\bar{G}_{xx_2}$ (together with a $(G_{xx})^{-1}$ or $(\bar{G}_{xx})^{-1}$ weight). These two solid edges will either appear in Γ_ω or become weights if x_1 or x_2 is identified with x due to newly added dotted edges in \mathcal{O}_{dot} operations. \square

If Γ_0 does not contain any weights or edges attached to x , then after Step 1 the structures of Γ_ω in (4.22) are already good enough for our purpose. In Steps 2 and 3, we aim to remove the Q_x label in $Q_x(\tilde{\Gamma}_\omega)$.

Step 2: In this step and Step 3, we will remove the Q_x label in

$$\Gamma_\omega Q_x(\tilde{\Gamma}_\omega) = \Gamma_\omega \tilde{\Gamma}_\omega - \Gamma_\omega P_x(\tilde{\Gamma}_\omega).$$

It suffices to write $P_x(\tilde{\Gamma}_\omega)$ into a sum of graphs without the P_x label. To this end, we will use the following lemma.

Lemma 4.12. *Let f be a differentiable function of G . We have that*

$$\begin{aligned} P_x [(G_{xx} - m)f(G)] &= P_x \left[m^2 \sum_\alpha s_{x\alpha} (G_{\alpha\alpha} - m) f(G) + m \sum_\alpha s_{x\alpha} (G_{\alpha\alpha} - m) (G_{xx} - m) f(G) \right] \\ &\quad - P_x \left[m \sum_\alpha s_{x\alpha} G_{\alpha x} \partial_{h_{\alpha x}} f(G) \right]. \end{aligned} \quad (4.23)$$

Given a graph \mathcal{G} taking the form (4.7), we have the following identity if $k_1 \geq 1$:

$$\begin{aligned}
P_x[\mathcal{G}] &= \sum_{i=1}^{k_2} |m|^2 P_x \left[\left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha y'_i} \right) \frac{\mathcal{G}}{G_{xy_1} \bar{G}_{xy'_i}} \right] + \sum_{i=1}^{k_3} m^2 P_x \left[\left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} G_{w_i \alpha} \right) \frac{\mathcal{G}}{G_{xy_1} G_{w_i x}} \right] \\
&+ \sum_{i=1}^{k_2} m P_x \left[(\bar{G}_{xx} - \bar{m}) \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha y'_i} \right) \frac{\mathcal{G}}{G_{xy_1} \bar{G}_{xy'_i}} \right] \\
&+ \sum_{i=1}^{k_3} m P_x \left[(G_{xx} - m) \left(\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} G_{w_i \alpha} \right) \frac{\mathcal{G}}{G_{xy_1} G_{w_i x}} \right] \\
&+ m P_x \left[\sum_{\alpha} s_{x\alpha} (G_{\alpha\alpha} - m) \mathcal{G} \right] + (k_1 - 1) m P_x \left[\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} G_{x\alpha} \frac{\mathcal{G}}{G_{xy_1}} \right] \\
&+ k_4 m P_x \left[\sum_{\alpha} s_{x\alpha} G_{\alpha y_1} \bar{G}_{\alpha x} \frac{\mathcal{G}}{G_{xy_1}} \right] - m P_x \left[\sum_{\alpha} s_{x\alpha} \frac{\mathcal{G}}{G_{xy_1} f(G)} G_{\alpha y_1} \partial_{h_{\alpha x}} f(G) \right]. \tag{4.24}
\end{aligned}$$

Proof. These two identities both follow from Gaussian integration by parts, and have been proved in Lemma 3.5 and Lemma 3.10 of [32]. \square

Similar to Definition 4.3, we can define an operator $\tilde{\mathcal{O}}_{weight}^{(x)}$ acting on a graph $P_x(\mathcal{G})$ as

$$\tilde{\mathcal{O}}_{weight}^{(x)}[P_x(\mathcal{G})] := \mathcal{O}_{weight}^{(x),1} \circ \mathcal{O}_{dot} \circ \tilde{\mathcal{O}}_{weight}^{(x),2} \circ \mathcal{O}_{weight}^{(x),1}[P_x(\mathcal{G})],$$

where $\tilde{\mathcal{O}}_{weight}^{(x),2}$ is an operator defined from (4.23). Also similar to Definition 4.4, we can define an operator $\tilde{\mathcal{O}}_{multi-e}^{(x)}$ acting on a graph $P_x(\mathcal{G})$ as

$$\tilde{\mathcal{O}}_{multi-e}^{(x)}[P_x(\mathcal{G})] := \mathcal{O}_{dot} \circ \tilde{\mathcal{O}}_{multi-e}^{(x),1}[P_x(\mathcal{G})],$$

where $\tilde{\mathcal{O}}_{multi-e}^{(x),1}$ is an operator defined from (4.24) (the $k_1 = 0$ case can be handled in the same way as cases (ii)–(iv) of Definition 4.4 and we omit the details).

If a normal regular graph $P_x(\mathcal{G})$ contains weights or solid edges attached to x , then we will apply $\tilde{\mathcal{O}}_{weight}^{(x)}$ or $\tilde{\mathcal{O}}_{multi-e}^{(x)}$ to it. We repeat these operations until all graphs do not contain weights or solid edges attached to x , and hence obtain the following lemma.

Lemma 4.13. *Suppose \mathcal{G} is a normal regular graph without P/Q , (x) or (-1) labels. Then we can expand $P_x(\mathcal{G})$ into a sum of $\mathcal{O}(1)$ many graphs:*

$$P_x(\mathcal{G}) = \sum_{\omega} P_x(\mathcal{G}_{\omega}) + \mathcal{G}_{err},$$

where \mathcal{G}_{ω} are normal regular graphs without weights or edges attached to x (and without P/Q , (x) or (-1) labels), and \mathcal{G}_{err} is a sum of normal regular graphs of scaling order $> D$.

Proof. We only describe the main argument for the proof without writing down all the details. Given a normal regular graph $P_x(\mathcal{G})$, it is easy to check that every graph in $\tilde{\mathcal{O}}_{weight}^{(x)}[P_x(\mathcal{G})]$ or $\tilde{\mathcal{O}}_{multi-e}^{(x)}[P_x(\mathcal{G})]$, say $P_x(\mathcal{G}_1)$, satisfies one of the following properties:

- $P_x(\mathcal{G}_1)$ has a strictly higher scaling order than $P_x(\mathcal{G}_0)$;
- $P_x(\mathcal{G}_1)$ contains strictly fewer weights or edges attached to x .

Hence applying the operations $\tilde{\mathcal{O}}_{weight}^{(x)}$ or $\tilde{\mathcal{O}}_{multi-e}^{(x)}$ for $C_{\mathcal{G},D}$ many times, each resulting graph either is of scaling order $> D$, or has no weights or edges attached to x . Here $C_{\mathcal{G},D} \in \mathbb{N}$ is a large constant depending only on D and the number of weights and edges attached to atom x in \mathcal{G} . \square

With Lemma 4.13, in Step 2 we can expand $Q_x(\tilde{\Gamma}_{\omega})$ as

$$Q_x(\tilde{\Gamma}_{\omega}) = \tilde{\Gamma}_{\omega} + \sum_{\zeta} P_x(\tilde{\Gamma}_{\omega,\zeta}) + \mathcal{G}_{err}, \tag{4.25}$$

where $\Gamma_{\omega,\xi}$ are normal regular graphs without weights or edges attached to x , and \mathcal{G}_{err} is a sum of graphs of scaling order $> D$.

Step 3: In this step, we expand the graphs $P_x(\tilde{\Gamma}_{\omega,\zeta})$ in (4.25). Suppose \mathcal{G} is a normal regular graph without weights or edges attached to x . Using the resolvent identity (4.17), we can write \mathcal{G} into a similar form as in (4.18):

$$\mathcal{G} = \mathcal{G}^{(x)} + \sum_{\omega} \mathcal{G}_{\omega},$$

where $\mathcal{G}^{(x)}$ is a graph whose weights and solid edges all have the same (x) label, and every graph \mathcal{G}_{ω} has a strictly higher scaling order than \mathcal{G} , at least two new solid edges connected with x , and some weights with label (-1) on x . Then we can expand $P_x(\mathcal{G})$ as

$$P_x(\mathcal{G}) = \mathcal{G} - \sum_{\omega} \mathcal{G}_{\omega} + \sum_{\omega} P_x(\mathcal{G}_{\omega}).$$

Next, as in Step 1, we apply (4.20) and (4.21) to remove all $G^{(x)}$, $(G_{xx})^{-1}$ and $(\bar{G}_{xx})^{-1}$ entries from \mathcal{G}_{ω} . Finally, we apply $\mathcal{O}_{weight}^{(x),1} \circ \mathcal{O}_{dot}$ to all resulting graphs to get a sum of normal regular graphs without regular weights on x . In sum, we obtain the following result.

Lemma 4.14. *Suppose \mathcal{G} is a normal regular graph without P/Q , (x) or (-1) labels. Moreover, suppose \mathcal{G} has no weights or edges attached to x . Then we can expand $P_x(\mathcal{G})$ into a sum of $O(1)$ many graphs:*

$$P_x(\mathcal{G}) = \mathcal{G} + \sum_{\xi} \mathcal{G}_{\xi} + \sum_{\gamma} P_x(\tilde{\mathcal{G}}_{\gamma}) + \mathcal{G}_{err},$$

where \mathcal{G}_{ξ} and $\tilde{\mathcal{G}}_{\gamma}$ are normal regular graphs without P/Q , (x) or (-1) labels, and \mathcal{G}_{err} is a sum of normal regular graphs of scaling order $> D$. Moreover, \mathcal{G}_{ξ} and $\tilde{\mathcal{G}}_{\gamma}$ are of strictly higher scaling order than \mathcal{G} , and have light weights or edges attached to the atom x .

With this lemma, we can expand $P_x(\tilde{\Gamma}_{\omega,\zeta})$ in (4.25) as

$$P_x(\tilde{\Gamma}_{\omega,\zeta}) = \tilde{\Gamma}_{\omega,\zeta} + \sum_{\xi} \Gamma_{\omega,\zeta,\xi} + \sum_{\gamma} P_x(\tilde{\Gamma}_{\omega,\zeta,\gamma}) + \mathcal{G}_{err},$$

where $\Gamma_{\omega,\zeta,\xi}$ and $\tilde{\Gamma}_{\omega,\zeta,\gamma}$ respectively satisfy the same properties as \mathcal{G}_{ξ} and $\tilde{\mathcal{G}}_{\gamma}$ in Lemma 4.11. Then we apply Step 2 to the graphs $P_x(\tilde{\Gamma}_{\omega,\zeta,\gamma})$ again. Repeating Steps 2 and 3 for $O(1)$ many times, we can finally expand $P_x(\tilde{\Gamma}_{\omega})$ into a sum of graphs without P_x labels plus graphs of scaling order $> D$.

Combining Steps 1–3, we obtain the following lemma on Q -expansions.

Lemma 4.15 (Q -expansions). *Suppose Γ_0 and $\tilde{\Gamma}_0$ in (4.16) are normal regular graph without P/Q , (x) or (-1) labels. Then \mathcal{G}_0 can be expanded into a sum of $O(1)$ many graphs:*

$$\mathcal{G}_0 = \sum_{\omega} \mathcal{G}_{\omega} + \sum_{\xi} Q_x(\tilde{\mathcal{G}}_{\xi}) + \mathcal{G}_{err}, \quad (4.26)$$

where \mathcal{G}_{ω} and $\tilde{\mathcal{G}}_{\xi}$ are normal regular graphs without P/Q , (x) or (-1) labels, and \mathcal{G}_{err} is a sum of normal regular graphs of scaling order $> D$. Moreover, these graphs satisfy the following properties.

- (i) Every graph on the right-hand side of (4.26) has a scaling order $\geq \text{ord}(\mathcal{G}_0)$.
- (ii) If there is a new atom in a graph on the right-hand side of (4.26), then it is connected to x through a path of wavy edges. Hence the expansion (4.26) is a local expansion.
- (iii) If \mathcal{G}_0 is doubly connected, then all graphs on the right-hand side of (4.26) are also doubly connected.
- (iv) If Γ_0 does not contain any weights or edges attached to x , then the scaling order of \mathcal{G}_{ω} is strictly higher than $\text{ord}(\mathcal{G}_0)$ for every ω . Furthermore, \mathcal{G}_{ω} contains at least one atom that belongs to the original graph Γ_0 and satisfies the following property: it is connected to x through a solid edge or it has been merged with x .

Proof. This lemma is an easy consequence of Lemmas 4.11, 4.13 and 4.14. We now give the main arguments without writing down all the details.

First, we show that the expansion (4.26) exists. Given \mathcal{G}_0 , we first expand it as in (4.22). Then we repeat Steps 2 and 3 to remove the Q_x label in $\Gamma_\omega Q_x(\tilde{\Gamma}_\omega)$. By Lemmas 4.13 and 4.14, after an iteration of Steps 2 and 3, every new graph either has no P/Q labels or has a strictly higher scaling order than the original graph. Hence after repeating Steps 2 and 3 for D many times, we can expand $\Gamma_\omega Q_x(\tilde{\Gamma}_\omega)$ into a sum of graphs without P/Q labels and graphs of scaling orders $> D$. This gives (4.26).

The properties (i) and (ii) are trivial. The proof of (iii) is similar to the one for Lemma 4.10. The property (iv) follows from Lemma 4.11. \square

The property (iv) of Lemma 4.15 is crucial to our global expansion strategy as we will explain in Section 6. Graphs with (x) and (-1) labels only appear in Q -expansions, and will not appear in any other part of the expansion process. Hence for the rest of this paper, unless mentioned otherwise, our graphs are assumed to have no (x) and (-1) labels.

5 PRE-DETERMINISTIC PROPERTY

The choice of the standard neutral atom is one of the most delicate parts of the global expansion defined in Section 4.3, and this subsection is devoted to this issue. Our goal is to define a rule to choose the t variable for every locally standard graph, so that the doubly connected property is preserved by global expansions. In this section, we will define a specific order of blue solid edges, called the *pre-deterministic order*, and we will show that the doubly connected property is preserved if we expand blue solid edges according to this order. As a convention, expansion of a blue solid edge refers to the expansion of a t -variable containing this edge.

In this section, we mostly consider molecular graphs with all red solid edges removed, because these edges are not used in the doubly connected property.

5.1 Isolated subgraphs

Using Definition 2.12, it is trivial to prove the following simple property.

Claim 5.1. *Let \mathcal{G} be a doubly connected graph satisfying Definition 2.12. Then in its molecular graph \mathcal{G}_M with all red solid edges removed, any subset of internal molecules are connected to other molecules (including external molecules) through at least one blue solid edge and one diffusive edge, or at least two diffusive edges.*

Then we define an isolated subgraph to be a subgraph induced on a subset of molecules that are connected to other molecules through *exactly two edges* in a molecular graph without red solid edges.

Definition 5.2 (Isolated subgraphs). *Let \mathcal{G} be a doubly connected graph and \mathcal{G}_M be its molecular graph with all red solid edges removed.*

- **Isolated subsets of molecule.** *A subset of internal molecules in \mathcal{G} , say \mathbf{M} , is isolated if and only if \mathbf{M} is connected to \mathbf{M}^c exactly by two edges in \mathcal{G}_M . Here the complement \mathbf{M}^c contains the internal molecules that are not in \mathbf{M} and all external molecules.*
- **Isolated subgraph.** *An isolated subgraph of \mathcal{G} is a subgraph induced on an isolated subset of molecules. Here by the “subgraph induced on a subset of molecules”, we mean the subgraph induced on the atoms in these molecules (recall Definition 2.3).*

Given any isolated subset of molecules \mathbf{M} , we can define an isolated subgraph induced on it, denoted by \mathcal{I}_M . Conversely, given an isolated subgraph \mathcal{I} , the molecules in it form an isolated subset of molecules, denoted by $\mathbf{M}(\mathcal{I})$. Furthermore, we define the concept of proper isolated subgraphs.

- **Proper isolated subgraph.** *Given any subset of molecules (which is not necessarily isolated), say \mathcal{S} , $\mathbf{M}_1 \subset \mathcal{S}$ is called a proper isolated subset if $\mathbf{M}_1 \neq \mathcal{S}$ and \mathbf{M}_1 is an isolated subset of molecules in \mathcal{G} . Moreover, a proper isolated subgraph of $\mathcal{G}|_{\mathcal{S}}$ refers to a subgraph induced on a proper isolated subset of molecules in \mathcal{S} .*

We call the set of all internal molecules the *maximal subset of internal molecules*, denoted by \mathbf{M}_{\max} . Correspondingly, the subgraph of \mathcal{G} induced on \mathbf{M}_{\max} is called the *maximal subgraph*, denoted by \mathcal{G}_{\max} . Whenever we say a proper isolated subset of molecules (resp. isolated subgraph) without specifying the superset, we mean a proper isolated subset (resp. isolated subgraph) of \mathbf{M}_{\max} (resp. \mathcal{G}_{\max}). Given any subset of molecules \mathcal{S} , we say an atom is inside \mathcal{S} if this atom belongs to a molecule in \mathcal{S} , and we say an edge is inside \mathcal{S} if its ending atoms are inside \mathcal{S} . Given two disjoint subsets of molecules \mathcal{S}_1 and \mathcal{S}_2 , an edge between \mathcal{S}_1 and \mathcal{S}_2 refers to an edge between an atom in \mathcal{S}_1 and an atom in \mathcal{S}_2 .

Every graph in our expansions has at least one edge between an internal atom and an external atom (recall property (ix) in Definition 3.2). Then from Definition 5.2, it is easy to get the following property.

Claim 5.3. *Let \mathcal{G} be a doubly connected graph such that there is at least one edge between its internal and external molecules in the molecular graph $\mathcal{G}_{\mathcal{M}}$ without red solid edges. Then for any two isolated subsets of molecules \mathbf{M}_1 and \mathbf{M}_2 in \mathcal{G} , we have that either one is a subset of the other or $\mathbf{M}_1 \cap \mathbf{M}_2 = \emptyset$.*

Proof. Suppose $\mathbf{M}_1 \not\subset \mathbf{M}_2$, $\mathbf{M}_2 \not\subset \mathbf{M}_1$ and $\mathbf{M}_1 \cap \mathbf{M}_2 \neq \emptyset$. First, assume that $\mathbf{M}_1 \cap \mathbf{M}_2$ is connected to $(\mathbf{M}_1 \cup \mathbf{M}_2)^c$ through a many edges with $a \in \{1, 2\}$ in $\mathcal{G}_{\mathcal{M}}$. Since \mathbf{M}_1 and \mathbf{M}_2 are isolated, $\mathbf{M}_1 \setminus \mathbf{M}_2$ connects to \mathbf{M}_1^c through $2 - a$ many edges and $\mathbf{M}_2 \setminus \mathbf{M}_1$ connects to \mathbf{M}_2^c through $2 - a$ many edges. Applying Claim 5.1, we get that $\mathbf{M}_1 \setminus \mathbf{M}_2$ connects to $\mathbf{M}_1 \cap \mathbf{M}_2$ through at least a many edges. This implies that \mathbf{M}_2 connects to \mathbf{M}_2^c through at least $a + 2 \geq 3$ many edges, contradicting the fact that \mathbf{M}_2 is isolated.

Now we assume that $\mathbf{M}_1 \cap \mathbf{M}_2$ is not connected to $(\mathbf{M}_1 \cup \mathbf{M}_2)^c$. Suppose $\mathbf{M}_1 \cap \mathbf{M}_2$ connects to $\mathbf{M}_1 \setminus \mathbf{M}_2$ through a many edges and to $\mathbf{M}_2 \setminus \mathbf{M}_1$ through b many edges. By Claim 5.1 and the fact that \mathbf{M}_1 and \mathbf{M}_2 are isolated, we have $0 \leq a \leq 2$, $0 \leq b \leq 2$ and $a + b \geq 2$. If $a = 0$, then $\mathbf{M}_1 \setminus \mathbf{M}_2$ connects to \mathbf{M}_1^c through two edges and $\mathbf{M}_1 \cap \mathbf{M}_2$ connects to $\mathbf{M}_2 \setminus \mathbf{M}_1$ through two edges, contradicting the fact that \mathbf{M}_1 is isolated. If $a = 2$, then $\mathbf{M}_2 \setminus \mathbf{M}_1$ is not connected to \mathbf{M}_2^c since \mathbf{M}_2 is isolated. This implies that $b = 2$ by applying Claim 5.1 to $\mathbf{M}_2 \setminus \mathbf{M}_1$. Since \mathbf{M}_1 is isolated, $\mathbf{M}_1 \setminus \mathbf{M}_2$ is also not connected to \mathbf{M}_1^c . Hence we get that $\mathbf{M}_1 \cup \mathbf{M}_2$ is disconnected from $(\mathbf{M}_1 \cup \mathbf{M}_2)^c$, which contradicts the assumption on $\mathcal{G}_{\mathcal{M}}$. Finally, we consider the case where $a = b = 1$, $\mathbf{M}_1 \setminus \mathbf{M}_2$ connects to \mathbf{M}_1^c through one edge and $\mathbf{M}_2 \setminus \mathbf{M}_1$ connects to \mathbf{M}_2^c through one edge. However, it is not hard to see that this case contradicts the doubly connected property. \square

This claim shows that there is a natural partial order of isolated subgraphs in a doubly connected graph satisfying Claim 5.3. In particular, we can define maximal and minimal subgraphs.

Definition 5.4. (i) *An isolated subgraph (resp. isolated subset of molecules) is said to be minimal if it has no proper isolated subgraphs (resp. proper isolated subsets). As a convention, if a graph \mathcal{G} does not contain any proper isolated subgraph, then the minimal isolated subgraph (MIS) refers to the maximal subgraph \mathcal{G}_{\max} .*

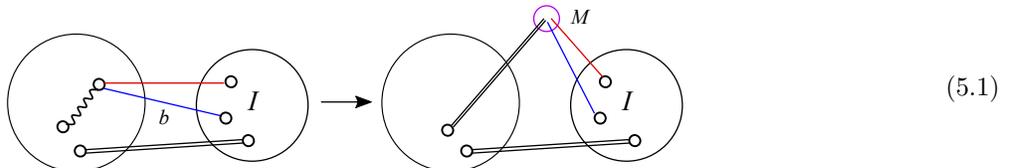
(ii) *Given a subset of molecules \mathcal{S} , an isolated subset \mathbf{M} of \mathcal{S} is said to be maximal if it is not a proper subset of any other proper isolated subset of \mathcal{S} . In this case, $\mathcal{I}_{\mathbf{M}}$ is called a maximal isolated subgraph of $\mathcal{G}|_{\mathcal{S}}$ induced on \mathcal{S} .*

5.2 Redundant edges

For the global expansions defined in Section 4.3, it is easy to see that expanding a blue solid edge inside a molecule will not break the doubly connected property. On the other hand, the doubly connected property may or may not be broken when we expand a blue solid edge between molecules, depending on whether this edge is *pivotal* or *redundant*.

Definition 5.5 (Pivotal edges and redundant edges). *We say a blue solid edge in a doubly connected graph \mathcal{G} is pivotal if after removing it, the remaining graph is not doubly connected anymore. Otherwise, this blue solid edge is said to be redundant.*

Example 5.6. In (5.1), the blue solid edge b connecting an isolated subgraph \mathcal{I} to its complement is pivotal:



In these graphs, inside the black circles are some subgraphs whose details are not drawn, and we did not indicate the directions of the solid edges for conciseness. If we replace the T -variable containing edge b in the first graph by a graph in (3.9), then we get the second graph, where the purple circle denotes a new molecule \mathcal{M} . It is easy to see that the second graph is not doubly connected anymore: in order to have a connected black net \mathcal{B}_{black} , we have to put the two diffusive edges into \mathcal{B}_{black} , but then there is no edge in the blue net \mathcal{B}_{blue} that connects \mathcal{M} and the molecules in \mathcal{I} to other molecules.

By definition, blue solid edges inside molecules are all redundant. Now we show that a redundant edge can be expanded without breaking the doubly connected property.

Lemma 5.7. *Suppose \mathcal{G} is a doubly connected graph containing a t_{x,y_1y_2} variable defined in (4.14), where the blue solid edge $G_{\alpha y_1}$ is redundant. If we replace t_{x,y_1y_2} with a graph on the right-hand side of (4.15) (including any recollision, Q , higher order or error graph), then the resulting graph is still doubly connected.*

Proof. We denote the blue solid edge $G_{\alpha y_1}$ as b . If we replace t_{x,y_1y_2} with $m\Theta_{xy_1}\overline{G}_{y_1y_2}$ or a graph in $m(\Theta\Sigma_T^{(n-1)}\Theta)_{xy_1}\overline{G}_{y_1y_2}$, then it corresponds to replacing the edge b with a diffusive edge in the molecular graph. Obviously, this will not break the doubly connected property because a diffusive edge can be also used in the blue net. Now suppose we replace t_{x,y_1y_2} with a graph, say $\tilde{\mathcal{G}}_{x,y_1y_2}$, in other terms. Since b is redundant, \mathcal{G} has a black net \mathcal{B}_{black} and a blue net \mathcal{B}_{blue} satisfying Definition 2.12 such that $\mathcal{B}_{blue} \setminus \{b\}$ is still a blue net. By property (x) of Definition 3.2, $\tilde{\mathcal{G}}_{x,y_1y_2}$ also contains a black net $\tilde{\mathcal{B}}_{black}$ and a blue net $\tilde{\mathcal{B}}_{blue}$ satisfying Definition 2.12. Moreover, by property (ix) of Definition 3.2, the atom x connects to the internal molecules of $\tilde{\mathcal{G}}_{x,y_1y_2}$ through a diffusive edge, say \tilde{b}_1 , while the atom y_1 connects to the internal molecules of $\tilde{\mathcal{G}}_{x,y_1y_2}$ through a blue solid or diffusive or dotted edge, say \tilde{b}_2 . Then $\mathcal{B}_{black} \cup \tilde{\mathcal{B}}_{black} \cup \{\tilde{b}_1\}$ and $(\mathcal{B}_{blue} \setminus \{b\}) \cup \tilde{\mathcal{B}}_{blue} \cup \{\tilde{b}_2\}$ are respectively the black net and blue net of the resulting graph if \tilde{b}_2 is not a dotted edge. If \tilde{b}_2 is a dotted edge, then the blue net can be chosen as $(\mathcal{B}_{blue} \setminus \{b\}) \cup \tilde{\mathcal{B}}_{blue}$ after merging the molecules connected by \tilde{b}_2 . In either case, the resulting graph is still doubly connected. \square

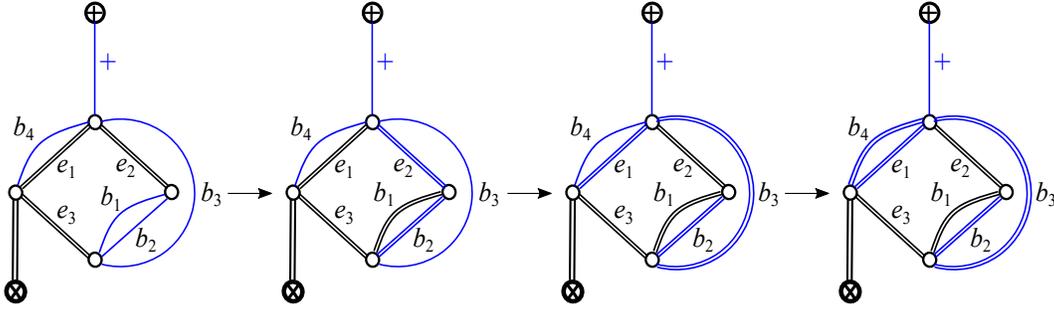
5.3 Pre-deterministic property

In the proof of Theorem 3.7, we need to expand T_{a,b_1b_2} into a sum of graphs that satisfy the properties in Definition 3.3. Hence for a graph that is not a recollision, higher order or Q graph, we want its maximal subgraph to be deterministic, so that the only random parts in the graph are two plus and minus G edges connected with \oplus and \ominus . On the other hand, since we want to maintain the doubly connected property during expansions, we are only allowed to expand redundant G edges. Hence, not all doubly connected graphs with non-deterministic maximal subgraphs can be expanded without breaking the doubly connected property. For example, in a doubly connected graph where both the black and blue nets are trees, all the blue solid edges between molecules are pivotal.

Now we want to identify a graphical property with which we can tell whether a graph is potentially expanded into deterministic graphs in the end without breaking the doubly connected property. We can obtain a necessary condition by looking at the leading terms of global expansions, where we replace t_{x,y_1y_2} in (4.14) with $m\Theta_{xy_1}\overline{G}_{y_1y_2}$. This corresponds to changing a plus G edge into a diffusive edge in the molecular graph. Hence we need to be able to change all plus G edges into diffusive edges one by one, such that the plus G edge for every expansion is redundant. This leads to the following definition.

Definition 5.8 (Pre-deterministic property). *We say a doubly connected graph \mathcal{G} is pre-deterministic if the following property holds. There exists an order of all internal blue solid edges, denoted by $b_1 \preceq b_2 \preceq \dots$, such that for any k , after changing the edges b_1, \dots, b_{k-1} into diffusive edges, the blue solid edge b_k becomes redundant. (Recall that internal edges refer to edges that do not connect to external atoms.) We will call this order of blue solid edges a pre-deterministic order.*

A pre-deterministic order is not necessarily unique. Moreover, we can always choose an order where blue solid edges inside molecules precede blue solid edges between molecules. If all internal blue solid edges in a graph \mathcal{G} are redundant, then \mathcal{G} is obviously a pre-deterministic graph. On the other hand, Definition 5.8 covers more general graphs. We use the following example to explain why we define pre-deterministic graphs in the above way, and why the order of blue solid edges is important:



Here all graphs are molecular graphs without red solid edges. Note that the edges b_1 and b_2 are redundant in the first graph, but b_3 and b_4 are not. Now we show that this graph is actually pre-deterministic. First, we replace b_1 and b_2 with diffusive edges. In the second graph, if we choose the black net as $\{e_1, e_3, b_1\}$ and the blue net as $\{e_2, b_2, b_3, b_4\}$, then the edge b_3 is redundant, and we can replace it with a diffusive edge in the third graph. In the third graph, if we choose the black net as $\{e_2, e_3, b_1\}$ and the blue net as $\{e_1, b_2, b_3, b_4\}$, then b_4 becomes redundant, and we can replace it with a diffusive edge in the fourth graph. This argument gives a pre-deterministic order $b_1 \preceq b_2 \preceq b_3 \preceq b_4$.

5.4 Sequentially pre-deterministic property

Not all graphs in our expansions satisfy the pre-deterministic property. Instead, we need to consider the following extension.

Definition 5.9 (Sequentially pre-deterministic property). *A graph \mathcal{G} is said to be sequentially pre-deterministic (SPD) if its molecular graph $\mathcal{G}_{\mathcal{M}}$ without red solid edges satisfies the following properties.*

- (i) $\mathcal{G}_{\mathcal{M}}$ is doubly connected in the sense of Definition 2.12.
- (ii) Any two proper isolated subgraphs \mathcal{I}_1 and \mathcal{I}_2 satisfy either $\mathcal{I}_1 \subset \mathcal{I}_2$ or $\mathcal{I}_2 \subset \mathcal{I}_1$.
- (iii) The minimal isolated subgraph of $\mathcal{G}_{\mathcal{M}}$ is pre-deterministic. Moreover, given an isolated subgraph \mathcal{I} , if we replace its maximal isolated subgraph, say \mathcal{I}' , plus the two external edges with a single diffusive edge, then \mathcal{I} becomes pre-deterministic. (Here by “external edges”, we mean the blue solid or diffusive edges connecting $\mathbf{M}(\mathcal{I}')$ to the two molecules, say \mathcal{M} and \mathcal{M}' , in the complement of $\mathbf{M}(\mathcal{I}')$; by “replace”, we mean that we remove \mathcal{I}' and its two external edges, and add a diffusive edge between \mathcal{M} and \mathcal{M}' . If $\mathcal{M} = \mathcal{M}'$, then this diffusive edge is inside \mathcal{M} and will not appear in the molecular graph.) Finally, if we replace the maximal isolated subgraph of $(\mathcal{G}_{\mathcal{M}})_{\max}$ (recall that $(\mathcal{G}_{\mathcal{M}})_{\max}$ is the maximal subgraph induced on all internal molecules) plus the two external edges with a single diffusive edge, then $(\mathcal{G}_{\mathcal{M}})_{\max}$ becomes pre-deterministic.

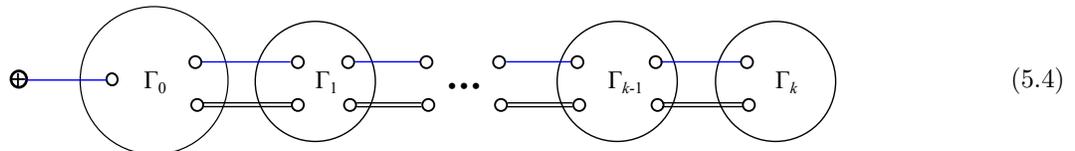
Now we discuss the meanings of properties (ii) and (iii). The property (ii) means that \mathcal{G} contains at most one sequence of proper isolated subgraphs, say

$$\mathcal{I}_k \subset \mathcal{I}_{k-1} \subset \cdots \subset \mathcal{I}_1 \subset \mathcal{G}_{\max}, \quad (5.2)$$

where \mathcal{I}_1 is the maximal isolated subgraph of \mathcal{G}_{\max} and for any j , \mathcal{I}_{j+1} is the maximal isolated subgraph of \mathcal{I}_j . In particular, any subgraph has at most one maximal isolated subgraph, so property (iii) is well-defined. Suppose that corresponding to (5.2), the sequence of proper isolated subsets of molecules is

$$\mathbf{M}_k \subset \mathbf{M}_{k-1} \subset \cdots \subset \mathbf{M}_1 \subset \mathbf{M}_{\max}, \quad \mathbf{M}_i := \mathbf{M}(\mathcal{I}_i), \quad 1 \leq i \leq k. \quad (5.3)$$

We draw a sequence of isolated subgraphs in the following figure, where inside each black circle is a subgraph Γ_i , which will be called a *component* in our proof, and we only draw the diffusive and blue solid edges between each isolated subgraph and its complement:



Here for definiteness, we draw a graph with one external blue solid edge, but generally there may be zero or more than one external edges. Moreover, the blue solid edges between components can be replaced by blue diffusive edges. In (5.4), the component Γ_k is the minimal isolated subgraph \mathcal{I}_k , the component Γ_i , $1 \leq i \leq k-1$, is the subgraph induced on $\mathbf{M}_i \setminus \mathbf{M}_{i+1}$, and Γ_0 is the subgraph induced on $\mathbf{M}_{\max} \setminus \mathbf{M}_1$. One can see that the isolated subgraphs in a SPD graph form a simple chain structure. Then property (iii) means that if we replace the MIS Γ_k and its two external edges with a diffusive edge, then the resulting graph is still SPD. In the new graph, replacing the MIS Γ_{k-1} and its two external edges with a diffusive edge again gives a SPD graph. Continuing this process, after replacing Γ_1 and its two external edges with a diffusive edge, Γ_0 becomes pre-deterministic.

The reason why we define the SPD property in the above way is due to our global expansion strategy below (cf. Strategy 6.6). We now describe one possible scenario to obtain a SPD graph. Initially, there is no proper isolated subgraph in a graph obtained from local expansions, and its maximal subgraph is pre-deterministic. Then we find the first redundant blue solid edge in a pre-deterministic order, replace a t -variable containing it with a graph, say $\tilde{\mathcal{G}}_1$, on the right-hand side of (4.15), and get a new graph \mathcal{G}_1 . If $\tilde{\mathcal{G}}_1$ contains a pre-deterministic maximal subgraph, then this subgraph becomes a pre-deterministic isolated subgraph \mathcal{I}_1 in graph \mathcal{G}_1 . Next we find the first blue solid edge in a pre-deterministic order of \mathcal{I}_1 , replace it with a graph, say $\tilde{\mathcal{G}}_2$, on the right-hand side of (4.15), and get a new graph. Continuing this process, we get a SPD graph with a sequence of isolated subgraphs in (5.2). At each step we expand the first blue solid edge in the minimal isolated subgraph. Moreover, replacing \mathcal{I}_{i+1} and its two external edges with a diffusive edge corresponds to replacing the first blue solid edge in a pre-deterministic order of \mathcal{I}_i by a diffusive edge, which still gives a pre-deterministic \mathcal{I}_i by Definition 5.8. This explains why we define property (iii) in such a way.

We now show that the SPD property is preserved under local expansions.

Lemma 5.10. *Let \mathcal{G} be a SPD graph. Then applying any expansion in Definitions 4.2, 4.3, 4.4, 4.5 and 4.6 to \mathcal{G} , the new graphs (including the Q -graphs) are all sequentially pre-deterministic.*

Proof. By Lemma 4.10, all new graphs are still doubly connected. It remains to check the properties (ii) and (iii) in Definition 5.9 for any new graph, say $\tilde{\mathcal{G}}$. Let $\tilde{\mathcal{G}}_{\mathcal{M}}$ be its molecular graph without red solid edges.

By Lemma 4.9, every molecule in $\tilde{\mathcal{G}}$ is obtained by merging some molecules in \mathcal{G} . We claim that any proper isolated subset of molecules, say \mathbf{M} , in $\tilde{\mathcal{G}}$ is obtained from merging a proper isolated subset of molecules in \mathcal{G} . In fact, suppose the molecules of \mathbf{M} are obtained from merging a subset of molecules \mathcal{S} that is not isolated in \mathcal{G} . Then \mathcal{S} is connected to \mathcal{S}^c through at least three edges, say b_1 , b_2 and b_3 , in the molecular graph $\mathcal{G}_{\mathcal{M}}$ without red solid edges. For $i = 1, 2, 3$, if b_i is a diffusive edge, then it is not affected in expansions and is still an external edge of \mathbf{M} in $\tilde{\mathcal{G}}_{\mathcal{M}}$. If b_i is a plus G edge in $\mathcal{G}_{\mathcal{M}}$ between molecules \mathcal{M}_1 and \mathcal{M}_2 , then either b_i is still a plus G edge between \mathcal{M}_1 and \mathcal{M}_2 in $\tilde{\mathcal{G}}_{\mathcal{M}}$, or b_i becomes a connected path of two plus G edges, say $b_{i,1}$ and $b_{i,2}$, between \mathcal{M}_1 and \mathcal{M}_2 . In the former case, b_i is an external edge of \mathbf{M} in $\tilde{\mathcal{G}}_{\mathcal{M}}$, and in the latter case, either $b_{i,1}$ or $b_{i,2}$ is an external edge of \mathbf{M} in $\tilde{\mathcal{G}}_{\mathcal{M}}$. In sum, we see that \mathbf{M} is connected to \mathbf{M}^c through at least three edges in $\tilde{\mathcal{G}}_{\mathcal{M}}$, which contradicts the assumption that \mathbf{M} is isolated.

Now with the above claim, we prove the property (ii) of Definition 5.9 for $\tilde{\mathcal{G}}$. Suppose two proper isolated subsets of molecules \mathbf{M}_1 and \mathbf{M}_2 in $\tilde{\mathcal{G}}$ are respectively obtained from merging two proper isolated subsets of molecules \mathbf{M}'_1 and \mathbf{M}'_2 in \mathcal{G} . Then we have either $\mathbf{M}_1 \subset \mathbf{M}_2$ if $\mathbf{M}'_1 \subset \mathbf{M}'_2$, or $\mathbf{M}_2 \subset \mathbf{M}_1$ if $\mathbf{M}'_2 \subset \mathbf{M}'_1$.

It remains to prove the property (iii) of Definition 5.9 for $\tilde{\mathcal{G}}$. In all expansions, it is not hard to see that there are only two types of operations that may affect the doubly connected structures:

- (A) merging a pair of molecules due to a newly added dotted or waved edge between them;
- (B) replacing a plus G edge b_0 between molecules \mathcal{M} and \mathcal{M}' with a path of two plus G edges—edge b between \mathcal{M} and \mathcal{M}'' and edge b' between \mathcal{M}' and \mathcal{M}'' —due to partial derivatives $\partial_{h_{\alpha x}}$ or $\partial_{h_{\beta \alpha}}$, where \mathcal{M}'' is a different molecule from \mathcal{M} and \mathcal{M}' .

All the other operations only act on local structures within molecules, and hence are irrelevant for our proof. Moreover, in case (B), we have assumed that \mathcal{M}'' is different from \mathcal{M} and \mathcal{M}' , because otherwise the molecular graph without red solid edges will be unchanged. To conclude the proof, it suffices to show that both operations (A) and (B) do not break the property (iii) of Definition 5.9.

Suppose the sequence of proper isolated subgraphs in \mathcal{G} is given by (5.2) and takes the form (5.4). In case (A), it is easy to see that merging a pair of molecules in the same component does not break the SPD

property. Now suppose we merge a pair of molecules in different components Γ_i and Γ_j with $i < j$. With a slight abuse of notation, we still denote the subgraph induced on \mathbf{M}_l by \mathcal{I}_l in $\tilde{\mathcal{G}}$. Then the sequence of isolated subgraphs in $\tilde{\mathcal{G}}$ is

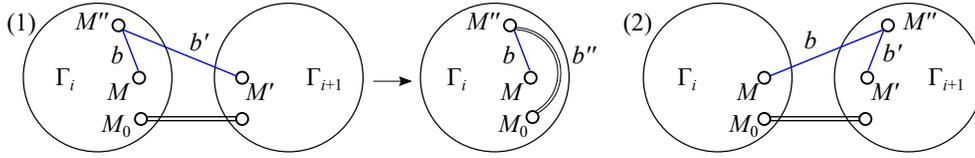
$$\mathcal{I}_k \subset \mathcal{I}_{k-1} \subset \cdots \subset \mathcal{I}_{j+1} \subset \mathcal{I}_i \subset \mathcal{I}_{i-1} \subset \cdots \subset \mathcal{I}_1.$$

In particular, \mathcal{I}_i is not isolated in $\tilde{\mathcal{G}}$ anymore if $j + 1 < l < i$. By the SPD property of \mathcal{G} , we immediately obtain the following property of $\tilde{\mathcal{G}}$: for $l \geq j + 1$ or $l \leq i - 1$, if we replace \mathcal{I}_{l+1} and its two external edges with a diffusive edge in the molecular graph of $\tilde{\mathcal{G}}$, then \mathcal{I}_l becomes pre-deterministic. It remains to show that after replacing \mathcal{I}_{j+1} and its two external edges with a diffusive edge, the subgraph \mathcal{I}_i becomes pre-deterministic. This is given by the following lemma, whose proof is postponed to Appendix A.

Lemma 5.11. *In the setting of (5.4), we merge a pair of molecules in different components Γ_i and Γ_j with $i < j$. Then after replacing \mathcal{I}_{j+1} and its two external edges with a diffusive edge in the molecular graph without red solid edges, the subgraph \mathcal{I}_i becomes pre-deterministic.*

Next we consider case (B). First, we assume that \mathcal{M} , \mathcal{M}' and \mathcal{M}'' are all inside Γ_i for some $0 \leq i \leq k$. Then all components are unchanged after operation (B), except the component Γ_i . By definition, after replacing \mathcal{I}_{i+1} and its two external edges with a diffusive edge, \mathcal{I}_i becomes pre-deterministic in \mathcal{G} , and suppose a pre-deterministic order of \mathcal{I}_i is $e_1 \preceq \cdots \preceq e_{\ell-1} \preceq b_0 \preceq e_{\ell+1} \preceq \cdots$. Then in $\tilde{\mathcal{G}}$, after replacing \mathcal{I}_{i+1} and its two external edges with a diffusive edge, $e_1 \preceq \cdots \preceq e_{\ell-1} \preceq b \preceq b' \preceq e_{\ell+1} \preceq \cdots$ is a pre-deterministic order in \mathcal{I}_i . Using this fact, we can readily check that $\tilde{\mathcal{G}}$ is still SPD.

Second, we assume that $\mathcal{M} \in \Gamma_i$, $\mathcal{M}' \in \Gamma_{i+1}$ and (1) $\mathcal{M}'' \in \Gamma_i$, or (2) $\mathcal{M}'' \in \Gamma_{i+1}$. Suppose we have replaced \mathcal{I}_{i+2} and its two external edges with a diffusive edge in \mathcal{I}_{i+1} and get the following graphs:



In case (1), \mathcal{I}_{i+1} is pre-deterministic because it is unchanged after the operation (B). In the second graph, we replace \mathcal{I}_{i+1} and its two external edges with a diffusive edge b'' . We show that the edge b is now redundant in \mathcal{I}_i . By the doubly connected property of \mathcal{G} , removing the subgraph \mathcal{I}_{i+1} and its two external edges still gives a doubly connected graph. Correspondingly, in the first graph of case (1), if we remove Γ_i , its two external edges and edge b , we still get a doubly connected graph. Hence the edge b is redundant in the second graph of case (1). Now if we replace b with a diffusive edge, then the path of diffusive edges b'' and b will play the role of a single diffusive edge between \mathcal{M}_0 and \mathcal{M} in \mathcal{I}_i , and hence \mathcal{I}_i becomes pre-deterministic by the property (iii) of Definition 5.9 for the original graph \mathcal{G} .

In case (2), \mathcal{I}_{i+1} is still pre-deterministic by choosing the edge b' as the last edge in a pre-deterministic order. Moreover, after replacing \mathcal{I}_{i+1} and its two external edges with a diffusive edge, \mathcal{I}_{i+1} becomes pre-deterministic by the property (iii) of Definition 5.9 for the original graph \mathcal{G} .

It remains to consider the case where \mathcal{M}'' is in a different component from both \mathcal{M} and \mathcal{M}' .

Lemma 5.12. *In the setting of (5.4), suppose a blue solid edge between molecules \mathcal{M} and \mathcal{M}' is replaced by a path of two blue solid edges from \mathcal{M} to \mathcal{M}'' and from \mathcal{M}'' to \mathcal{M}' . Let the new graph be $\tilde{\mathcal{G}}$, and with a slight abuse of notation, we still denote the subgraphs induced on \mathbf{M}_l by \mathcal{I}_l in $\tilde{\mathcal{G}}$. Suppose \mathcal{M}'' is inside component Γ_j . Then we have the following five cases for the molecular graph $\tilde{\mathcal{G}}_{\mathcal{M}}$ without red solid edges.*

- (i) *If $\mathcal{M}, \mathcal{M}' \in \Gamma_i$ and $i < j$, then \mathcal{I}_{j+1} is the maximal isolated subgraph of \mathcal{I}_i . Moreover, after replacing \mathcal{I}_{j+1} and its two external edges with a diffusive edge, the subgraph \mathcal{I}_i becomes pre-deterministic.*
- (ii) *If $\mathcal{M}, \mathcal{M}' \in \Gamma_i$ and $i > j$, then \mathcal{I}_{i+1} is the maximal isolated subgraph of \mathcal{I}_j . Moreover, after replacing \mathcal{I}_{i+1} and its two external edges with a diffusive edge, the subgraph \mathcal{I}_j becomes pre-deterministic.*
- (iii) *If $\mathcal{M} \in \Gamma_i$, $\mathcal{M}' \in \Gamma_{i+1}$ and $i < j$, then \mathcal{I}_{i+1} is the maximal isolated subgraph of \mathcal{I}_i , and \mathcal{I}_{j+1} is the maximal isolated subgraph of \mathcal{I}_{i+1} . Moreover, after replacing \mathcal{I}_{j+1} and its two external edges with a diffusive edge, the subgraph \mathcal{I}_{i+1} becomes pre-deterministic.*

(iv) If $\mathcal{M} \in \Gamma_i$, $\mathcal{M}' \in \Gamma_{i+1}$ and $i > j$, then \mathcal{I}_{i+1} is the maximal isolated subgraph of \mathcal{I}_j . Moreover, after replacing \mathcal{I}_{i+1} and its two external edges with a diffusive edge, the subgraph \mathcal{I}_j becomes pre-deterministic.

(v) If \mathcal{M} is an external molecule and $\mathcal{M}' \in \Gamma_0$, then \mathcal{I}_{j+1} is the maximal proper isolated subgraph. Moreover, after replacing \mathcal{I}_{j+1} and its two external edges with a diffusive edge, the maximal subgraph $\tilde{\mathcal{G}}_{\max}$ becomes pre-deterministic.

The proof of Lemma 5.12 will be postponed to Appendix A. Similar to case (A), combining Lemma 5.12 with the SPD property of the original graph \mathcal{G} , we can readily show that the new graph obtained from the operation (B) is still SPD. We omit the details. This concludes Lemma 5.10. \square

Similar to Lemma 5.10, we have the following result for Q -expansions.

Lemma 5.13. *Let \mathcal{G}_0 in (4.16) be a SPD graph. Then applying the Q -expansions in Section 4.4, the new graphs (including the Q -graphs) are all SPD.*

Proof. The proof of this lemma is similar to the one for Lemma 5.10 by using Lemmas 5.11 and 5.12, because Q -expansions are also local expansions as those in Lemma 5.10. We omit the details. \square

6 PROOF OF THEOREM 3.7 AND COROLLARY 3.8

6.1 Proof of Corollary 3.8

Given the n -th order T -equation constructed in Theorem 3.7, we can solve (3.11) to get that

$$T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = m \left(\frac{1}{1 - \Theta_{\Sigma^{(n)}}} \Theta \right)_{\mathbf{a} \mathbf{b}_1} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} + \sum_x \left(\frac{1}{1 - \Theta_{\Sigma^{(n)}}} \right)_{\mathbf{a} x} \left[(\mathcal{R}_{IT}^{(n)})_{x, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{A}_{IT}^{(>n)})_{x, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{Q}_{IT}^{(n)})_{x, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{E}rr'_{n,D})_{x, \mathbf{b}_1 \mathbf{b}_2} \right]. \quad (6.1)$$

By the property (iv) of Definition 3.3, we can write that

$$\begin{aligned} (\mathcal{R}_{IT}^{(n)})_{x, \mathbf{b}_1 \mathbf{b}_2} &= \sum_y \Theta_{xy} (\mathcal{G}_R^{(n)})_{y, \mathbf{b}_1 \mathbf{b}_2}, & (\mathcal{A}_{IT}^{(>n)})_{x, \mathbf{b}_1 \mathbf{b}_2} &= \sum_y \Theta_{xy} (\mathcal{G}_A^{(>n)})_{y, \mathbf{b}_1 \mathbf{b}_2}, \\ (\mathcal{Q}_{IT}^{(n)})_{x, \mathbf{b}_1 \mathbf{b}_2} &= \sum_y \Theta_{xy} (\mathcal{G}_Q^{(n)})_{y, \mathbf{b}_1 \mathbf{b}_2}, & (\mathcal{E}rr'_{n,D})_{x, \mathbf{b}_1 \mathbf{b}_2} &= \sum_y \Theta_{xy} (\mathcal{G}_{err}^{(n,D)})_{y, \mathbf{b}_1 \mathbf{b}_2}, \end{aligned}$$

for some sums of graphs $\mathcal{G}_R^{(n)}$, $\mathcal{G}_A^{(>n)}$, $\mathcal{G}_Q^{(n)}$ and $\mathcal{G}_{err}^{(n,D)}$. Using the definition (1.18), we can write (6.1) as

$$T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = m \Theta_{\mathbf{a} \mathbf{b}_1}^{(n)} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} + \sum_x \Theta_{\mathbf{a} x}^{(n)} \left[(\mathcal{G}_R^{(n)})_{x, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{G}_A^{(>n)})_{x, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{G}_Q^{(n)})_{x, \mathbf{b}_1 \mathbf{b}_2} + (\mathcal{G}_{err}^{(n,D)})_{x, \mathbf{b}_1 \mathbf{b}_2} \right]. \quad (6.2)$$

We expand $\Theta^{(n)}$ as

$$\Theta^{(n)} = \sum_{k=0}^D (\Theta_{\Sigma^{(n)}})^k \Theta + \Theta_{err}^{(n)}, \quad \Theta_{err}^{(n)} := \sum_{k>D} (\Theta_{\Sigma^{(n)}})^k \Theta. \quad (6.3)$$

The terms $(\Theta_{\Sigma^{(n)}})^k \Theta$ can be expanded into sums of labelled diffusive edges, and we regard $(\Theta_{err}^{(n)})_{xy}$ as a new type of diffusive edge of scaling order $\geq 2(D+2)$ between atoms x and y . Then we plug the expansion (6.3) into (6.2) and rearrange the resulting graphs as follows. First, all graphs containing $\Theta_{err}^{(n)}$ and graphs from $\sum_x \Theta_{\mathbf{a} x}^{(n)} (\mathcal{G}_{err}^{(n,D)})_{x, \mathbf{b}_1 \mathbf{b}_2}$ will be included into $(\mathcal{E}rr_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$. For other graphs,

- the term $m \Theta_{\mathbf{a} \mathbf{b}_1}^{(n)} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2}$ will give the first two terms on the right-hand side of (3.1) and some higher order graphs in $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$;
- the term $\sum_x \Theta_{\mathbf{a} x}^{(n)} (\mathcal{G}_R^{(n)})_{x, \mathbf{b}_1 \mathbf{b}_2}$ will give $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and some higher order graphs in $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$;

- the term $\sum_x \Theta_{ax}^{(n)}(\mathcal{G}_A^{(>n)})_{x,b_1b_2}$ will give higher order graphs in $(\mathcal{A}_T^{(>n)})_{a,b_1b_2}$;
- the term $\sum_x \Theta_{ax}^{(n)}(\mathcal{G}_Q^{(n)})_{x,b_1b_2}$ will give graphs in $(\mathcal{Q}_T^{(n)})_{a,b_1b_2}$.

This concludes Corollary 3.8.

6.2 Globally standard graphs

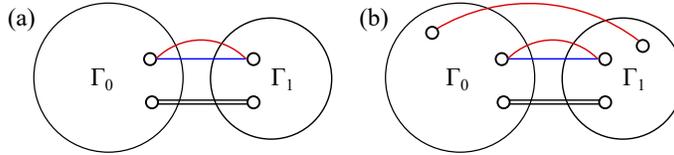
For the rest of this section, we focus on proving Theorem 3.7. In this subsection, we introduce the concept of *globally standard graphs*. By taking into account the external red solid edges connected with isolated subgraphs, we define the following concept of weakly and strongly isolated subgraphs.

Definition 6.1 (Weakly and strongly isolated subgraphs). *An isolated subset of molecules \mathbf{M} is said to be strongly isolated if there is at most one red solid edge between \mathbf{M} and \mathbf{M}^c , and the subgraph $\mathcal{I}_{\mathbf{M}}$ induced on \mathbf{M} is called a strongly isolated subgraph. Otherwise, \mathbf{M} and $\mathcal{I}_{\mathbf{M}}$ are said to be weakly isolated (i.e. a weakly isolated subgraph is an isolated subgraph that is not strongly isolated).*

With Definition 5.9 and Definition 6.1, we define globally standard graphs.

Definition 6.2 (Globally standard graphs). *A graph is said to be globally standard if it is SPD, and every proper isolated subgraph of it is weakly isolated.*

The reason for introducing globally standard graphs is to avoid *non-expandable graphs*, i.e. graphs that cannot be expanded without breaking the doubly connected property. As an example, we consider the following two graphs, where Γ_1 is strongly isolated in (a) and weakly isolated in (b):



Suppose both graphs (a) and (b) are SPD with Γ_1 being the minimal isolated subgraph. If Γ_1 contains blue solid edges, then we can either perform local expansions or expand the first blue solid edge in a pre-deterministic order of Γ_1 . Now suppose Γ_1 does not contain any internal blue solid edge, then it is not locally standard in graph (b) because there are more external red solid edges than blue solid edges. Hence we can perform local expansions to graph (b). On the other hand, if both Γ_0 and Γ_1 in (a) are deterministic, then graph (a) is locally standard and only contains a pivotal blue solid edge, so it cannot be expanded without breaking the doubly connected property. Such a graph may not be included into one of the six terms on the right-hand side of (3.11). In sum, the SPD property in Definition 6.2 gives a canonical order of blue solid edges to expand, while the weakly isolated property guarantees that our expansions will not give non-expandable graphs.

Now we state some additional properties satisfied by the graphs in the T -expansion and T -equation. Recall the definition of minimal isolated subgraphs (MIS) in Definition 5.4.

Definition 6.3 (T -expansion and T -equation: additional properties). *The graphs in Definition 3.2 satisfy the following additional properties.*

(i) *Every graph in $(\mathcal{R}_T^{(n)})_{a,b_1b_2}$ is globally standard.*

(ii) *Every graph in $(\mathcal{A}_T^{(>n)})_{a,b_1b_2}$ is SPD.*

(iii) *Every Q -graph in $(\mathcal{Q}_T^{(n)})_{a,b_1b_2}$ is SPD. Moreover, the atom in the Q -label of a Q -graph belongs to the MIS, i.e. all solid edges and weights have the same Q -label Q_x for an atom x inside the MIS.*

$(\mathcal{R}_{IT}^{(n)})_{a,b_1b_2}$, $(\mathcal{A}_{IT}^{(>n)})_{a,b_1b_2}$ and $(\mathcal{Q}_{IT}^{(n)})_{a,b_1b_2}$ in Definition 3.3 also satisfy these properties.

By this definition, the higher order and Q graphs in the T -expansion and T -equation may contain strongly isolated subgraphs, but the recollision graphs do not. The heuristic reason is as follows. We only expand globally standard graphs, and we want to show that an expansion of a globally standard graph still gives

globally standard graphs plus some graphs that are not needed to be expanded further (i.e. recollision, Q , higher order and error graphs). Suppose we substitute a t -variable with a recollision graph \mathcal{G} in $\mathcal{R}_T^{(n-1)}$. In order for the resulting graph to be globally standard, \mathcal{G} cannot contain any strongly isolated subgraph. This explains why recollision graphs have to be weakly isolated. If we substitute a T -variable with a graph in $\mathcal{A}_T^{(n-1)}$, then the resulting graph will be of scaling order $> n$ and we will not expand this graph further. Hence we do not require this graph to be globally standard. Finally, if we substitute a T -variable with a Q -graph \mathcal{G} in $\mathcal{Q}_T^{(n-1)}$ and get a graph, say \mathcal{G}_0 , then we need to perform Q -expansions to \mathcal{G}_0 . Suppose a Q -expansion of \mathcal{G}_0 is given by (4.26). By the property (iv) of Lemma 4.15, there will be solid edges connecting the atom in the Q -label of \mathcal{G} , say x , to old atoms in the original graph. Since x belongs to the MIS of \mathcal{G} , one can see that the strongly isolated subgraphs in \mathcal{G}_0 before the Q -expansion are not strongly isolated anymore in graphs \mathcal{G}_ω after the Q -expansion. The rigorous argument will be given in the proof of Lemma 6.5 below.

With Lemma 5.10, we can easily show that local expansions preserve the globally standard property.

Lemma 6.4. *Let \mathcal{G} be a globally standard graph without any P/Q labels.*

- (i) *Apply any expansion in Definitions 4.2, 4.3, 4.4, 4.5 and 4.6 to \mathcal{G} . The new graphs (including the Q -graphs) are all globally standard.*
- (ii) *Apply any expansion in Definitions 4.3, 4.4, 4.5 and 4.6 on an atom in the MIS of \mathcal{G} . In each new Q -graph, the atom in the Q -label also belongs to the MIS.*

Proof. By Lemma 5.10, the new graphs are all SPD. Let $\tilde{\mathcal{G}}$ be one of the new graphs. As shown in the proof of Lemma 5.10, any proper isolated subset of molecules \mathbf{M} in $\tilde{\mathcal{G}}$ is obtained from merging a proper isolated subset of molecules, say \mathbf{M}_0 , in \mathcal{G} . Moreover, it is easy to see that the number of external red solid edges of \mathbf{M} in $\tilde{\mathcal{G}}$ is larger than or equal to the number of external red solid edges of \mathbf{M}_0 in \mathcal{G} . Since \mathbf{M}_0 is weakly isolated in \mathcal{G} , we get that \mathbf{M} is also weakly isolated in $\tilde{\mathcal{G}}$. This concludes (i). The property (ii) can be checked readily using the Definitions 4.3, 4.4, 4.5 and 4.6. \square

The following lemma is key to our proof. Roughly speaking, it shows that the globally standard property is preserved if we expand the *first* blue solid edge in a pre-deterministic order of the MIS.

Lemma 6.5. *Suppose \mathcal{G} is a globally standard graph without P/Q labels. Let \mathcal{I}_k be the MIS of \mathcal{G} . Consider a t_{x,y_1y_2} variable in \mathcal{G} defined by (4.14), so that the blue solid edge $G_{\alpha y_1}$ is the first blue solid edge in a pre-deterministic order of \mathcal{I}_k .*

- (1) *If we replace t_{x,y_1y_2} with a graph in the first two terms on the right-hand side of (4.15), then the resulting graph, say $\tilde{\mathcal{G}}$, has no P/Q labels and is globally standard. Moreover, $\tilde{\mathcal{G}}$ either has a strictly higher scaling order than \mathcal{G} , or is obtained by replacing t_{x,y_1y_2} with $m_{\Theta_{xy_1}} \tilde{\mathcal{G}}_{y_1y_2}$.*
- (2) *If we replace t_{x,y_1y_2} with a graph $(\mathcal{G}_R)_{x,y_1y_2}$ in $(\tilde{\mathcal{R}}_T^{(n-1)})_{x,y_1y_2}$, then the resulting graph has no P/Q labels, is globally standard and has a scaling order $\geq \text{ord}(\mathcal{G}) + 1$.*
- (3) *If we replace t_{x,y_1y_2} with a graph $(\mathcal{G}_A)_{x,y_1y_2}$ in $(\mathcal{A}_T^{(>n-1)})_{x,y_1y_2}$, then the resulting graph has no P/Q labels, is SPD and has a scaling order $\geq \text{ord}(\mathcal{G}) + n - 2$.*
- (4) *Suppose we replace t_{x,y_1y_2} with a graph $(\mathcal{G}_Q)_{x,y_1y_2}$ in $(\mathcal{Q}_T^{(n-1)})_{x,y_1y_2}$ and get a graph $\tilde{\mathcal{G}}$. Then applying the Q -expansions, we can expand it into a sum of $O(1)$ many graphs:*

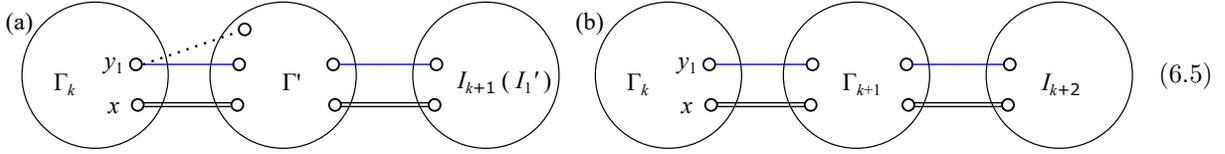
$$\tilde{\mathcal{G}} = \sum_{\omega} \mathcal{G}_{\omega} + \mathcal{Q} + \mathcal{G}_{err}, \quad (6.4)$$

where every \mathcal{G}_{ω} has no P/Q labels, is globally standard and has a scaling order $\geq \text{ord}(\mathcal{G}) + 1$; \mathcal{Q} is a sum of Q -graphs, each of which is SPD and has a MIS containing the atom in the Q -label; \mathcal{G}_{err} is a sum of doubly connected graphs of scaling orders $> D$.

- (5) *If we replace t_{x,y_1y_2} with a graph $(\mathcal{G}_{err})_{x,y_1y_2}$ in $(\mathcal{E}rr_{n-1,D})_{x,y_1y_2}$, then the resulting graph is doubly connected and has a scaling order $\geq \text{ord}(\mathcal{G}) + D - 1$.*

Proof. The proofs of (1), (3) and (5) are simple by using the properties in Definitions 3.2 and 6.3. We focus on the proofs of (2) and (4).

Proof of (2): We denote the new graph by $\tilde{\mathcal{G}}$. Then we have the following graph (a), where we only show a case which has a dotted edge connected with y_1 in $(\mathcal{G}_R)_{x,y_1y_2}$. There are also cases with a dotted edge connected with y_2 . With a slight abuse of notation, we have used x and y_1 to denote the respective molecules that contain atoms x and y_1 .



The graph (a) gives the isolated molecular subgraph \mathcal{I}_k in $\tilde{\mathcal{G}}$ with all red solid edges removed, where we have not merged the molecules connected by the dotted edge. Inside the back circles are some subgraphs, where Γ_k contains the molecules in \mathcal{I}_k of the original graph \mathcal{G} , $\mathcal{I}'_1 = \mathcal{I}_{k+1}$ is the first proper isolated subgraph in $(\mathcal{G}_R)_{x,y_1y_2}$ and also the $(k+1)$ -th proper isolated subgraph in $\tilde{\mathcal{G}}$, and Γ' contains the molecules in $(\mathcal{G}_R)_{x,y_1y_2}$ that are not in \mathcal{I}'_1 . The graph (b) is obtained by removing the dotted edge from graph (a) and renaming the subgraphs.

First, $\text{ord}(\tilde{\mathcal{G}}) \geq \text{ord}(\mathcal{G}) + 1$ follows immediately from the fact that $(\mathcal{G}_R)_{x,y_1y_2}$ has scaling order ≥ 3 . Second, using the fact that both \mathcal{G} and $(\mathcal{G}_R)_{x,y_1y_2}$ have no proper strongly isolated subgraphs, we immediately get that $\tilde{\mathcal{G}}$ also does not contain any proper strongly isolated subgraph. It remains to prove the SPD property of $\tilde{\mathcal{G}}$. With Lemma 5.11, it suffices to show that graph (b) in (6.5), denoted by $\tilde{\mathcal{G}}_b$, is SPD. In this graph, we have renamed \mathcal{I}_{k+1} in (a) as \mathcal{I}_{k+2} and Γ' as Γ_{k+1} . Notice that Γ_{k+1} , \mathcal{I}_{k+2} and the two edges between them form the isolated subgraph \mathcal{I}_{k+1} in $\tilde{\mathcal{G}}_b$.

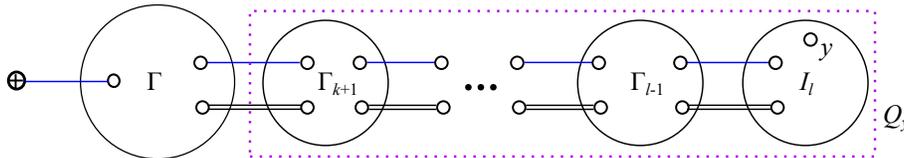
Now we verify the properties (i)–(iii) of Definition 5.9 for $\tilde{\mathcal{G}}_b$. The property (i) follows from Lemma 5.7. Using the SPD property of $(\mathcal{G}_R)_{x,y_1y_2}$ given by Definition 6.3, we get that there is at most one sequence of isolated graphs in \mathcal{I}_k . Together with the SPD property of \mathcal{G} and the fact that \mathcal{I}_k is the MIS of \mathcal{G} , it concludes the property (ii) for $\tilde{\mathcal{G}}_b$. It remains to prove the property (iii). Suppose the sequence of proper isolated subgraphs in $\tilde{\mathcal{G}}_b$ is

$$\mathcal{I}_l \subset \cdots \subset \mathcal{I}_{k+2} \subset \mathcal{I}_{k+1} \subset \mathcal{I}_k \subset \cdots \subset \mathcal{I}_1, \quad \text{for some } l \geq k, \quad (6.6)$$

and for simplicity of notation, we denote the maximal subgraph by \mathcal{I}_0 . For $j \geq k+1$, if we replace \mathcal{I}_{j+1} and its two external edges with a diffusive edge, then \mathcal{I}_j becomes pre-deterministic because $(\mathcal{G}_R)_{x,y_1y_2}$ is SPD. For $j \leq k-1$, if we replace \mathcal{I}_{j+1} and its two external edges with a diffusive edge, then \mathcal{I}_j becomes pre-deterministic because \mathcal{G} is SPD. Finally, if we replace \mathcal{I}_{k+1} and its two external edges with a diffusive edge, then it corresponds to changing the first blue solid edge in a pre-deterministic order of \mathcal{I}_k into a diffusive edge. Hence \mathcal{I}_k becomes pre-deterministic by Definition 5.8. In sum, we get that $\tilde{\mathcal{G}}_b$ is SPD, which concludes statement (2) of Lemma 6.5.

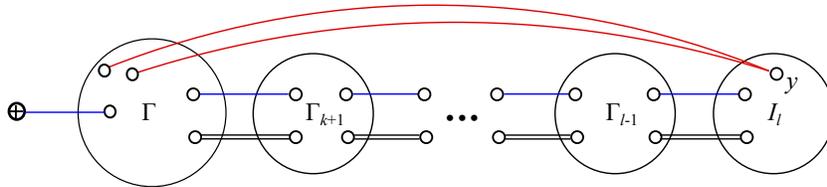
Proof of (4): Using a similar argument as the one for $\tilde{\mathcal{G}}_b$, we get that $\tilde{\mathcal{G}}$ is SPD. Then the SPD property of the graphs on the right-hand side of (6.4) follow from Lemma 5.13. The conditions on scaling orders and the fact that the atom in the Q -label of a Q -graph belongs to the MIS follow from Lemma 4.15. It remains to prove the weakly isolated property of (possible) proper isolated subgraphs in \mathcal{G}_ω .

We assume that $(\mathcal{G}_Q)_{x,y_1y_2}$ indeed contains strongly isolated subgraphs, since otherwise the proof will be trivial. Then we have the following molecular graph without red solid edges:



Here all solid edges and weights inside the purple dashed rectangle have the same Q_y label for an atom y in the MIS, denoted by \mathcal{I}_l for some $l \geq k$. Inside the back circles are some subgraphs, where Γ contains the molecules in the original graph \mathcal{G} , and Γ_i 's are components corresponding to the isolated subgraphs in

$(\mathcal{G}_Q)_{x,y_1y_2}$. Again we denote the isolated subgraphs of $\tilde{\mathcal{G}}$ by (6.6). Then by property (iv) of Lemma 4.15, every \mathcal{G}_ω has atoms in Γ or external atoms so that (a) they connect to y through red solid edges, (b) they connect to y through blue solid edges, or (c) they have been merged with y . In cases (b) and (c), the subgraphs \mathcal{I}_i , $k+1 \leq i \leq l$, are not isolated anymore. In case (a), we have the following graph (or some variants of it, where we are not trying to draw all possible cases):



In this case, any subgraph \mathcal{I}_i , $k+1 \leq i \leq l$, is weakly isolated if it is still an isolated subgraph in \mathcal{G}_ω . In sum, we see that \mathcal{G}_ω does not contain proper strongly isolated subgraphs, and hence is globally standard. \square

6.3 Global expansion strategy

Lemma 6.5 gives a canonical choice of the standard neutral atom in a global expansion of a globally standard graph, that is, we choose an ending atom of the first blue solid edge in a pre-deterministic order of the MIS. With this choice, we define the global expansion strategy for the proof of Theorem 3.7 in this subsection.

Fix any $n \in \mathbb{N}$. As an induction hypothesis, suppose we have obtained the $(n-1)$ -th order T -expansion. Then we define the following stopping rules. We stop the expansion of a graph if it is a normal regular graph and satisfies at least one of the following properties:

- (S1) it is a \oplus/\ominus -recollision graph;
- (S2) its scaling order is at least $n+1$;
- (S3) it is a Q -graph;
- (S4) it is *non-expandable*, that is, it is locally standard and has no redundant blue solid edge.

If a graph has a deterministic maximal subgraph, then it is non-expandable. On the other hand, in a non-expandable graph that is not deterministic, we cannot expand a plus G edge without breaking the doubly connected property. Now we give our global expansion strategy.

Strategy 6.6 (Global expansion strategy). Fix any $n \in \mathbb{N}$ and large $D > n$. Given the above stopping rules (S1)–(S4), we apply the following strategy.

Step 0: We start with the second order T -expansion (3.8), and apply local expansions to obtain a linear combination of new graphs, each of which either satisfies the stopping rules (S1)–(S3) already, or is locally standard. At this step, there is only one internal molecule in every graph, which is trivially globally standard.

Step 1: Given a globally standard input graph, we perform the local expansions in Definitions 4.3, 4.4, 4.5 and 4.6 on atoms in the minimal isolated subgraph (MIS). We send the resulting graphs that already satisfy the stopping rules (S1)–(S4) to the outputs. Every remaining graph is globally standard by Lemma 6.4, and its MIS is locally standard (i.e. the MIS has no weights and every atom in it either has degree 0 or is a standard neutral atom by Definition 4.8).

Step 2: Given a globally standard input graph \mathcal{G} with a locally standard MIS, say \mathcal{I}_k , we find a t_{x,y_1y_2} or $t_{y_1y_2,x}$ variable defined in (4.14), so that α is a standard neutral atom in \mathcal{I}_k and the blue solid edge $G_{\alpha y_1}$ or $G_{y_1 \alpha}$ is the first blue solid edge in a pre-deterministic order of \mathcal{I}_k . If we cannot find such a t -variable, then we stop expanding the input graph.

Step 3: We apply the global expansions defined in Section 4.3 to the t_{x,y_1y_2} or $t_{y_1y_2,x}$ variable chosen in Step 2. More precisely, we first replace t_{x,y_1y_2} (or $t_{y_1y_2,x}$) with (4.15) (or an expression obtained by taking transpositions of all G entries in (4.15)). Then we apply the Q -expansions defined in Section 4.4 to graphs that take the form (4.16), where both Γ_0 and $\tilde{\Gamma}_0$ are non-trivial. We send the resulting graphs that already satisfy the stopping rules (S1)–(S4) to the outputs. The remaining graphs are all globally standard by Lemma 6.5, and we send them back to Step 1.

Using the definition of globally standard graphs, it is easy to show that if an output graph from the above strategy does not satisfy the stopping rules (S1)–(S3), then it must have a deterministic maximal subgraph.

Lemma 6.7. *Let $\mathcal{G}_{\alpha, b_1 b_2}$ be an output graph from the global expansion strategy 6.6. If $\mathcal{G}_{\alpha, b_1 b_2}$ does not satisfy stopping rules (S1)–(S3), then it has a deterministic maximal subgraph with a doubly connected structure.*

Proof. By Lemma 6.4 and Lemma 6.5, we know that $\mathcal{G}_{\alpha, b_1 b_2}$ is globally standard. Under the assumption of this lemma, $\mathcal{G}_{\alpha, b_1 b_2}$ either is non-expandable or does not contain a t -variable required by Step 2 of Strategy 6.6. In either case, $\mathcal{G}_{\alpha, b_1 b_2}$ contains a locally standard MIS, say \mathcal{I}_k , which, by the pre-deterministic property of \mathcal{I}_k , does not contain any internal blue solid edge.

Now we consider two cases. First, suppose \mathcal{I}_k is a proper isolated subgraph. Due to the weakly isolated property, \mathcal{I}_k is connected with at least two external red solid edges and at most one blue solid edge. Hence \mathcal{I}_k contains a non-standard neutral atom, which gives a contradiction. Second, suppose \mathcal{I}_k is indeed the maximal subgraph of $\mathcal{G}_{\alpha, b_1 b_2}$. Then \mathcal{I}_k is locally standard and does not contain any internal blue solid edges, so it is deterministic. \square

With Lemma 6.5, we show that Strategy 6.6 will stop after $O(1)$ many iterations.

Lemma 6.8. *The expansions in Strategy 6.6 will stop after at most C_n many iterations of Steps 1–3, where C_n denotes a large constant depending on n . All graphs from these expansions are doubly connected. If a graph satisfies the stopping rule (S1)/(S2)/(S3) and has scaling order $\leq D$, then it satisfies the property (i)/(ii)/(iii) of Definition 6.3.*

Proof. Let \mathcal{G} be an input graph for Step 3 of Strategy 6.6. Its scaling order must be larger than or equal to the scaling orders of the graphs in (3.9), i.e. $\text{ord}(\mathcal{G}) \geq 3$. Hence the new graphs from case (3) of Lemma 6.5 are SPD and have scaling orders $\geq n + 1$, so it satisfies the property (ii) of Definition 6.3; the new graphs from case (5) of Lemma 6.5 are doubly connected and have scaling orders $\geq D + 2$. Furthermore, the new graphs from cases (1) and (2) of Lemma 6.5 are globally standard, so they satisfy the property (i)/(ii) of Definition 6.3 if they satisfy the stopping rule (S1)/(S2). Finally, in equation (6.4), the graphs in \mathcal{Q} satisfy the stopping rule (S3) and the property (iii) of Definition 6.3; the graphs in \mathcal{G}_{err} are doubly connected and have scaling orders $\geq D + 1$; the graphs \mathcal{G}_ω are globally standard, so they satisfy the property (i)/(ii) of Definition 6.3 if they satisfy the stopping rule (S1)/(S2). Combining the above discussions with Lemma 6.4 for local expansions in Step 1 of Strategy 6.6, we conclude the second and third statements.

Now we prove the first statement. Let \mathcal{G}_0 be a graph from Step 0. We construct inductively a tree diagram \mathcal{T} for the expansions of \mathcal{G}_0 as follows. Let \mathcal{G}_0 be the root. Given a graph \mathcal{G} represented by a vertex of the tree, its children are the graphs obtained from an iteration of Steps 1–3 of Strategy 6.6 acting on \mathcal{G} . Suppose a graph \mathcal{G} satisfies a stopping rule, then we stop the expansion and \mathcal{G} has no children on \mathcal{T} . Let the height of \mathcal{T} be the maximum distance between the root and a leaf of \mathcal{T} . To show that the expansions will stop after C_n many iterations of Steps 1–3, it is equivalent to show that \mathcal{T} is a finite tree with height $\leq C_n$.

Let $\mathcal{G}_0 \rightarrow \mathcal{G}_1 \rightarrow \mathcal{G}_2 \rightarrow \dots \rightarrow \mathcal{G}_h$ be a self-avoiding path from the root to a leaf. Let $k_0 = 0$. After having defined k_i , let $k_{i+1} := h \wedge \min\{j > k_i : \text{ord}(\mathcal{G}_j) > \text{ord}(\mathcal{G}_{k_i})\}$. Then the increasing sequence $\{k_0, k_1, k_2, \dots\}$ has length at most n , because a graph of scaling order $\geq n + 1$ satisfies the stopping rule (S2) and has no children. Moreover, we claim that $|k_{i+1} - k_i| \leq n$. First, by Lemma 6.5, if a new graph after an iteration of Steps 1–3 has the same scaling order as the input graph, then it must have one fewer blue solid edge than the input graph. Second, by the property (ii) of Definition 2.5, the number of internal atoms in \mathcal{G}_{k_i} is less than or equal to the number of waved and diffusive edges, which gives that the number of blue solid edges in \mathcal{G}_{k_i} is at most n . These two facts together conclude the claim. In sum, we have shown that $h \leq n^2$, i.e. the height of \mathcal{T} is at most n^2 . \square

6.4 Proof of Theorem 3.7

In this subsection, we prove Theorem 3.7 using the results in Sections 6.2 and 6.3. To summarize, we have proved the following facts.

- (I) The expansions of $T_{\alpha, b_1 b_2}$ will stop and give $O(1)$ many new graphs (Lemma 6.8).
- (II) If a new graph from the expansions satisfies the stopping rule (S1)/(S2)/(S3), then it satisfies the property (i)/(ii)/(iii) of Definition 6.3 (Lemma 6.8).

(III) If a new graph from the expansions does not satisfy the stopping rules (S1)–(S3), then it has a deterministic doubly connected maximal subgraph (Lemma 6.7).

Now we complete the proof of Theorem 3.7 using induction. We have obtained the second order T -expansion and T -equation in (3.8). Fix any $2 \leq n \leq M$. Suppose for all $2 \leq k \leq n-1$, we have constructed the k -th order T -equation using Strategy 6.6, shown the properties (1.20)–(1.22) of \mathcal{E}_{n-1} by Lemma 3.9, and obtained the k -th order T -equation using Corollary 3.8. Now applying Strategy 6.6, we obtain the following expansion of T_{a,b_1b_2} :

$$T_{a,b_1b_2} = m\Theta_{ab_1}\bar{G}_{b_1b_2} + \sum_x (\Theta\Sigma^{(n)})_{ax} t_{x,b_1b_2} + (\tilde{\mathcal{R}}_{IT}^{(n)})_{a,b_1b_2} + (\mathcal{A}_{IT}^{(>n)})_{a,b_1b_2} + (\mathcal{Q}_{IT}^{(n)})_{a,b_1b_2} + (\mathcal{E}rr'_{n,D})_{a,b_1b_2}.$$

Denoting

$$(\mathcal{R}_{IT}^{(n)})_{a,b_1b_2} = (\tilde{\mathcal{R}}_{IT}^{(n)})_{a,b_1b_2} - \sum_x (\Theta\Sigma^{(n)})_{ax} |m|^2 \sum_\alpha s_{x\alpha} G_{\alpha b_1} \bar{G}_{\alpha b_2} (1 - \mathbf{1}_{\alpha \neq b_1} \mathbf{1}_{\alpha \neq b_2}),$$

the above equation can be rewritten as

$$\begin{aligned} T_{a,b_1b_2} &= m\Theta_{ab_1}\bar{G}_{b_1b_2} + \sum_x (\Theta\Sigma^{(n)})_{ax} T_{x,b_1b_2} + (\mathcal{R}_{IT}^{(n)})_{a,b_1b_2} + (\mathcal{A}_{IT}^{(>n)})_{a,b_1b_2} \\ &\quad + (\mathcal{Q}_{IT}^{(n)})_{a,b_1b_2} + (\mathcal{E}rr'_{n,D})_{a,b_1b_2}. \end{aligned} \quad (6.7)$$

By the above three facts (I)–(III), we have shown that (6.7) satisfies Definitions 3.3 and 6.3, except for the following properties:

- in the decomposition (3.12) of $\mathcal{R}_{IT}^{(n)}$, $\mathcal{R}_{IT,l}$, $4 \leq l \leq n-1$, are the same expressions as those in lower order T -equations;
- in the decomposition (3.13) of $\mathcal{Q}_{IT}^{(n)}$, $\mathcal{Q}_{IT,l}$, $4 \leq l \leq n-1$, are the same expressions as those in lower order T -equations;
- in the decomposition (3.14) of $\Sigma^{(n)}$, \mathcal{E}_l , $4 \leq l \leq n-1$, are the same self-energies as those in lower order T -equations.

We decompose the graphs $\Sigma^{(n)}$, $\mathcal{R}_{IT}^{(n)}$ and $\mathcal{Q}_{IT}^{(n)}$ in (6.7) according to scaling orders as

$$\Sigma^{(n)} = \hat{\Sigma}^{(n-1)} + \mathcal{E}_n, \quad \mathcal{R}_{IT}^{(n)} = \hat{\mathcal{R}}_{IT}^{(n-1)} + \mathcal{R}_{IT,n}, \quad \mathcal{Q}_{IT}^{(n)} = \hat{\mathcal{Q}}_{IT}^{(n-1)} + \mathcal{Q}_{IT,n} + \mathcal{Q}_{IT}^{(>n)}, \quad (6.8)$$

where $\hat{\Sigma}^{(n-1)}$, $\hat{\mathcal{R}}_{IT}^{(n-1)}$ and $\hat{\mathcal{Q}}_{IT}^{(n-1)}$ are sums of graphs of scaling orders $\leq n-1$, \mathcal{E}_n , $\mathcal{R}_{IT,n}$ and $\mathcal{Q}_{IT,n}$ are sums of graphs of scaling order n , and $\mathcal{Q}_{IT}^{(>n)}$ is a sum of Q -graphs of scaling order $> n$. To conclude the proof, it suffices to prove that

$$\hat{\Sigma}^{(n-1)} = \Sigma^{(n-1)}, \quad \hat{\mathcal{R}}_{IT}^{(n-1)} = \mathcal{R}_{IT}^{(n-1)}, \quad \hat{\mathcal{Q}}_{IT}^{(n-1)} = \mathcal{Q}_{IT}^{(n-1)}, \quad (6.9)$$

if we perform the expansions in a *proper way*. In order to have (6.9), we perform almost the same $(n-1)$ -th and n -th order expansions of T_{a,b_1b_2} in parallel, with the only difference being the cutoff order in the stopping rule: the cutoff order is $n-1$ for the $(n-1)$ -th order expansion strategy, and n for the n -th order expansion strategy. We now give a more precise description of the expansion procedure.

After the r -th step expansion (where one step refers to a local expansion in Section 4.2, a Q -expansion in Section 4.4 or a substitution in global expansions), we denote by $\mathfrak{G}_r^{(n-1)}$ and $\mathfrak{G}_r^{(n)}$ the collections of scaling order $\leq n-1$ graphs in the $(n-1)$ -th and n -th order expansion processes, respectively. We trivially have $\mathfrak{G}_0^{(n-1)} = \mathfrak{G}_0^{(n)}$. Suppose $\mathfrak{G}_r^{(n-1)} = \mathfrak{G}_r^{(n)}$ for an $r \in \mathbb{N}$. Then given any graph in $\mathcal{G} \in \mathfrak{G}_r^{(n-1)}$, we perform the $(r+1)$ -th step expansion as follows.

- If we apply a local expansion to \mathcal{G} in the $(n-1)$ -th order expansion process, then we apply the same expansion to the same weight or edge of \mathcal{G} in the n -th order expansion process.
- If \mathcal{G} is of the form (4.16), then we apply exactly the same Q -expansion to it in both the $(n-1)$ -th and n -th order expansion processes.

- Suppose in the $(n-1)$ -th order expansion processes, we replace a t_{x,y_1y_2} variable in \mathcal{G} with an $(n-2)$ -th order T -expansion (i.e. (4.15) with $n-1$ replaced by $n-2$). Then in the n -th order expansion, we replace the same t_{x,y_1y_2} variable with (4.15). By (3.2), (3.5) and (3.6), we have that

$$\begin{aligned}\Sigma_T^{(n-1)} - \Sigma_T^{(n-2)} &= \Sigma_{T,n-1}, & \mathcal{R}_T^{(n-1)} - \mathcal{R}_T^{(n-2)} &= \mathcal{R}_{T,n-1}, \\ \mathcal{Q}_T^{(k-1)} - \mathcal{Q}_T^{(k-2)} &= \mathcal{Q}_{T,k-1} + \mathcal{Q}_T^{(>k-1)} - \mathcal{Q}_T^{(>k-2)}.\end{aligned}$$

Hence the $(n-2)$ -th order version of (4.15) is different from (4.15) only in the following terms:

$$\begin{aligned}m(\Theta\Sigma_{T,n-1}\Theta)_{xy_1}\overline{G}_{y_1y_2}, & \quad (\mathcal{R}_{T,n-1})_{x,y_1y_2}, & \quad (\mathcal{Q}_{T,n-1} + \mathcal{Q}_T^{(>n-1)} - \mathcal{Q}_T^{(>n-2)})_{x,y_1y_2}, \\ (\mathcal{A}_T^{(>n-2)})_{x,y_1y_2}, & \quad (\mathcal{A}_T^{(>n-1)})_{x,y_1y_2}, & \quad (\mathcal{E}rr_{n-1,D})_{x,y_1y_2}, & \quad (\mathcal{E}rr_{n,D})_{x,y_1y_2}.\end{aligned}$$

However, if we have replaced t_{x,y_1y_2} with a graph in one of these terms, then the resulting graph must be of scaling order at least n . Such graphs will not be included into $\mathfrak{G}_{r+1}^{(n-1)}$ or $\mathfrak{G}_{r+1}^{(n)}$.

In sum, we see that $\mathfrak{G}_{r+1}^{(n-1)} = \mathfrak{G}_{r+1}^{(n)}$ as long as we perform the n -th order expansions in the above way. By induction in r , we get that (6.9) holds, which concludes the proof.

7 PROOF OF THEOREM 3.6

Recall the following standard large deviation estimates in Lemma 7.1, which show that the resolvent entries are controlled T -variables. The bound (7.2) was proved in equation (3.20) of [33], and (7.3) was proved in Lemma 5.3 of [12]. Given a matrix M , we will use $\|M\|_{\max} = \max_{i,j} |M_{ij}|$ to denote its maximum norm.

Lemma 7.1. *Suppose for a constant $\delta_0 > 0$ and deterministic parameter $W^{-d/2} \leq \Phi \leq W^{-\delta_0}$ we have that*

$$\|G(z) - m(z)\|_{\max} \prec W^{-\delta_0}, \quad \|T\|_{\max} \prec \Phi^2, \quad (7.1)$$

uniformly in $z \in \mathbf{D}$ for a subset $\mathbf{D} \subset \mathbb{C}_+$. Then

$$\mathbf{1}_{x \neq y} |G_{xy}(z)|^2 \prec T_{xy}(z) \quad (7.2)$$

uniformly in $x, y \in \mathbb{Z}_L^d$ and $z \in \mathbf{D}$, and

$$|G_{xx}(z) - m(z)| \prec \Phi \quad (7.3)$$

uniformly in $x \in \mathbb{Z}_L^d$ and $z \in \mathbf{D}$.

Now we state the three main ingredients, Lemmas 7.2, 7.3 and 7.4, for the proof of Theorem 3.6. First, we have an initial estimate when $\eta = 1$, whose proof will be given in Section 8.

Lemma 7.2 (Initial estimate). *Under the assumptions of Theorem 3.6, for any $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $\eta = 1$, we have that*

$$|G_{xy}(z) - m(z)\delta_{xy}|^2 \prec B_{xy}, \quad \forall x, y \in \mathbb{Z}_L^d. \quad (7.4)$$

Second, we have a continuity estimate in Lemma 7.3, whose proof will be given in Section 9. It allows us to get some a priori estimates on $G(z)$ from the local law (3.16) on $G(\tilde{z})$ for \tilde{z} with a larger imaginary part $\text{Im } \tilde{z} = W^{\varepsilon_0} \text{Im } z$, where $\varepsilon_0 > 0$ is a small constant.

Lemma 7.3 (Continuity estimates). *Under the assumptions of Theorem 3.6, suppose that*

$$|G_{xy}(\tilde{z}) - m(\tilde{z})\delta_{xy}|^2 \prec B_{xy}(\tilde{z}), \quad \forall x, y \in \mathbb{Z}_L^d, \quad (7.5)$$

with $\tilde{z} = E + i\tilde{\eta}$ for some $E \in (-2 + \kappa, 2 - \kappa)$ and $\tilde{\eta} \in [W^{2+\varepsilon}/L^2, 1]$. Then we have that

$$\max_{x,x_0} \frac{1}{K^d} \sum_{y:|y-x_0| \leq K} (|G_{xy}(z)|^2 + |G_{yx}(z)|^2) \prec \left(\frac{\tilde{\eta}}{\eta}\right)^2 \frac{1}{W^4 K^{d-4}}, \quad (7.6)$$

uniformly in $K \in [W, L/2]$ and $z = E + i\eta$ with $W^{2+\varepsilon}/L^2 \leq \eta \leq \tilde{\eta}$. Moreover, for any constant $\varepsilon_0 \in (0, d/20)$, we have that

$$\|G(z) - m(z)\|_{\max} \prec W^{-d/2+\varepsilon_0}, \quad (7.7)$$

uniformly in $z = E + i\eta$ with $\max\{W^{-\varepsilon_0}\tilde{\eta}, W^{2+\varepsilon}/L^2\} \leq \eta \leq \tilde{\eta}$.

Compared with (3.16), the ℓ^∞ bound (7.7) is sharp up to a factor W^{ε_0} . The estimate (7.6) is an averaged bound instead of an entrywise bound and the right-hand side of (7.6) loses an W^2/K^2 factor when compared with the sharp averaged bound $W^{-2}K^{-(d-2)}$. We need to use the following lemma to improve the weaker estimates (7.6) and (7.7) to the stronger local law (3.16). Its proof will be given in Section 8. Note that (7.6) verifies the assumption (7.8) as long as we have $W^{-\varepsilon_0}\tilde{\eta} \leq \eta \leq \tilde{\eta}$.

Lemma 7.4 (Entrywise bounds on T -variables). *Suppose the assumptions of Theorem 3.6 hold. Fix any $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $\eta \in [W^{2+\varepsilon}/L^2, 1]$. Suppose for some constant $\varepsilon_0 > 0$, (7.7) and the following estimate hold:*

$$\max_{x, x_0} \frac{1}{K^d} \sum_{y: |y-x_0| \leq K} (|G_{xy}(z)|^2 + |G_{yx}(z)|^2) \prec \frac{W^{2\varepsilon_0}}{W^4 K^{d-4}}, \quad (7.8)$$

for all $K \in [W, L/2]$. As long as ε_0 is sufficiently small (depending on n and c_0 in (3.15)), we have that

$$T_{xy}(z) \prec B_{xy}, \quad \forall x, y \in \mathbb{Z}_L^d. \quad (7.9)$$

Combining the above three lemmas, we can complete the proof of Theorem 3.6 using a bootstrapping argument on a sequence of multiplicatively decreasing η given in (7.10). The details have been given in Section 5.2 of [32]. For the reader's convenience, we repeat the main argument here.

Proof of Theorem 3.6. Fix any $E \in (-2 + \kappa, 2 - \kappa)$. We define the following sequence of decreasing η for a small constant $\varepsilon_0 > 0$:

$$\eta_k := \max(W^{-k\varepsilon_0}, W^{2+\varepsilon}/L^2), \quad 0 \leq k \leq \ell_0, \quad (7.10)$$

where ℓ_0 is the smallest integer such that $W^{-\ell_0\varepsilon_0} \leq W^{2+\varepsilon}/L^2$. By definition, $\eta_{k+1} = W^{-\varepsilon_0}\eta_k$ for $k \leq \ell_0 - 1$ and we always have $\eta_{\ell_0} = W^{2+\varepsilon}/L^2$. Now we prove Theorem 3.6 through an induction on k . First, by Lemma 7.2, (3.16) holds with $z = z_0 = E + i\eta_0$. Then suppose (3.16) holds with $z = z_k := E + i\eta_k$ for some $0 \leq k \leq \ell_0 - 1$. By Lemma 7.3, (7.7) and (7.8) hold for all $z = E + i\eta$ with $\eta_{k+1} \leq \eta \leq \eta_k$. Then applying Lemma 7.4, we obtain that (7.9) holds with $z = z_{k+1}$. Now using Lemma 7.1, we can conclude (3.16) with $z = z_{k+1}$. Repeating the induction for ℓ_0 steps, we obtain that

- (i) (3.16) holds for all z_k with $0 \leq k \leq \ell_0$;
- (ii) (7.7) and (7.8) hold for all $z = E + i\eta$ with $\eta_{\ell_0} \leq \eta \leq 1$.

To conclude Theorem 3.6, we need to extend (3.16) uniformly to all $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $\eta \in [\eta_{\ell_0}, 1]$. This is a standard perturbation and union bound argument, so we omit the details. \square

8 HIGH MOMENT ESTIMATE

In this section, we prove Lemma 7.2 and Lemma 7.4. Their proofs use the same idea, that is, we bound the high moment $\mathbb{E}T_{xy}(z)^p$ for any fixed $p \in \mathbb{N}$ using the n -th order T -expansion. First, Lemma 7.4 follows immediately from the high moment estimate in Lemma 8.1, which will be proved in Section 8.2.

Lemma 8.1. *Suppose the assumptions of Lemma 7.4 hold. Assume that*

$$T_{xy} \prec B_{xy} + \tilde{\Phi}^2, \quad \forall x, y \in \mathbb{Z}_L^d, \quad (8.1)$$

for a deterministic parameter $\tilde{\Phi}$ satisfying $0 \leq \tilde{\Phi} \leq W^{-\delta}$ for a constant $\delta > 0$. Then for any fixed $p \in \mathbb{N}$, we have that

$$\mathbb{E}T_{xy}(z)^p \prec (B_{xy} + W^{-c}\tilde{\Phi}^2)^p \quad (8.2)$$

for a constant $c > 0$ depending only on d and c_0 in (3.15).

Proof of Lemma 7.4. By (7.7), we have that (8.1) holds with $\tilde{\Phi} = \tilde{\Phi}_0 := W^{-d/2+\varepsilon_0}$. Then combining (8.2) with Markov's inequality, we obtain that

$$T_{xy}(z) \prec B_{xy} + W^{-c}\tilde{\Phi}_0^2.$$

Hence (8.1) holds with a smaller parameter $\tilde{\Phi} = \tilde{\Phi}_1 := W^{-c/2}\tilde{\Phi}_0$. Applying Lemma 8.1 and Markov's inequality again, we obtain that

$$T_{xy}(z) \prec B_{xy} + W^{-c}\tilde{\Phi}_1^2 = B_{xy} + W^{-2c}\tilde{\Phi}_0^2.$$

Now for any fixed $D > 0$, iterating the above argument for $\lceil D/c \rceil$ many times, we obtain that

$$T_{xy}(z) \prec B_{xy} + W^{-D}.$$

This concludes (7.9) as long as D is large enough. \square

8.1 Estimates of doubly connected graphs

The proof of Lemma 8.1 will use some important estimates on doubly connected graphs stated in this subsection. First, inspired by the maximum bound (7.7), the weak averaged bound (7.8) and the local law (3.16), the following weak and strong norms were introduced in [32].

Definition 8.2. Given a $\mathbb{Z}_L^d \times \mathbb{Z}_L^d$ matrix \mathcal{A} and some fixed $a, b > 0$, we define its weak- (a, b) norm as

$$\|\mathcal{A}\|_{w;(a,b)} := W^{ad/2} \max_{x,y \in \mathbb{Z}_L^d} |\mathcal{A}_{xy}| + \sup_{K \in [W, L/2]} \left(\frac{W}{K}\right)^b K^{ad/2} \max_{x, x_0 \in \mathbb{Z}_L^d} \frac{1}{K^d} \sum_{y: |y-x_0| \leq K} (|\mathcal{A}_{xy}| + |\mathcal{A}_{yx}|),$$

and its strong- (a, b) norm as

$$\|\mathcal{A}\|_{s;(a,b)} := \max_{x,y \in \mathbb{Z}_L^d} \left(\frac{W}{\langle x-y \rangle}\right)^b \langle x-y \rangle^{ad/2} |\mathcal{A}_{xy}|.$$

It is easy to check that $\|B\|_{s;(2,2)} \prec 1$, $\|G(z) - m(z)I_N\|_{s;(1,1)} \prec 1$ if (3.16) holds, and $\|G(z) - m(z)I_N\|_{w;(1,2)} \prec W^{\varepsilon_0}$ if (7.7) and (7.8) hold. We now introduce a positive random variable $\Psi_{xy}(\tau, D)$ for a small constant $\tau > 0$ and a large constant $D > 0$, which was defined in [33, Definition 3.4]:

$$\Psi_{xy}^2 \equiv \Psi_{xy}^2(\tau, D) := W^{-D} + \max_{\substack{|x_1-x| \leq W^{1+\tau} \\ |y_1-y| \leq W^{1+\tau}}} s_{x_1 y_1} + W^{-(2+2\tau)d} \sum_{|x_1-x| \leq W^{1+\tau}} \sum_{|y_1-y| \leq W^{1+\tau}} |G_{x_1 y_1}|^2. \quad (8.3)$$

It is easy to check that $\|\Psi(z)\|_{w;(1,2)} \prec \|G(z) - m(z)I_N\|_{w;(1,2)} + 1$ and $\|\Psi(z)\|_{s;(1,1)} \prec \|G(z) - m(z)I_N\|_{s;(1,1)} + 1$ as long as D is large enough. The motivation for introducing the Ψ variable is as follows: given two atoms $x_1, x_2 \in \mathbb{Z}_L^d$, suppose $y_1 \neq y_2$ satisfy that

$$|y_1 - x_1| \leq W^{1+\tau/2}, \quad |y_2 - x_2| \leq W^{1+\tau/2}. \quad (8.4)$$

Then under the setting of Lemma 7.1, by applying (7.2) twice we obtain that

$$\begin{aligned} |G_{y_1 y_2}(z)|^2 &\prec T_{y_1 y_2}(z) = |m|^2 s_{y_1 y_2} |G_{y_2 y_2}(z)|^2 + |m|^2 \sum_{\alpha \neq y_2} s_{y_1 \alpha} |G_{y_2 \alpha}(\bar{z})|^2 \\ &\prec s_{y_1 y_2} + \sum_{\alpha \neq y_2} s_{y_1 \alpha} T_{y_2 \alpha}(\bar{z}) \leq s_{y_1 y_2} + \sum_{\alpha, \beta} s_{y_1 \alpha} s_{y_2 \beta} |G_{\alpha \beta}(z)|^2 \\ &\leq W^{-D} + s_{y_1 y_2} + W^{-2d} \sum_{|\alpha - y_1| \leq W^{1+\tau/2}} \sum_{|\beta - y_2| \leq W^{1+\tau/2}} |G_{\alpha \beta}(z)|^2 \leq W^{2d\tau} \Psi_{x_1 x_2}^2(\tau, D), \end{aligned} \quad (8.5)$$

where we also used (1.9) and the identity $G_{xy}(z) = \overline{G_{yx}(\bar{z})}$ in the derivation. In particular, if y_1 and y_2 are in the same molecules as x_1 and x_2 , respectively, then (8.4) holds, since otherwise the graph will be smaller than W^{-D} for any fixed $D > 0$ by (1.9) and (2.3). Hence (8.5) shows that all the G edges between

two molecules containing atoms x_1 and x_2 can be bounded by the same variable $\Psi_{x_1x_2}$. This fact will be convenient for our proof.

In this paper, we only use weak or strong- (a, b) norms with $a \leq 2$. In this case, it is not hard to check that the strong- (a, b) norm is strictly stronger than the weak- (a, b) norm. By Definition 8.2, we immediately get the bounds

$$\max_{x, y \in \mathbb{Z}_L^d} |\mathcal{A}_{xy}| \leq W^{-ad/2} \|\mathcal{A}\|_{w;(a,b)}, \quad (8.6)$$

$$\max_{x, x_0 \in \mathbb{Z}_L^d} \frac{1}{K^d} \sum_{y: |y-x_0| \leq K} (|\mathcal{A}_{xy}| + |\mathcal{A}_{yx}|) \leq \frac{1}{W^b K^{ad/2-b}} \|\mathcal{A}\|_{w;(a,b)}, \quad \text{for all } K \in [W, L/2], \quad (8.7)$$

$$|\mathcal{A}_{xy}| \leq \frac{1}{W^b \langle x-y \rangle^{ad/2-b}} \|\mathcal{A}\|_{s;(a,b)}. \quad (8.8)$$

Using these estimates, we can easily prove the following bounds.

Claim 8.3. *Let a and b be two positive constants satisfying that*

$$ad/2 - b - 2 \geq 0. \quad (8.9)$$

Given any two matrices $\mathcal{A}^{(1)}$ and $\mathcal{A}^{(2)}$, we have that

$$\sum_x \mathcal{A}_{x\beta}^{(1)} \cdot \prod_{i=1}^k B_{xy_i} \prec W^{-ad/2} \Gamma(y_1, \dots, y_k) \cdot \|\mathcal{A}^{(1)}\|_{w;(a,b)}, \quad (8.10)$$

$$\sum_x \mathcal{A}_{x\alpha}^{(1)} \mathcal{A}_{x\beta}^{(2)} \cdot \prod_{i=1}^k B_{xy_i} \prec W^{-ad/2} \Gamma(y_1, \dots, y_k) \cdot \frac{1}{W^b \langle x-y \rangle^{ad/2-b}} \cdot \|\mathcal{A}^{(1)}\|_{s;(a,b)} \|\mathcal{A}^{(2)}\|_{s;(a,b)}, \quad (8.11)$$

$$\sum_x \mathcal{A}_{x\alpha}^{(1)} \mathcal{A}_{x\beta}^{(2)} \cdot \prod_{i=1}^k B_{xy_i} \prec W^{-ad/2} \Gamma(y_1, \dots, y_k) \mathcal{A}_{\alpha\beta} \cdot \|\mathcal{A}^{(1)}\|_{w;(a,b)} \|\mathcal{A}^{(2)}\|_{w;(a,b)}, \quad (8.12)$$

where $\mathcal{A}_{\alpha\beta}$ is a positive variable satisfying $\|\mathcal{A}\|_{w;(a,b)} \leq 1$ and $\Gamma(y_1, \dots, y_k)$ is defined by

$$\Gamma(y_1, \dots, y_k) := \sum_{i=1}^k \prod_{j \neq i} B_{y_i y_j}. \quad (8.13)$$

Proof. The proof of this claim is basic by using (8.6)–(8.8), so we omit the details. The reader can also refer to the proof of Claim 6.11 in [32] for a formal proof. \square

The following lemma gives useful estimates on doubly connected graphs.

Lemma 8.4 (Lemma 6.10 of [32]). *Suppose $d \geq 8$ and \mathcal{G} is a doubly connected normal regular graph without external atoms. Pick any two atoms of \mathcal{G} and fix their values $x, y \in \mathbb{Z}_L^d$. Then the resulting graph \mathcal{G}_{xy} satisfies that*

$$|\mathcal{G}_{xy}| \prec W^{-(n_{xy}-3)d/2} B_{xy} \mathcal{A}_{xy} \cdot \|G(z) - m(z)I_N\|_{w;(1,2)}^{n_{xy}-2}, \quad (8.14)$$

and

$$|\mathcal{G}_{xy}| \prec W^{-(n_{xy}-3)d/2} B_{xy}^{3/2} \cdot \|G(z) - m(z)I_N\|_{s;(1,1)}^{n_{xy}-2}, \quad (8.15)$$

where $n_{xy} := \text{ord}(\mathcal{G}_{xy})$ is the scaling order of \mathcal{G}_{xy} and \mathcal{A}_{xy} is some positive variable satisfying $\|\mathcal{A}\|_{w;(1,2)} \prec 1$. If we fix an atom $x \in \mathcal{G}$, then the resulting graph \mathcal{G}_x satisfies that

$$|\mathcal{G}_x| \prec W^{-\text{ord}(\mathcal{G}_x) \cdot d/2} \cdot \|G(z) - m(z)I_N\|_{w;(1,2)}^{n_{xy}-2}. \quad (8.16)$$

The above bounds hold also for the graph \mathcal{G}^{abs} , which is obtained by replacing every component (including edges, weights and coefficients) in \mathcal{G} with its absolute value and ignoring all P or Q labels (if any).

Deterministic doubly connected graphs satisfy better bounds than Lemma 8.4, because all edges in their blue nets are now (labelled) diffusive edges, whose strong- $(2, 2)$ norms are bounded by $O_{\prec}(1)$.

Lemma 8.5 (Corollary 6.12 of [32]). *Suppose $d \geq 6$ and \mathcal{G} is a deterministic doubly connected normal regular graph without external atoms. Pick any two atoms of \mathcal{G} and fix their values $x, y \in \mathbb{Z}_L^d$. Then the resulting graph \mathcal{G}_{xy} satisfies that*

$$|\mathcal{G}_{xy}| \prec W^{-(n_{xy}-4)d/2} B_{xy}^2, \quad (8.17)$$

where $n_{xy} := \text{ord}(\mathcal{G}_{xy})$ is the scaling order of \mathcal{G}_{xy} . This bound holds also for the graph \mathcal{G}^{abs} , which is obtained by replacing every component (including edges and coefficients) in \mathcal{G} with its absolute value.

8.2 Proof of Lemma 8.1

In this subsection, we prove Lemma 8.1 using the n -th order T -expansion.

Proof of Lemma 8.1. We rename the indices x and y as \mathbf{a} and \mathbf{b} , respectively. Moreover, following the notation in (2.4), we represent \mathbf{a} and \mathbf{b} by \otimes and \oplus in graphs. Applying (3.1) to a $T_{\mathbf{ab}}$ in $\mathbb{E}T_{\mathbf{ab}}^p$, we obtain that

$$\begin{aligned} \mathbb{E}T_{\mathbf{ab}}^p &= \mathbb{E}T_{\mathbf{ab}}^{p-1} \left[m\Theta_{\mathbf{ab}} + m(\Theta\Sigma_T^{(n)}\Theta)_{\mathbf{ab}} \right] \bar{G}_{\mathbf{bb}} + \mathbb{E}T_{\mathbf{ab}}^{p-1} (\mathcal{R}_T^{(n)})_{\mathbf{a},\mathbf{bb}} \\ &\quad + \mathbb{E}T_{\mathbf{ab}}^{p-1} (\mathcal{A}_T^{(>n)})_{\mathbf{a},\mathbf{bb}} + \mathbb{E}T_{\mathbf{ab}}^{p-1} (\mathcal{Q}_T^{(n)})_{\mathbf{a},\mathbf{bb}} + \mathbb{E}T_{\mathbf{ab}}^{p-1} (\mathcal{E}rr_{n,D})_{\mathbf{a},\mathbf{bb}}. \end{aligned} \quad (8.18)$$

Using (1.14) and (3.7), we can bound the first term on the right-hand side as

$$\mathbb{E}T_{\mathbf{ab}}^{p-1} \left[m\Theta_{\mathbf{ab}} + m(\Theta\Sigma_T^{(n)}\Theta)_{\mathbf{ab}} \right] \bar{G}_{\mathbf{bb}} \prec B_{\mathbf{ab}} \mathbb{E}T_{\mathbf{ab}}^{p-1}. \quad (8.19)$$

Next we claim that

$$(\mathcal{R}_T^{(n)})_{\mathbf{a},\mathbf{bb}} \prec W^{-d/2+\varepsilon_0} B_{\mathbf{ab}}. \quad (8.20)$$

Let $\mathcal{G}_{\mathbf{ab}}$ be a graph in $(\mathcal{R}_T^{(n-1)})_{\mathbf{ab}}$. By Definition 3.2, it has dotted edges connected with \oplus , has a (labelled) diffusive edge connected with \otimes , is of scaling order ≥ 3 , and is doubly connected. Now merging \oplus with the internal atoms that are connected to it through dotted edges, we can write $\mathcal{G}_{\mathbf{ab}}$ as

$$\mathcal{G}_{\mathbf{ab}} = \sum_x \Theta_{\mathbf{ax}} (\mathcal{G}_0)_{x\mathbf{b}},$$

where the Θ edge can also be replaced by a labelled diffusive edge and $(\mathcal{G}_0)_{x\mathbf{b}}$ is a graph satisfying the assumptions of Lemma 8.4. Then using (1.14) (or (2.8) if $\Theta_{\mathbf{ax}}$ is replaced by a labelled diffusive edge), (8.14) and $\|G(z) - m(z)I_N\|_{w;(1,2)} \prec W^{\varepsilon_0}$ by the assumptions of Lemma 7.4, we can bound that

$$|\mathcal{G}_{\mathbf{ab}}| \prec W^{(n_{x\mathbf{b}}-3)(-d/2+\varepsilon_0)+\varepsilon_0} \sum_x B_{\mathbf{ax}} B_{x\mathbf{b}} \mathcal{A}_{x\mathbf{b}} \prec W^{(n_{x\mathbf{b}}-2)(-d/2+\varepsilon_0)} B_{\mathbf{ab}}, \quad (8.21)$$

where $n_{x\mathbf{b}} := \text{ord}((\mathcal{G}_0)_{x\mathbf{b}})$, $\mathcal{A}_{x\mathbf{b}}$ is a positive variable satisfying $\|\mathcal{A}\|_{w;(1,2)} \prec 1$, and in the last step we used (8.10) with $(a, b) = (1, 2)$. Using (8.21) and the fact that $n_{x\mathbf{b}} \geq 3$, we conclude (8.20). Now with (8.20), we can bound the second term on the right-hand side of (8.18) as

$$\mathbb{E}T_{\mathbf{ab}}^{p-1} (\mathcal{R}_T^{(n)})_{\mathbf{a},\mathbf{bb}} \prec W^{-d/2+\varepsilon_0} B_{\mathbf{ab}} \mathbb{E}T_{\mathbf{ab}}^{p-1}. \quad (8.22)$$

It remains to bound the last three terms on the right-hand side of (8.18). This can be done with the following two claims.

Claim 8.6. *Under the setting of Lemma 8.1, we have that*

$$(\mathcal{A}_T^{(>n)})_{\mathbf{a},\mathbf{bb}} \prec W^{(n-1)(-d/2+\varepsilon_0)} \frac{L^2}{W^2} (B_{\mathbf{ab}} + \tilde{\Phi}^2), \quad (8.23)$$

and

$$(\mathcal{E}rr_{n,D})_{\mathbf{a},\mathbf{bb}} \prec W^{D(-d/2+\varepsilon_0)} \frac{L^2}{W^2} (B_{\mathbf{ab}} + \tilde{\Phi}^2). \quad (8.24)$$

Claim 8.7. *Under the setting of Lemma 8.1, we have that*

$$\mathbb{E}T_{\mathbf{ab}}^{p-1} (\mathcal{Q}_T^{(n)})_{\mathbf{a},\mathbf{bb}} \prec \sum_{k=2}^p \left[W^{-d/4+\varepsilon_0/2} (B_{\mathbf{ab}} + \tilde{\Phi}^2) \right]^k \mathbb{E}T_{\mathbf{ab}}^{p-k}. \quad (8.25)$$

We postpone the proofs of these two claims until we complete the proof of Lemma 8.1. Using Claim 8.6 and the condition (3.15), we get that

$$\begin{aligned} \mathbb{E}T_{\text{ab}}^{p-1} \left[(\mathcal{A}_T^{(>n)})_{\text{a,bb}} + (\mathcal{E}rr_{n,D})_{\text{a,bb}} \right] &\prec W^{(n-1)(-d/2+\varepsilon_0)} \frac{L^2}{W^2} (B_{\text{ab}} + \tilde{\Phi}^2) \mathbb{E}T_{\text{ab}}^{p-1} \\ &\leq W^{-c_0+(n-1)\varepsilon_0} (B_{\text{ab}} + \tilde{\Phi}^2) \mathbb{E}T_{\text{ab}}^{p-1}. \end{aligned} \quad (8.26)$$

Combining (8.19), (8.22), (8.25) and (8.26), and using Hölder's inequality $\mathbb{E}T_{\text{ab}}^{p-k} \leq (\mathbb{E}T_{\text{ab}}^p)^{\frac{p-k}{p}}$, we can bound (8.18) as

$$\mathbb{E}T_{\text{ab}}^p \prec (B_{\text{ab}} + W^{-c}\tilde{\Phi}^2) (\mathbb{E}T_{\text{ab}}^p)^{\frac{p-1}{p}} + \sum_{k=2}^p \left[W^{-c}(B_{\text{ab}} + \tilde{\Phi}^2) \right]^k (\mathbb{E}T_{\text{ab}}^p)^{\frac{p-k}{p}}, \quad (8.27)$$

where $c := \min(c_0 - (n-1)\varepsilon_0, d/4 - \varepsilon_0/2)$ is a positive constant as long as ε_0 is sufficiently small. Applying Young's inequality to every term on the right-hand side, we get that

$$\mathbb{E}T_{\text{ab}}^p \prec W^\varepsilon (B_{\text{ab}} + W^{-c}\tilde{\Phi}^2)^p + W^{-\varepsilon} \mathbb{E}T_{\text{ab}}^p \quad \Rightarrow \quad \mathbb{E}T_{\text{ab}}^p \prec W^\varepsilon (B_{\text{ab}} + W^{-c}\tilde{\Phi}^2)^p, \quad (8.28)$$

for any constant $\varepsilon > 0$. Since ε is arbitrary, we conclude (8.2). \square

For convenience of our proof, we introduce the following notation of Ω variables, which satisfy the same properties needed for the proof as off-diagonal G edges.

Notation 8.8. *We will use Ω to denote matrices of non-negative random variables satisfying $\|\Omega\|_{w;(1,2)} \prec W^{\varepsilon_0}$ and*

$$\Omega_{xy} \prec B_{xy}^{1/2} + \tilde{\Phi}. \quad (8.29)$$

In the setting of Lemma 8.1, $|G_{xy} - m\delta_{xy}|$ and Ψ_{xy} in (8.3) are both Ω variables.

Now we claim the following useful fact: if $\Omega^{(1)}$ and $\Omega^{(2)}$ satisfy Notation 8.8, then

$$\Omega_{\alpha\beta} := \frac{W^{d/2-\varepsilon_0}}{\Gamma(y_1, \dots, y_k)} \sum_x \Omega_{x\alpha}^{(1)} \Omega_{x\beta}^{(2)} \cdot \prod_{i=1}^k B_{xy_i} \quad \text{also satisfies Notation 8.8.} \quad (8.30)$$

First, notice that by (8.12), we have $\|\Omega\|_{w;(1,2)} \prec W^{\varepsilon_0}$. It remains to prove that Ω satisfies (8.29). Consider two regions $\mathcal{I}_1 := \{x : \langle x-\alpha \rangle \geq \langle x-\beta \rangle\}$ and $\mathcal{I}_2 := \{x : \langle x-\alpha \rangle < \langle x-\beta \rangle\}$. On \mathcal{I}_1 , we have $\langle x-\alpha \rangle \geq \langle \alpha-\beta \rangle/2$, which gives that

$$\Omega_{x\alpha}^{(1)} \prec B_{x\alpha}^{1/2} + \tilde{\Phi} \lesssim B_{\alpha\beta}^{1/2} + \tilde{\Phi}.$$

Together with (8.10), it gives that

$$\sum_{x \in \mathcal{I}_1} \Omega_{x\alpha}^{(1)} \Omega_{x\beta}^{(2)} \cdot \prod_{i=1}^k B_{xy_i} \prec (B_{\alpha\beta}^{1/2} + \tilde{\Phi}) \sum_{x \in \mathcal{I}_1} \Omega_{x\beta}^{(2)} \cdot \prod_{i=1}^k B_{xy_i} \prec (B_{\alpha\beta}^{1/2} + \tilde{\Phi}) \cdot W^{-d/2+\varepsilon_0} \Gamma(y_1, \dots, y_k).$$

We have a similar bound for the sum over \mathcal{I}_2 . This concludes (8.30). In the proof, it is more convenient to use the following form of (8.30):

$$\sum_x \Omega_{x\alpha}^{(1)} \Omega_{x\beta}^{(2)} \cdot \prod_{i=1}^k B_{xy_i} = W^{-d/2+\varepsilon_0} \Gamma(y_1, \dots, y_k) \Omega_{\alpha\beta}, \quad (8.31)$$

for some Ω satisfying Notation 8.8.

Proof of Claim 8.6. We only need to consider the graphs in $(\mathcal{A}_T^{(>n)})_{\text{ab}}$ that are not \oplus -recollision graphs, because \oplus -recollision graphs have been shown to satisfy (8.21). Any such graph \mathcal{G}_{ab} can be written into

$$\mathcal{G}_{\text{ab}} = \sum_{x, y_1, y_2} \Theta_{\text{ax}}(\mathcal{G}_0)_{x, y_1 y_2} G_{y_1 \text{b}} \bar{G}_{y_2 \text{b}}, \quad \mathcal{G}_{\text{ab}} = \sum_{x, y_1} \Theta_{\text{ax}}(\mathcal{G}_0)_{xy} |G_{y \text{b}}|^2, \quad \mathcal{G}_{\text{ab}} = \sum_{x, y} \Theta_{\text{ax}}(\mathcal{G}_0)_{xy} \Theta_{y \text{b}}, \quad (8.32)$$

or some forms obtained by setting x to be equal to y , y_1 or y_2 and by replacing the Θ edges with labelled diffusive edges. Here the graphs \mathcal{G}_0 are doubly connected graphs without external atoms. Using (8.14), we can bound the second and third terms of (8.32) as

$$\begin{aligned} |\mathcal{G}_{\mathbf{ab}}| &\prec W^{(n_{xy}-3)(-d/2+\varepsilon_0)+\varepsilon_0} \sum_{x,y} B_{\mathbf{ax}} B_{xy} \mathcal{A}_{xy} (B_{y\mathbf{b}} + \tilde{\Phi}^2) \lesssim W^{(n_{xy}-2)(-d/2+\varepsilon_0)} \sum_y B_{\mathbf{ay}} (B_{y\mathbf{b}} + \tilde{\Phi}^2) \\ &\lesssim W^{(n_{xy}-2)(-d/2+\varepsilon_0)} \left(\frac{1}{W^4 \langle \mathbf{a} - \mathbf{b} \rangle^{d-4}} + \frac{L^2}{W^2} \tilde{\Phi}^2 \right) \lesssim W^{(n-1)(-d/2+\varepsilon_0)} \frac{L^2}{W^2} (B_{\mathbf{ab}} + \tilde{\Phi}^2), \end{aligned} \quad (8.33)$$

where $n_{xy} := \text{ord}((\mathcal{G}_0)_{xy})$. Here in the second and third steps we used (8.10) and the simple bounds

$$\sum_y B_{\mathbf{ay}} B_{y\mathbf{b}} \lesssim \frac{1}{W^4 \langle \mathbf{a} - \mathbf{b} \rangle^{d-4}}, \quad \sum_y B_{\mathbf{ay}} \lesssim \frac{L^2}{W^2},$$

and in the fourth step we used $\text{ord}((\mathcal{G}_0)_{xy}) = \text{ord}(\mathcal{G}_{\mathbf{ab}}) \geq n+1$ and $\langle \mathbf{a} - \mathbf{b} \rangle \lesssim L$. It remains to bound the first expression in (8.32). (Some variants of (8.32) obtained by setting x to be equal to y , y_1 or y_2 and by replacing the Θ edges with labelled diffusive edges can be estimated in similar ways, so we omit the details.)

By (1.9), (1.14), (2.3) and (2.8), we have the following maximum bounds on deterministic edges:

$$\begin{aligned} \max_{x,y} s_{xy} &= O(W^{-d}), \quad \max_{x,y} |S_{xy}^\pm| = O(W^{-d}), \quad \max_{x,y} \Theta_{xy} \prec W^{-d}, \\ \max_{x,y} |(\Theta \mathcal{E}_{2k_1} \Theta \mathcal{E}_{2k_2} \Theta \cdots \Theta \mathcal{E}_{2k_l} \Theta)_{xy}| &\prec W^{-kd/2}, \end{aligned} \quad (8.34)$$

where $k := \sum_{i=1}^l 2k_i - 2(l-1)$. For simplicity of presentation, we will use $\alpha \sim_{\mathcal{M}} \beta$ to mean that ‘‘atoms α and β belong to the same molecule’’. Suppose there are ℓ internal molecules \mathcal{M}_i , $1 \leq i \leq \ell$, in \mathcal{G}_0 . We choose one atom in each \mathcal{M}_i , say x_i , as a representative. For definiteness, we assume that x , y_1 and y_2 belong to different molecules. Otherwise, the proof will be easier and we omit the details. Throughout the following proof, we fix a small constant $\tau > 0$ and a large constant $D > 0$. For any $\alpha \sim_{\mathcal{M}} x_i$, it suffices to assume that

$$|\alpha - x_i| \leq W^{1+\tau/2}, \quad (8.35)$$

because otherwise the graph is smaller than W^{-D} . Then under the assumption (8.35), for $\alpha_i \sim_{\mathcal{M}} x_i$ and $\alpha_j \sim_{\mathcal{M}} x_j$, by (1.14), (8.5) and (2.8) we have that

$$|G_{\alpha_i \alpha_j}| \prec W^{d\tau} \Psi_{x_i x_j}(\tau, D), \quad \Theta_{\alpha_i \alpha_j} \prec B_{y_i y_j} \lesssim W^{(d-2)\tau/2} B_{x_i x_j}. \quad (8.36)$$

$$|(\Theta \mathcal{E}_{2k_1} \Theta \mathcal{E}_{2k_2} \Theta \cdots \Theta \mathcal{E}_{2k_l} \Theta)_{\alpha_i \alpha_j}| \prec W^{-(k-2)d/2+(d-2)\tau/2} B_{x_i x_j}. \quad (8.37)$$

The above estimates show that we can bound edges between different molecules with Ψ or B variables that only contain the representative atoms x_i in their indices.

We first bound the edges between different molecules. Due to the doubly connected property of \mathcal{G}_0 , we can pick two spanning trees of the black and blue nets, which we refer to as the *black tree* and *blue tree*, respectively. We bound the *internal edges* that are not in the two trees by their maximum norms:

- (i) we bound each solid edge that is not in the blue tree by $O_{\prec}(W^{-d/2+\varepsilon_0})$;
- (ii) we bound each diffusive edge that is not in the black and blue trees by $O_{\prec}(W^{-d})$;
- (iii) we bound each labelled diffusive edge that is not in the black and blue trees by $O_{\prec}(W^{-kd/2})$, where k is the scaling order of this edge.

We bound the external edges and edges of the two trees as follows:

- (iv) the blue solid and diffusive edges in the two trees and the external edges $\Theta_{\mathbf{ax}}$, $G_{y_1 \mathbf{b}}$ and $\overline{G}_{y_2 \mathbf{b}}$ are bounded using (8.36) and (8.37).

In this way, we can bound that

$$|\mathcal{G}_{\mathbf{ab}}| \prec W^{-n_1 d/2 + n_2 \tau + n_3 \varepsilon_0} \sum_{x_1, \dots, x_\ell} \Gamma_{\text{global}}(x_1, \dots, x_\ell) \prod_{i=1}^{\ell} |\mathcal{G}_{x_i}^{(i)}|, \quad (8.38)$$

where $W^{-n_1 d/2 + n_2 \tau + n_3 \varepsilon_0}$ is a factor coming from the above items (i)–(iv); Γ_{global} is a product of blue solid edges that represent Ψ entries, and (black or blue) double-line edges that represent B entries; every $\mathcal{G}_{x_i}^{(i)}$ is the subgraph inside the molecule \mathcal{M}_i , which has x_i as an external atom. The local structure $\mathcal{G}_{x_i}^{(i)}$ can be bounded as follows:

- we bound each wavy or diffusive edge by $O_{\prec}(W^{-d})$ using the maximum bounds in (8.34);
- we bound each labelled diffusive edge by $O_{\prec}(W^{-kd/2})$, where k is its scaling order;
- we bound each off-diagonal G edge and light G weight by $O_{\prec}(W^{-d/2 + \varepsilon_0})$;
- each summation over an internal atom in $\mathcal{M}_i \setminus \{x_i\}$ gives a $W^{(1+\tau/2)d}$ factor due to (8.35).

Thus with the definition of scaling order in (2.11), we get that

$$|\mathcal{G}_{x_i}^{(i)}| \prec W^{-\text{ord}(\mathcal{G}_{x_i}^{(i)}) \cdot d/2 + l_i \varepsilon_0 + k_i d \tau/2}, \quad (8.39)$$

where l_i is the number of off-diagonal G edges and light weights in $\mathcal{G}_{x_i}^{(i)}$, and k_i is the number of internal atoms. Finally, for convenience of proof, we bound every diffusive edge in the *blue* (but not black) tree of $\Gamma_{global}(x_1, \dots, x_\ell)$ as

$$B_{x_i x_j} \leq W^{-d/2} B_{x_i x_j}^{1/2}. \quad (8.40)$$

(This is solely because we can express both the Ψ and $B^{1/2}$ entries using the Notation 8.8.) Plugging (8.39) and (8.40) into (8.38), we obtain that

$$\mathcal{G}_{\mathbf{ab}} \prec W^{(n_{\mathbf{ab}} - \ell - 1)(-d/2 + \varepsilon_0) + n_4 \tau} (\mathcal{G}_{\mathbf{ab}})_{aux}, \quad (8.41)$$

where $n_{\mathbf{ab}} := \text{ord}(\mathcal{G}_{\mathbf{ab}})$, $n_4 := n_2 + \sum_{i=1}^{\ell} k_i d/2$, and $n_{\mathbf{ab}} - \ell - 1$ in the exponent can be obtained by counting the number of $W^{-d/2}$ factors from the above argument. Here we also used the following fact: by property (ii) of Definition 2.5, the number of internal atoms in $\mathcal{G}_{\mathbf{ab}}$ is at most the number of wavy and diffusive edges, and hence the number of W^{ε_0} factors coming from off-diagonal G edges and light weights is less than or equal to the number of $W^{-d/2}$ factors. $(\mathcal{G}_{\mathbf{ab}})_{aux}$ is an auxiliary graph satisfying the following properties:

- $(\mathcal{G}_{\mathbf{ab}})_{aux}$ has two external atoms \mathbf{a} and \mathbf{b} , and ℓ internal atoms x_i , $1 \leq i \leq \ell$, which are the representative atoms of the internal molecules of $\mathcal{G}_{\mathbf{ab}}$;
- every double-line edge between atoms x and y represents a B_{xy} factor, and every blue solid edge between atoms x and y represents a variable satisfying the Notation 8.8;
- there is a spanning tree of black double-line edges, and \otimes is connected to an internal atom through a double-line edge (which corresponds to the edge Θ_{ax} in $\mathcal{G}_{\mathbf{ab}}$);
- there is a spanning tree of blue solid edges, and \oplus is connected to internal atoms through two blue solid edges (which correspond to the edges $G_{y_1 \mathbf{b}}$ and $\overline{G}_{y_2 \mathbf{b}}$ in $\mathcal{G}_{\mathbf{ab}}$).

Now we choose an atom connected to \oplus as the root of the blue spanning tree. Then we sum over the internal atoms in $(\mathcal{G}_{\mathbf{ab}})_{aux}$ from the leaves to this root. Without loss of generality, assume that we sum over the internal atoms according to the order $\sum_{x_\ell} \dots \sum_{x_2} \sum_{x_1}$, such that atom x_ℓ is the root. For simplicity of notations, we denote all blue solid edges appearing in the proof by Ω , including the Ψ and $B^{1/2}$ edges in $(\mathcal{G}_{\mathbf{ab}})_{aux}$ and new edges coming from applications of (8.30). All these Ω variables satisfy the Notation 8.8, and their exact forms may change from one line to another.

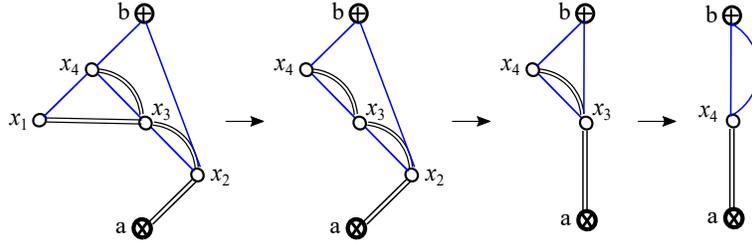
We sum over the internal atoms one by one. For the sum over x_1 , using (8.31) (if x_1 is connected with \oplus) or (8.10) (if x_1 is not connected with \oplus), we can bound $(\mathcal{G}_{\mathbf{ab}})_{aux}$ as

$$(\mathcal{G}_{\mathbf{ab}})_{aux} \prec W^{-d/2 + \varepsilon_0} \sum_{k=1}^{n_1} (\mathcal{G}_{\mathbf{ab},k}^{(1)})_{aux}, \quad (8.42)$$

where $(\mathcal{G}_{\mathbf{ab},k}^{(1)})_{aux}$ are auxiliary graphs obtained by replacing the edges connected to x_1 with the graphs on the right-hand side of (8.31) or (8.10), and n_1 is the number of atoms connected to x_1 through double-line edges. More precisely, after summing over x_1 , we get rid of the blue solid edge connected with x_1 . If \oplus and x_1 are

connected through a blue solid edge in $(\mathcal{G}_{ab})_{aux}$, then in each new graph \oplus is connected to the parent of x_1 on the blue tree through a blue solid edge. Moreover, suppose w_1, \dots, w_{n_1} are the atoms connected to x_1 through double-line edges. Then corresponding to the n_1 terms in $\Gamma(w_1, \dots, w_{n_1})$, the atoms w_1, \dots, w_{n_1} are now connected to one of them, say w_k , through double-line edges in new graphs, which leads to the n_1 different choices in (8.42). Now we observe that every new graph $(\mathcal{G}_{ab,k}^{(1)})_{aux}$ is doubly connected in the following sense: there is a black spanning tree connecting all the internal atoms and \otimes , and a disjoint blue spanning tree connecting all the internal atoms and \oplus . Furthermore, there are at least two blue solid edges connected with \oplus in $(\mathcal{G}_{ab,k}^{(1)})_{aux}$.

Then we sum over the atoms $x_2, \dots, x_{\ell-1}$ one by one using (8.31) or (8.10). At each step, we gain a $W^{-d/2+\varepsilon_0}$ factor and reduce a graph into a sum of several new graphs, each of which has one fewer atom, a black spanning tree connecting all the internal atoms and \otimes , a blue spanning tree connecting all the internal atoms and \oplus , and two blue solid edges connected with \oplus . In the following figure, we give an example of the graph reduction process by summing over the internal atoms x_1, x_2, x_3 .



Finally, we get a graph with only one internal atom x_l , one double-line edge between \otimes and x_l , and two blue solid edges between \oplus and x_l . Then using (8.29), we can bound (8.41) as

$$|\mathcal{G}_{ab}| \prec W^{(n_{ab}-2)(-d/2+\varepsilon_0)+n_4\tau} \sum_{x_\ell} B_{ax_\ell} \left(B_{x_\ell b} + \tilde{\Phi}^2 \right) \lesssim W^{(n-1)(-d/2+\varepsilon_0)+n_4\tau} \frac{L^2}{W^2} \left(B_{ab} + \tilde{\Phi}^2 \right),$$

where we used $n_{ab} \geq n+1$ and a similar argument as in (8.33). Since τ is arbitrary, we can bound the first case in (8.32) by the right-hand side of (8.23). This concludes the proof. \square

Proof of Claim 8.7. We only consider the graphs in $(\mathcal{Q}_T^{(n)})_{a,b,b}$ that are not \oplus -recollision graphs, because \oplus -recollision graphs are much easier to deal with and we omit the details. Let \mathcal{G}_{ab} be such a Q -graph. We need to bound the graph $\mathbb{E}T_{ab}^{p-1}\mathcal{G}_{ab}$. In the following proof, we call the $2(p-1)$ solid edges in T_{ab}^{p-1} *external solid edges*, and we regard the atoms x in $T_{ab} = |m|^2 \sum_x s_{ax} |G_{xb}|^2$ as an atom in the external \otimes molecule.

We perform the Q -expansions in Section 4.4 to $T_{ab}^{p-1}\mathcal{G}_{ab}$ and get that

$$\mathbb{E}T_{ab}^{p-1}\mathcal{G}_{ab} = \mathbb{E} \sum_{k=2}^p T_{ab}^{p-k} \sum_{\omega} (\mathcal{G}_{\omega}^{(k)})_{ab} + \mathbb{E} \sum_{k=2}^p T_{ab}^{p-k} \sum_{\zeta} (\mathcal{G}_{err,\zeta}^{(k)})_{ab}. \quad (8.43)$$

Every $(\mathcal{G}_{\omega}^{(k)})_{ab}$ is a normal regular graph satisfying the following properties.

- (1) $(\mathcal{G}_{\omega}^{(k)})_{ab}$ contains no P/Q labels.
- (2) It is doubly connected.
- (3) \otimes is connected to internal molecules through a (labelled) diffusive edge.
- (4) Let the atom in the Q -label of \mathcal{G}_{ab} be α . There are r , $k-1 \leq r \leq 2(k-1)$, external edges (coming from $(k-1)$ many T_{ab} variables) that become paths of two external solid edges in the molecular graph from the \otimes molecule to the molecule containing α and then to the \oplus molecule.
- (5) Besides the external solid edges in (4), the internal molecules are also connected to \oplus through a diffusive edge, or two blue and red solid edges (which correspond to the two solid edges connected with \oplus in \mathcal{G}_{ab}). In the latter case, we call the two solid edges *special solid edges*.

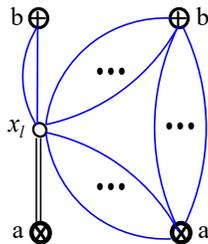
Every graph $(\mathcal{G}_{err,\zeta}^{(k)})_{ab}$ is of scaling order $> 2k + D$ and satisfies the above properties (2)–(5) (but it may contain P/Q labels). For convenience of presentation, whenever we refer to external solid edges in the following proof, they do not include the special solid edges in (5). For the rest of the proof, we will focus on $(\mathcal{G}_\omega^{(k)})_{ab}$, while the graphs $(\mathcal{G}_{err,\zeta}^{(k)})_{ab}$ can be bounded in the same way. Moreover, we only consider the hardest case where (a) there are no dotted edges connected with \oplus or \otimes in $(\mathcal{G}_\omega^{(k)})_{ab}$; (b) in the above item (5), \oplus is connected to the internal molecules through a blue solid edge and a red solid edge. Other cases where (a) or (b) does not hold are all easier to bound.

We will follow similar arguments as in the above proof of Claim 8.6. More precisely, given any graph $(\mathcal{G}_\omega^{(k)})_{ab}$, we first pick two spanning trees of the black and blue nets. Then we bound the internal edges that are not in the two trees by their maximum norms, and bound the local structures inside all internal molecules by (8.39). Furthermore, we bound the external edges, special solid edges and the internal edges that are in the two trees using (8.36), (8.37) and (8.40). Again we can reduce the problem to bounding an auxiliary graph $(\mathcal{G}_{ab})_{aux}$ satisfying the following properties:

- (i) $(\mathcal{G}_\omega^{(k)})_{ab}$ has two external atoms \mathbf{a} and \mathbf{b} , and ℓ internal atoms x_i , $1 \leq i \leq \ell$, which are the representative atoms of the internal molecules;
- (ii) each double-line edge between atoms x and y represents a B_{xy} factor, and each blue solid edge between atoms x and y represents a variable satisfying the Notation 8.8;
- (iii) each external or special solid edge between two molecules in $(\mathcal{G}_\omega^{(k)})_{ab}$ is replaced by an external blue solid edge between the representative atoms of these molecules in $(\mathcal{G}_{ab})_{aux}$;
- (iv) the maximal subgraph of $(\mathcal{G}_{ab})_{aux}$ induced on the internal atoms has a spanning tree of black double-line edges and a spanning tree of blue solid edges;
- (v) in $(\mathcal{G}_{ab})_{aux}$, \otimes is connected to the internal atoms through a black double-line edge, and \oplus is connected to the internal atoms through two special blue solid edges;
- (vi) in $(\mathcal{G}_{ab})_{aux}$, there are $2(k-1) - r$ blue solid edges between \mathbf{a} and \mathbf{b} , r blue solid edges between \mathbf{a} and x_ℓ , and r blue solid edges between \mathbf{b} and x_ℓ , where x_ℓ is the representative atom of the molecule containing α .

Since $(\mathcal{G}_\omega^{(k)})_{ab} \prec (\mathcal{G}_{ab})_{aux}$, we only need to estimate $(\mathcal{G}_{ab})_{aux}$. We choose the atom x_ℓ , the representative atom of the molecule containing α , as the root of the blue spanning tree. Then we sum over the internal atoms in $(\mathcal{G}_{ab})_{aux}$ from leaves to this root. Without loss of generality, assume that we sum over the internal atoms according to the order $\sum_{x_\ell} \cdots \sum_{x_2} \sum_{x_1}$. For simplicity of notations, we denote all blue solid edges appearing in the proof by Ω , including the edges in the original graph $(\mathcal{G}_{ab})_{aux}$ and new edges coming from applications of (8.30). All these Ω variables satisfy the Notation 8.8, and their exact forms may change from one line to another. Suppose the two special blue solid edges in (v) connect \oplus to atoms x_i and x_j , respectively. We have the following two cases.

Case 1: Suppose the unique path on the blue spanning tree from x_i to x_j passes through x_ℓ . Then, similar to the proof of Claim 8.6, we sum over the internal atoms one by one and reduce the graphs using (8.10) and (8.31). Finally, we get the following graph with $2(k-1) - r$ blue solid edges between \otimes and \oplus , and only one internal atom x_ℓ , which is connected with \otimes through a black double-line edge and r external solid edges, and with \oplus through two special solid edges and r external solid edges. (To have a clearer picture, we draw two copies of the \otimes and \oplus atoms in the graph.)



Denote this graph by $(\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux}$. To estimate $(\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux}$, we consider two regions $\mathcal{I}_1 := \{x_\ell : \langle x_\ell - \mathbf{a} \rangle \geq \langle x_\ell - \mathbf{b} \rangle\}$ and $\mathcal{I}_2 := \{x : \langle x_\ell - \mathbf{a} \rangle < \langle x_\ell - \mathbf{b} \rangle\}$. Then we can bound that

$$\begin{aligned} (\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux} &\leq \left(\sum_{x_\ell \in \mathcal{I}_1} + \sum_{x_\ell \in \mathcal{I}_2} \right) (B_{\mathbf{a}x_\ell} |\Omega_{x_\ell \mathbf{b}}|^2) (|\Omega_{\mathbf{a}x_\ell}|^r |\Omega_{x_\ell \mathbf{b}}|^r) |\Omega_{\mathbf{ab}}|^{2k-2-r} \\ &\prec \left[\sum_{x_\ell \in \mathcal{I}_1} B_{\mathbf{a}x_\ell} (B_{x_\ell \mathbf{b}} + \tilde{\Phi}^2) |\Omega_{x_\ell \mathbf{b}}|^r + \sum_{x_\ell \in \mathcal{I}_2} B_{\mathbf{a}x_\ell} (B_{x_\ell \mathbf{b}} + \tilde{\Phi}^2) |\Omega_{\mathbf{a}x_\ell}|^r \right] (B_{\mathbf{ab}}^{1/2} + \tilde{\Phi})^{2k-2}, \end{aligned} \quad (8.44)$$

where in the second step we used (8.29), $\langle x_\ell - \mathbf{a} \rangle \geq \langle \mathbf{a} - \mathbf{b} \rangle / 2$ on \mathcal{I}_1 and $\langle x_\ell - \mathbf{b} \rangle \geq \langle \mathbf{a} - \mathbf{b} \rangle / 2$ on \mathcal{I}_2 . We bound the sum over \mathcal{I}_1 as

$$\begin{aligned} \sum_{x_\ell \in \mathcal{I}_1} B_{\mathbf{a}x_\ell} (B_{x_\ell \mathbf{b}} + \tilde{\Phi}^2) |\Omega_{x_\ell \mathbf{b}}|^r &\prec W^{(r-1)(-d/2+\varepsilon_0)} \sum_{x_\ell \in \mathcal{I}_1} B_{\mathbf{a}x_\ell} (B_{x_\ell \mathbf{b}} + \tilde{\Phi}^2) \Omega_{x_\ell \mathbf{b}} \\ &\prec W^{r(-d/2+\varepsilon_0)} (B_{\mathbf{ab}} + \tilde{\Phi}^2), \end{aligned} \quad (8.45)$$

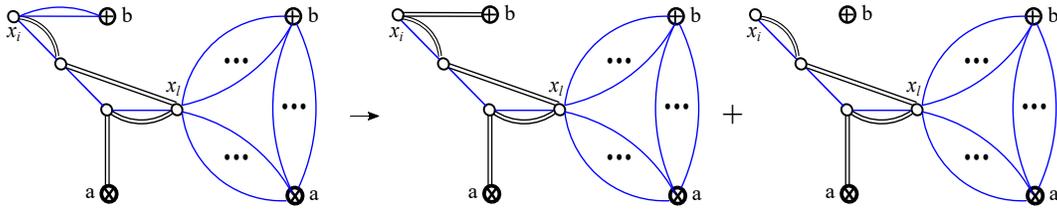
where we used (8.6) in the first step, and (8.10) in the second step with $(a, b) = (1, 2)$ and $\|\Omega\|_{w;(1,2)} \prec W^{\varepsilon_0}$. We have a similar bound for the sum over \mathcal{I}_2 . Hence we get that

$$(\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux} \prec W^{r(-d/2+\varepsilon_0)} (B_{\mathbf{ab}} + \tilde{\Phi}^2) (B_{\mathbf{ab}}^{1/2} + \tilde{\Phi})^{2k-2} \lesssim W^{r(-d/2+\varepsilon_0)} (B_{\mathbf{ab}} + \tilde{\Phi}^2)^k. \quad (8.46)$$

Case 2: Suppose the unique path on the blue spanning tree from x_i to x_j does not pass through x_ℓ . Then, similar to the proof of Claim 8.6, we sum over the internal atoms one by one and reduce the graphs using (8.10) and (8.31). At certain step, we will get a graph where the two special blue solid edges are connected with the same internal atom, say x_i . Denote this graph by $(\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux}$. Now applying (8.29) to the two special edges, we can bound $(\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux}$ by

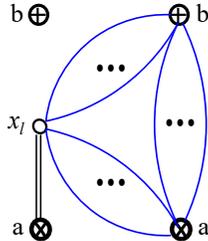
$$(\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux} \prec (\tilde{\mathcal{G}}_{\mathbf{ab}}^{(1)})_{aux} + \tilde{\Phi}^2 (\tilde{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux}, \quad (8.47)$$

where $(\tilde{\mathcal{G}}_{\mathbf{ab}}^{(1)})_{aux}$ is obtained by replacing the two special edges with a double-line edge between x_i and \oplus , and $(\tilde{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux}$ is obtained by removing the two special edges. In the following figure, we draw an example of graphs $(\tilde{\mathcal{G}}_{\mathbf{ab}})_{aux}$, $(\tilde{\mathcal{G}}_{\mathbf{ab}}^{(1)})_{aux}$ and $(\tilde{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux}$.



There is a $\tilde{\Phi}^2$ factor associated with the third graph $(\tilde{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux}$, but we did not draw it.

Similar to the proof of Claim 8.6, we sum over the internal atoms of $(\tilde{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux}$ from leaves to the root x_ℓ on the blue tree and reduce the graphs using (8.10) at each step. We will finally get the following graph with only one internal atom x_ℓ :

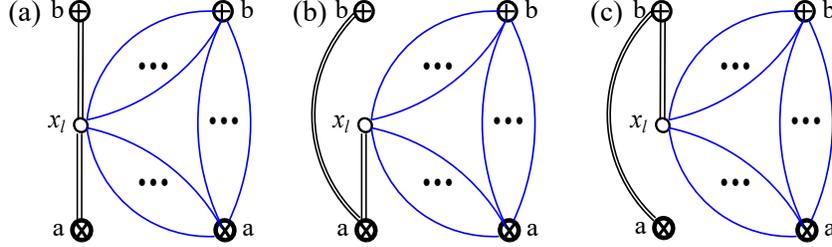


Denote this graph by $(\hat{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux}$. Using similar arguments as in (8.44) and (8.45), we can bound that

$$(\tilde{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux} \prec (\hat{\mathcal{G}}_{\mathbf{ab}}^{(2)})_{aux} \prec \left(\sum_{x_\ell \in \mathcal{I}_1} B_{\mathbf{a}x_\ell} |\Omega_{x_\ell \mathbf{b}}|^r + \sum_{x_\ell \in \mathcal{I}_2} B_{\mathbf{a}x_\ell} |\Omega_{\mathbf{a}x_\ell}|^r \right) (B_{\mathbf{ab}}^{1/2} + \tilde{\Phi})^{2k-2}$$

$$\begin{aligned}
&\prec \left(\sum_{x_\ell \in \mathcal{I}_1} B_{ax_\ell} \Omega_{x_\ell b} + \sum_{x_\ell \in \mathcal{I}_2} B_{ax_\ell} \Omega_{ax_\ell} \right) W^{(r-1)(-d/2+\varepsilon_0)} \left(B_{ab}^{1/2} + \tilde{\Phi} \right)^{2k-2} \\
&\prec W^{r(-d/2+\varepsilon_0)} \left(B_{ab} + \tilde{\Phi}^2 \right)^{k-1}. \tag{8.48}
\end{aligned}$$

To estimate the graph $(\tilde{\mathcal{G}}_{ab}^{(1)})_{aux}$, we also sum over its internal atoms from leaves to the root x_ℓ on the blue tree and reduce the graphs using (8.10) at each step. After each summation, we will get a sum of several new graphs, each of which has a black spanning tree that connects all the internal atoms and the atoms \otimes and \oplus . In the end, we get a sum of graphs with only one internal atom x_ℓ . Each of these graphs must take one of the following three forms:



Graph (a), denoted by $(\hat{\mathcal{G}}_{ab}^{(a)})_{aux}$, can be bounded using similar arguments as in (8.44) and (8.45):

$$(\hat{\mathcal{G}}_{ab}^{(a)})_{aux} \prec W^{r(-d/2+\varepsilon_0)} B_{ab} \left(B_{ab} + \tilde{\Phi}^2 \right)^{k-1}.$$

Graph (b), denoted by $(\hat{\mathcal{G}}_{ab}^{(b)})_{aux}$, can be bounded by

$$(\hat{\mathcal{G}}_{ab}^{(b)})_{aux} \prec B_{ab} (\hat{\mathcal{G}}_{ab}^{(2)})_{aux} \prec W^{r(-d/2+\varepsilon_0)} B_{ab} \left(B_{ab} + \tilde{\Phi}^2 \right)^{k-1}.$$

It is trivial to see that this bound also holds for graph (c) denoted by $(\hat{\mathcal{G}}_{ab}^{(c)})_{aux}$. Combining these estimates, we obtain that

$$(\tilde{\mathcal{G}}_{ab}^{(1)})_{aux} \prec (\hat{\mathcal{G}}_{ab}^{(a)})_{aux} + (\hat{\mathcal{G}}_{ab}^{(b)})_{aux} + (\hat{\mathcal{G}}_{ab}^{(c)})_{aux} \prec W^{r(-d/2+\varepsilon_0)} B_{ab} \left(B_{ab} + \tilde{\Phi}^2 \right)^{k-1}. \tag{8.49}$$

Plugging (8.48) and (8.49) into (8.47), we get the estimate (8.46) in case 2.

Finally, combining the above two cases, we conclude from (8.46) that

$$(\mathcal{G}_\omega^{(k)})_{ab} \prec (\mathcal{G}_{ab})_{aux} \prec (\tilde{\mathcal{G}}_{ab})_{aux} \prec W^{r(-d/2+\varepsilon_0)} \left(B_{ab} + \tilde{\Phi}^2 \right)^k \prec \left[W^{-d/4+\varepsilon_0/2} \left(B_{ab} + \tilde{\Phi}^2 \right) \right]^k,$$

where we used $k \geq 2$ and $r \geq k-1 \geq k/2$ in the last step. Inserting this estimate into (8.43), we can conclude Claim 8.7. \square

8.3 Proof of Lemma 7.2

The proof of Lemma 7.2 is similar to (and actually much easier than) the one for Lemma 7.4. In the $\eta = 1$ case, by (1.14) we have that for any small constant $\tau > 0$ and large constant $D > 0$,

$$\Theta_{xy} \leq \frac{W^\tau}{W^d} \mathbf{1}_{|x-y| \leq W^{1+\tau}} + O(W^{-D}). \tag{8.50}$$

In other words, the Θ edge is typically a ‘‘short edge’’ of length $O_\prec(W)$. Moreover, the following local law on $G(z)$ was proved in [13, 14].

Lemma 8.9 (Theorem 2.3 of [13] and Theorem 2.1 of [14]). *Suppose the assumptions of Theorem 1.3 hold. For any constants $\kappa, \varepsilon > 0$, the local law*

$$\max_{x,y} |G_{xy}(z) - \delta_{xy} m(z)| \prec (W^d \eta)^{-1/2} \tag{8.51}$$

holds uniformly in $z = E + i\eta$ with $E \in (-2 + \kappa, 2 - \kappa)$ and $\eta \in [W^{-d+\varepsilon}, 1]$.

With (8.51) as the a priori estimate, to conclude Lemma 7.2, it suffices to prove the following high moment estimate similar to (8.2): if (8.1) holds, then

$$\mathbb{E}T_{xy}(z)^p \prec (B_{xy} + W^{-d/4}\tilde{\Phi}^2)^p. \quad (8.52)$$

To prove (8.52), we use the second order T -expansion (3.8). Using (8.50), (8.51) and (8.1), we can easily bound that

$$(\mathcal{A}_T^{(>2)})_{a,bb} \prec W^{-d/2} \sum_{x:|x-a|\leq W^{1+\tau}} \frac{W^\tau}{W^d} (B_{xb} + \tilde{\Phi}^2) + W^{-D} \prec W^{-d/2+2d\tau} (B_{ab} + \tilde{\Phi}^2).$$

Moreover, we can prove that

$$\mathbb{E}T_{ab}^{p-1}(\mathcal{Q}_T^{(2)})_{a,bb} \prec \sum_{k=2}^p \left[W^{-d/4+d\tau} (B_{xy} + \tilde{\Phi}^2) \right]^k \mathbb{E}T_{ab}^{p-k}.$$

We omit the details since the proof is similar to (and actually much easier than) the one for Claim 8.7. With the above two estimates, we can obtain an estimate similar to (8.27), which gives (8.52) by the argument in (8.28).

9 CONTINUITY ESTIMATE

9.1 Proof of Lemma 7.3

Define the subset of indices $\mathcal{I} = \{y : |y - x_0| \leq K\}$ for $x_0 \in \mathbb{Z}_L^d$ and $K \in [W, L/2]$. Then we define the $\mathcal{I} \times \mathcal{I}$ positive definite Hermitian matrix $A = (A_{yy'} : y, y' \in \mathcal{I})$ by

$$A_{y'y} := \frac{G_{y'y}(\tilde{z}) - \overline{G_{yy'}(\tilde{z})}}{2i}. \quad (9.1)$$

In the proof of Lemma 5.3 in [32], we have obtained the following estimates:

$$\sum_{y \in \mathcal{I}} |G_{xy}(z)|^2 \lesssim \sum_{y \in \mathcal{I}} |G_{xy}(\tilde{z})|^2 + \left(\frac{\tilde{\eta}}{\eta}\right)^2 \|A\|_{\ell^2 \rightarrow \ell^2}, \quad (9.2)$$

$$\sum_{y \in \mathcal{I}} |G_{yx}(z)|^2 \lesssim \sum_{y \in \mathcal{I}} |G_{yx}(\tilde{z})|^2 + \left(\frac{\tilde{\eta}}{\eta}\right)^2 \|A\|_{\ell^2 \rightarrow \ell^2}, \quad (9.3)$$

with high probability. Using (7.5), we can bound that

$$\sum_{y \in \mathcal{I}} (|G_{xy}(\tilde{z})|^2 + |G_{yx}(\tilde{z})|^2) \prec 1 + \sum_{y \in \mathcal{I}} B_{xy} \lesssim \frac{K^2}{W^2}. \quad (9.4)$$

In this section, we will prove the following bound.

Lemma 9.1. *Suppose the assumptions of Lemma 7.3 hold. Then for any fixed $p \in \mathbb{N}$ and small constant $\varepsilon > 0$, the matrix A in (9.1) satisfies that*

$$\mathbb{E} \operatorname{Tr} (A^{2p}) \leq K^d \left(W^\varepsilon \frac{K^4}{W^4} \right)^{2p-1}. \quad (9.5)$$

With Lemma 9.1, we obtain that

$$\mathbb{E} \|A\|_{\ell^2 \rightarrow \ell^2}^{2p} \leq \mathbb{E} \operatorname{Tr} (A^{2p}) \leq K^d \left(W^\varepsilon \frac{K^4}{W^4} \right)^{2p-1}.$$

Since p can be arbitrarily large, using Markov's inequality we obtain that

$$\|A\|_{\ell^2 \rightarrow \ell^2} \prec \frac{K^4}{W^4}. \quad (9.6)$$

Inserting (9.4) and (9.6) into (9.2) and (9.3), we conclude (7.6). The proof of (7.7) uses a standard perturbation and union bound argument, which has been given in [32]. Hence we omit the details.

9.2 Non-universal T -expansion

The rest of this section is devoted to proving Lemma 9.1. Recall that the matrix A is defined using $G(\tilde{z})$. Hence all G edges in the following proof represent $G(\tilde{z})$ entries, and they satisfy the local law (7.5). The proof of Lemma 9.1 is based on an intricate expansion strategy of the graphs in $\text{Tr}(A^{2p})$, which is an extension of Strategy 6.6. In this subsection, we establish the first tool for our proof, that is, the *non-universal T -expansion*. We will expand the n -th order T -expansion into a sum of deterministic graphs (more precisely, graphs whose maximal subgraphs are deterministic) and Q -graphs. In other words, we will further expand the graphs in $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{A}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ into deterministic graphs plus Q -graphs. As we will see later, the expansion is called *non-universal* because it depends on L explicitly, and the graphs in the expansion are bounded properly only when the condition (3.15) holds.

To get a non-universal T -expansion, we apply Strategy 6.6 to $(\mathcal{R}_{IT}^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{A}_{IT}^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ with the following stopping rule: we will stop expanding a graph when it has a deterministic maximal subgraph, it is a Q -graph, or its scaling order is larger than a large enough constant $D > 0$. However, there is one scenario which is not covered by Strategy 6.6, that is, at a certain step we have to expand a pivotal edge and hence break the double connected property. This is the main difficulty with the proof. We will design an expansion strategy so that in the end all the graphs that are not doubly connected in the non-universal T -expansion can be bounded properly under the condition (3.15).

Although some graphs may not be doubly connected, all graphs in our expansions will automatically have a black net. On the other hand, the subset of blue and red solid edges may not contain a spanning tree and can be separated into disjoint components. For simplicity, we summarize these properties in the following definition.

Definition 9.2. *We say a subgraph \mathcal{G} without external atoms has (at most) $k_0 \equiv k_0(\mathcal{G})$ many components if there exist three disjoint subsets of edges in the molecular graph $\mathcal{G}_{\mathcal{M}}$ satisfying the following properties.*

- (i) \mathcal{B}_{black} is a black net consisting of diffusive edges.
- (ii) \mathcal{B}_{blue} is a subset consisting of blue solid (i.e. plus G) and diffusive edges.
- (iii) \mathcal{R}_{red} is a subset consisting of red solid (i.e. minus G) edges.
- (iv) There are k_0 disjoint components in the molecular subgraph consisting of the edges in $\mathcal{B}_{blue} \cup \mathcal{R}_{red}$. (By definition, a component means a subgraph in which any two molecules are connected to each other by a path of edges in $\mathcal{B}_{blue} \cup \mathcal{R}_{red}$, and which is connected to no additional molecules in the rest of the graph.)

A graph \mathcal{G} with external atoms is said to have k_0 many components if its maximal subgraph induced on internal atoms has k_0 many components. We will call the edges in \mathcal{B}_{blue} and \mathcal{B}_{red} as blue edges and red edges, respectively.

If a graph has only one component, then Lemma 8.4 applies to it. In general, we have the following lemma for graphs with more than one component.

Lemma 9.3. *Under the assumptions of Lemma 7.3, let \mathcal{G} be a normal regular graph without external atoms and with (at most) k_0 components in the sense of Definition 9.2. Pick any two atoms of \mathcal{G} and fix their values $x, y \in \mathbb{Z}_L^d$. Then the resulting graph \mathcal{G}_{xy} satisfies that*

$$|\mathcal{G}_{xy}| \prec \left(\frac{L^2}{W^2} \right)^{k_0-1} \frac{W^{-(n_{xy}-2)d/2}}{\langle x-y \rangle^d}, \quad (9.7)$$

where $n_{xy} := \text{ord}(\mathcal{G}_{xy})$ is the scaling order of \mathcal{G}_{xy} . This bound holds also for the graph \mathcal{G}^{abs} .

Proof. The proof is similar to the one for Lemma 8.4 in [32] and the one for Claim 8.6 in Section 8. Hence we only explain the main difference instead of writing down all the details. First, we pick a spanning tree of black edges in \mathcal{B}_{black} , and a spanning tree of blue and red edges in $\mathcal{B}_{blue} \cup \mathcal{R}_{red}$ for each component. Then similar to the proof of Claim 8.6, we can reduce the problem to bounding an auxiliary graph $(\mathcal{G}_{xy})_{aux}$ satisfying the following properties:

- \mathcal{G}_{xy} has two external atoms x and y , and ℓ internal atoms x_i , $1 \leq i \leq \ell$, which are the representative atoms of the internal molecules;

- there is a spanning tree of black double-line edges connecting all atoms, where a double-line edge between atoms α and β represents a $B_{\alpha\beta}$ factor;
- there is a spanning tree of blue solid edges connecting all atoms in each of the k_0 components, where a blue solid edge between atoms α and β represents a $B_{\alpha\beta}^{1/2}$ factor.

In obtaining the auxiliary graph, we also bound the red solid edges in the spanning trees of the k_0 components by $B^{1/2}$ factors. This is different from the proof of Claim 8.6, where we bound all red solid edges by their maximum norms.

For any spanning tree of blue solid edges in a component of $(\mathcal{G}_{xy})_{aux}$, we choose an atom in it as the root. If a blue tree contains x or y , then we choose x or y as the root. For definiteness, we assume that x and y belong to different blue trees in the following proof. The case where x and y belong to the same tree can be handled in a similar way, and we omit the details. Now we sum over the atoms in a spanning tree from leaves to the root. Similar to the proof of Claim 8.6, we bound each sum using (8.10) and (8.11) with $(a, b) = (1, 1)$. After summing over all internal atoms in one component except for the root, we turn to the blue spanning tree of the next component and sum over its internal atoms from leaves to the chosen root. After summing over the non-root atoms in all components, we obtain a graph, say $(\tilde{\mathcal{G}}_{xy})_{aux}$, satisfying the following properties:

- it has two external atoms x , y and $k_0 - 2$ internal atoms, which are the roots of the k_0 blue trees;
- it has a spanning tree of black diffusive edges connecting all atoms.

We sum over the internal atoms, say x_1, \dots, x_{k_0-2} , of $(\tilde{\mathcal{G}}_{xy})_{aux}$ one by one, and bound each sum using the simple estimate

$$\sum_{x_i} \prod_{i=1}^k B_{x_i y_k} \lesssim \frac{L^2}{W^2} \Gamma(y_1, \dots, y_k). \quad (9.8)$$

In $(\tilde{\mathcal{G}}_{xy})_{aux}$, we have a black spanning tree connecting all internal atoms. By (9.8), after each summation, we get some new graphs, each of which has one fewer internal atom, an additional L^2/W^2 factor and a black spanning tree connecting all atoms. After summing over all the $k_0 - 2$ internal atoms, we get a graph where x is connected to y through a double-line edge, i.e.,

$$(\tilde{\mathcal{G}}_{xy})_{aux} \prec \left(\frac{L^2}{W^2} \right)^{k_0-2} B_{xy} \lesssim \left(\frac{L^2}{W^2} \right)^{k_0-1} \frac{1}{\langle x - y \rangle^d}.$$

Finally, by counting the number of $W^{-d/2}$ factors carefully, we can obtain (9.7). \square

For our purpose, the weakest bound required for a graph \mathcal{G}_{xy} satisfying the setting of Lemma 9.3 is $\langle x - y \rangle^{-d}$. Hence we need to make sure that the factor $W^{-(n_{xy}-2)d/2}$ is small enough to cancel the $(L^2/W^2)^{k_0-1}$ factor. By condition (3.15), if we have $n_{xy} \geq (n-1) \cdot (k_0-1) + 2$, then (9.7) gives

$$|\mathcal{G}_{xy}| \prec \frac{W^{-(k_0-1)c_0}}{\langle x - y \rangle^d}.$$

Thus in expansions, we need to make sure that the scaling order of every graph is sufficiently high depending on the number of components in it. For this purpose, we introduce the following helpful tool.

Definition 9.4 (Ghost edges). *We use a green dashed edge between atoms x and y to represent a W^2/L^2 factor, and we call such an edge a ghost edge. We do not count ghost edges when calculating the scaling order of a graph, i.e. the scaling order of a ghost edge is 0. Moreover, the doubly connected property in Definition 2.12, the SPD property in Definition 5.9, and the globally standard property in Definition 6.2 can be extended to graphs with ghost edges by including these edges into blue nets.*

To keep graph values unchanged, whenever we add a ghost edge to a graph, we always multiply it by L^2/W^2 to cancel this edge. In a doubly connected graph with k_0 ghost edges, removing all of them gives at most $k_0 + 1$ many components. Hence with Lemma 9.3, we immediately obtain the following estimate.

Lemma 9.5. *Under the assumptions of Lemma 7.3, let \mathcal{G} be a doubly connected normal regular graph without external atoms and with k_{gh} ghost edges. Pick any two atoms of \mathcal{G} and fix their values $x, y \in \mathbb{Z}_L^d$. Then the resulting graph \mathcal{G}_{xy} satisfies that*

$$|\mathcal{G}_{xy}| \prec \left(\frac{L^2}{W^2} \right)^{k_{\text{gh}}} \frac{W^{-(n_{xy}-2)d/2}}{\langle x-y \rangle^d}, \quad (9.9)$$

where $n_{xy} := \text{ord}(\mathcal{G}_{xy})$ is the scaling order of \mathcal{G}_{xy} . This bound holds also for the graph \mathcal{G}^{abs} .

Ghost edges are introduced to deal with expansions of pivotal blue solid edges (recall Definition 5.5). We have avoided such expansions in the proof of Theorem 3.7, but they are necessary for constructing the non-universal T -expansion. Roughly speaking, when we expand a pivotal blue solid edge in a graph, we will add a ghost edge between its two ending atoms and multiply the graph by L^2/W^2 to keep the graph value unchanged. Then this pivotal edge becomes redundant, and we can make use of the tools developed in Sections 5 and 6. In this way, we do not need to rebuild a new set of graphical tools from scratch. However, different from Strategy 6.6, we also need to keep track of the scaling orders of our graphs carefully to make sure that they are high enough to cancel the L^2/W^2 factors associated with the ghost edges. To deal with this issue, we will introduce some new graphical tools.

To define the non-universal T -expansion, we first define the *generalized SPD property*, extending the SPD property in Definition 5.9. For simplicity of notations, we call an isolated subgraph plus its external edges (including the ending atoms of them) the *closure* of this isolated subgraph.

Definition 9.6 (Generalized SPD property). *A graph \mathcal{G} with ghost edges is said to be a generalized sequentially pre-deterministic graph if the following properties hold.*

- (i) \mathcal{G} is doubly connected by including its ghost edges into the blue net.
- (ii) \mathcal{G} contains at most one sequence of proper isolated subgraphs with non-deterministic closures. (By definition, an isolated subgraph has a non-deterministic closure if this subgraph contains G edges and weights inside it, or it is connected with at least one external G edge.)
- (iii) The maximal subgraph \mathcal{G}_{max} (resp. an isolated subgraph \mathcal{I}) of \mathcal{G} is pre-deterministic if it has no proper isolated subgraph with non-deterministic closure. Otherwise, let \mathcal{I}' be its maximal isolated subgraph with non-deterministic closure. If we replace the closure of \mathcal{I}' with a diffusive edge in the molecular graph without red solid edges, then \mathcal{G}_{max} (resp. \mathcal{I}) becomes pre-deterministic.

The only difference from Definition 5.9 is that property (ii) of Definition 9.6 is restricted to the sequence of isolated subgraphs with non-deterministic closures. In other words, a proper isolated subgraph of \mathcal{G} may have several other sequences of *deterministic* isolated subgraphs. Now we are ready to state the main result of this subsection on non-universal T -expansions.

Lemma 9.7 (Non-universal T -expansion). *Suppose the assumptions of Lemma 7.3 hold. For any large constant $D > 0$, $T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be expanded into a sum of $\mathcal{O}(1)$ many graphs:*

$$\begin{aligned} T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} &= m \Theta_{\mathbf{a} \mathbf{b}_1} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} + \sum_{\mu} B_{\mathbf{a} \mathbf{b}_1}^{(\mu)} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} f_{\mu}(G_{\mathbf{b}_1 \mathbf{b}_1}) + \sum_{\nu} \tilde{B}_{\mathbf{a} \mathbf{b}_2}^{(\nu)} G_{\mathbf{b}_2 \mathbf{b}_1} \tilde{f}_{\nu}(G_{\mathbf{b}_2 \mathbf{b}_2}) \\ &\quad + \sum_{\mu} \mathcal{B}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)} g_{\mu}(G_{\mathbf{b}_1 \mathbf{b}_1}, G_{\mathbf{b}_2 \mathbf{b}_2}, \bar{G}_{\mathbf{b}_1 \mathbf{b}_2}, G_{\mathbf{b}_2 \mathbf{b}_1}) + \mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} + \text{Err}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}. \end{aligned} \quad (9.10)$$

The graphs on the right-hand side depend on n , D , W and L directly, and satisfy the following properties.

- (i) $\text{Err}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is an error term satisfying $\text{Err}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} \prec W^{-D}$.
- (ii) $B_{\mathbf{a} \mathbf{b}_1}^{(\mu)}$ and $\tilde{B}_{\mathbf{a} \mathbf{b}_2}^{(\nu)}$ are deterministic graphs satisfying

$$|B_{\mathbf{a} \mathbf{b}_1}^{(\mu)}| \prec W^{-c_1} B_{\mathbf{a} \mathbf{b}_1}, \quad |\tilde{B}_{\mathbf{a} \mathbf{b}_2}^{(\nu)}| \prec W^{-c_1} B_{\mathbf{a} \mathbf{b}_2}, \quad (9.11)$$

under the condition (3.15), where $c_1 := \min(c_0, d/2)$.

(iii) $\mathcal{B}_{\mathbf{ab}_1}^{(\mu)}$ are deterministic graphs of the form $\sum_x \widehat{B}_{\mathbf{ax}}^{(\mu)} \mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)}$, where $\widehat{B}_{\mathbf{ax}}^{(\mu)}$ satisfies

$$|\widehat{B}_{\mathbf{ax}}^{(\mu)}| \prec B_{\mathbf{ax}}, \quad (9.12)$$

and $\mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)}$ is doubly connected with x, \mathbf{b}_1 and \mathbf{b}_2 regarded as internal atoms and satisfies

$$\text{ord}(\mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)}) \geq k_{\text{gh}}(\mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)}) \cdot (n-1) + 2. \quad (9.13)$$

Here $k_{\text{gh}}(\mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)})$ denotes the number of ghost edges in $\mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)}$.

(iv) f_μ are monomials of $G_{\mathbf{b}_1 \mathbf{b}_1}$ and $\overline{G}_{\mathbf{b}_1 \mathbf{b}_1}$, \tilde{f}_ν are monomials of $G_{\mathbf{b}_2 \mathbf{b}_2}$ and $\overline{G}_{\mathbf{b}_2 \mathbf{b}_2}$, and g_μ are monomials of $G_{\mathbf{b}_1 \mathbf{b}_1}$, $\overline{G}_{\mathbf{b}_1 \mathbf{b}_1}$, $G_{\mathbf{b}_2 \mathbf{b}_2}$, $\overline{G}_{\mathbf{b}_2 \mathbf{b}_2}$, $\overline{G}_{\mathbf{b}_1 \mathbf{b}_2}$ and $G_{\mathbf{b}_2 \mathbf{b}_1}$.

(v) $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a sum of $O(1)$ many Q -graphs, denoted by $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}$, satisfying the following properties.

(a) $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}$ is a generalized SPD graph.

(b) The atom in the Q -label of $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}$ belongs to the MIS with non-deterministic closure, denoted by \mathcal{I}_{min} . In other words, we can write that

$$\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)} = \left(\frac{L^2}{W^2} \right)^{k_{\text{gh}}(\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)})} \sum_{\alpha} Q_{\alpha}(\Gamma^{(\omega)}),$$

where $k_{\text{gh}}(\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)})$ denotes the number of ghost edges in $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}$, $\Gamma^{(\omega)}$ is a graph without P/Q labels, and the internal atom α is inside \mathcal{I}_{min} .

(c) The scaling order of $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}$ satisfies that

$$\text{ord}(\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}) \geq k_{\text{gh}}(\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}) \cdot (n-1) + 2. \quad (9.14)$$

(vi) Each $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}^{(\omega)}$ has a deterministic graph $\mathcal{B}_{\mathbf{ax}}^{(\omega)}$ between \otimes and an internal atom x , where $\mathcal{B}_{\mathbf{ax}}^{(\omega)}$ satisfies

$$|\mathcal{B}_{\mathbf{ax}}^{(\omega)}| \prec B_{\mathbf{ax}}. \quad (9.15)$$

Moreover, there is at least an edge, which is either blue solid or diffusive or dotted, connected to \oplus , and there is at least an edge, which is either red solid or diffusive or dotted, connected to \ominus .

To prove Lemma 9.7, we start with the n -th order T -expansion (3.1). The term $m(\Theta \Sigma_T^{(n)} \Theta)_{\mathbf{ab}_1} \overline{G}_{\mathbf{b}_1 \mathbf{b}_2}$ can be included into the second term on the right-hand side of (9.10), $(\mathcal{Q}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be included into $\mathcal{Q}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, and $(\mathcal{E}rr_{n,D})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be included into $\mathcal{E}rr_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$. It remains to expand the graphs in $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$. We again use the Strategy 6.6, but with some modifications to handle the ghost edges and to keep track of the scaling order of every graph (see Strategy 9.8 below).

To describe the expansion strategy, we now define the stopping rules. Given a graph \mathcal{G} , we define

$$\text{size}(\mathcal{G}) := \left(\frac{L^2}{W^2} \right)^{k_{\text{gh}}(\mathcal{G})} W^{-\text{ord}(\mathcal{G}) \cdot d/2}, \quad (9.16)$$

where $k_{\text{gh}}(\mathcal{G})$ denotes the number of ghost edges in \mathcal{G} . By Lemma 9.5, we have $|\mathcal{G}| \prec \text{size}(\mathcal{G})$ if \mathcal{G} is doubly connected with ghost edges. Given the large constant D in Lemma 9.7, we stop expanding a graph \mathcal{G} if it is normal regular and satisfies at least one of the following properties:

(T1) \mathcal{G} has a deterministic maximal subgraph that is locally standard (i.e. if there is an internal atom connected with external edges, it must be standard neutral);

(T2) $\text{size}(\mathcal{G}) \leq W^{-D}$;

(T3) \mathcal{G} is a Q -graph.

Then, similar to Strategy 6.6, the core of the expansion strategy for the proof of Lemma 9.7 is still to expand the plus G edges according to a pre-deterministic order in the MIS with non-deterministic closure. However, there is a key difference that we have to expand a pivotal blue solid edge connected with an isolated subgraph at a certain step. To deal with this issue, we add a ghost edge between the ending atoms of the pivotal edge which we want to expand. Then this blue solid edge becomes redundant, and we can expand it in the same way as Step 3 of Strategy 6.6. However, we need to make sure that every graph, say \mathcal{G} , from the expansion has a scaling order satisfying

$$\text{ord}(\mathcal{G}) \geq (n-1) \cdot k_{\text{gh}}(\mathcal{G}) + 2.$$

Now we define the following expansion strategy.

Strategy 9.8. Given a large constant $D > 0$ and a generalized SPD graph \mathcal{G} without P/Q labels, we perform one step of expansion as follows. Let \mathcal{I}_k be the MIS with non-deterministic closure.

Case 1: If \mathcal{I}_k is not locally standard, then we perform the local expansions in Definitions 4.3, 4.4, 4.5 and 4.6 on an atom in \mathcal{I}_k . We send the resulting graphs that already satisfy the stopping rules (T1)–(T3) to the outputs. Every remaining graph has a locally standard MIS with non-deterministic closure and satisfies the generalized SPD property by Lemma 5.10.

Case 2: Suppose \mathcal{I}_k is locally standard. We find a t_{x,y_1y_2} or $t_{y_1y_2,x}$ variable defined in (4.14), so that α is a standard neutral atom in \mathcal{I}_k and the edge $G_{\alpha y_1}$ or $G_{y_1 \alpha}$ is the first blue solid edge in a pre-deterministic order of \mathcal{I}_k . Then we apply the expansion in Step 3 of Strategy 6.6 (except that we will use (4.15) with $n-1$ replaced by n).

Case 3: Suppose \mathcal{I}_k is deterministic, strongly isolated in \mathcal{I}_{k-1} (cf. Definition 6.1), and locally standard. (In other words, \mathcal{I}_k contains a standard neutral atom connected with two external blue and red solid edges.) Suppose b_1 is the edge $G_{\alpha y_1}$ or $G_{y_1 \alpha}$ in (4.14), with α being the standard neutral atom in \mathcal{I}_k . We add a ghost edge between α and y_1 and multiply the graph by L^2/W^2 . In the resulting graph, the edge b_1 becomes redundant if we include the newly added ghost edge into the blue net. Then we apply the expansion in Step 3 of Strategy 6.6 (except that we will use (4.15) with $n-1$ replaced by n). We will show that each Q -graph from this expansion satisfies the property (v) of Lemma 9.7, and each non- Q graph, say \mathcal{G}' , satisfies

$$\text{ord}(\mathcal{G}') \geq (n-1) \cdot k_{\text{gh}}(\mathcal{G}') + 2,$$

so that $\text{size}(\mathcal{G}')$ is under control.

We will show that by applying the Strategy 9.8 repeatedly until all graphs satisfy the stopping rules (T1)–(T3), we can obtain the expansion (9.10). For this purpose, we define the *generalized globally standard property*, extending the globally standard property in Definition 6.2.

Definition 9.9 (Generalized globally standard graphs). *We say a graph \mathcal{G} is generalized globally standard (GGs) if it is a generalized SPD graph and satisfies at least one of the following properties.*

(A) \mathcal{G} satisfies

$$\text{ord}(\mathcal{G}) \geq (n-1) \cdot [k_{\text{gh}}(\mathcal{G}) + 1] + 2. \quad (9.17)$$

(B) \mathcal{G} satisfies

$$\text{ord}(\mathcal{G}) \geq (n-1) \cdot k_{\text{gh}}(\mathcal{G}) + 2. \quad (9.18)$$

Let \mathcal{I}_k be the minimal strongly isolated subgraph with non-deterministic closure. (In other words, \mathcal{I}_k may contain weakly isolated subgraphs, but a strongly isolated subgraph of \mathcal{I}_k must have a deterministic closure.) There exists a ghost edge, say g_0 , inside \mathcal{I}_k such that the following property holds.

(B1) *Let \mathcal{I}' be the minimal isolated subgraph of \mathcal{I}_k that contains g_0 . (\mathcal{I}' can be \mathcal{I}_k if g_0 is not inside any proper isolated subgraph of \mathcal{I}_k .) If we replace the closure of the maximal proper isolated subgraph of \mathcal{I}' and all other blue solid edges in \mathcal{I}' with diffusive edges, then g_0 becomes redundant.*

Similar to the proof of Theorem 3.7 in Section 6, Lemma 9.7 follows from the following two observations:

- if the input graph is GGS, then after one step of expansion in Strategy 9.8, all the resulting non- Q graphs are still GGS and all the Q -graphs satisfy property (v) of Lemma 9.7;
- the expansion of T_{a,b_1b_2} will stop after $O(1)$ many iterations of Strategy 9.8.

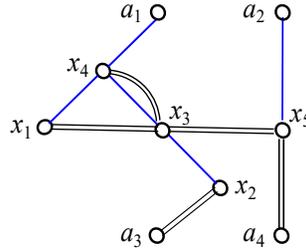
We postpone the detailed proof of Lemma 9.7 to Appendix B.

9.3 Generalized doubly connected property

In this subsection, we develop another tool for the proof of Lemma 9.1, that is, a *generalized doubly connected property* of graphs with external atoms, which extends the doubly connected property in Definition 2.12.

Definition 9.10 (Generalized doubly connected property). *A graph \mathcal{G} with external molecules is said to be generalized doubly connected if its molecular graph satisfies the following property. There exist a collection, say \mathcal{B}_{black} , of diffusive edges, and another collection, say \mathcal{B}_{blue} , of blue solid, diffusive or ghost edges such that: (a) $\mathcal{B}_{black} \cap \mathcal{B}_{blue} = \emptyset$, (b) every internal molecule connects to external molecules through two disjoint paths: a path of edges in \mathcal{B}_{black} and a path of edges in \mathcal{B}_{blue} .*

Given a generalized doubly connected graph \mathcal{G} , after removing its external molecules we *may not* get a doubly connected graph in the sense of Definition 2.12 (i.e., the maximal subgraph of \mathcal{G} consisting of internal molecules may not have a black net and a blue net). For example, the following graph is a generalized doubly connected graph with external molecules a_1, a_2, a_3, a_4 , and internal molecules x_1, x_2, x_3, x_4, x_5 , but it is not doubly connected.



However, by Definition 9.10, if we merge all external molecules in a generalized doubly connected graph into a single internal molecule, then we will get a doubly connected graph in the sense of Definition 2.12.

Generalized doubly connected graphs satisfy the following bound.

Lemma 9.11. *Under the assumptions of Lemma 7.3, let \mathcal{G} be a generalized doubly connected normal regular graph. Then it satisfies the bound*

$$|\mathcal{G}| \prec \left(\frac{L^2}{W^2} \right)^{k_{gh}(\mathcal{G})} W^{-\text{ord}(\mathcal{G}) \cdot d/2}. \quad (9.19)$$

Proof. The proof of this lemma is similar to the one for Lemma 9.3. With the generalized doubly connected property of \mathcal{G} , we can choose disjoint black spanning trees and blue spanning trees with external molecules so that each internal molecule connects to an external molecule through a *unique black path* on a black tree, and to an external molecule through a *unique blue path* on a blue tree. We can again reduce the problem to bounding an auxiliary graph \mathcal{G}_{aux} consisting of these black and blue trees. Then we sum over the internal atoms in \mathcal{G}_{aux} from leaves of the blue trees to the roots of them. We bound the summation over each internal atom using (8.10) with $(a, b) = (1, 1)$ (if the blue edge in the summation is bounded by a $B^{1/2}$ entry), or (9.8) (if the blue edge in the summation is bounded by W^2/L^2). After each summation, we get a sum of new graphs that are still generalized doubly connected. Finally, after summing over all internal atoms, we get the bound (9.19). We omit the details of the proof. \square

The following lemma will be used in the proof of Lemma 9.1. It bounds the average of a deterministic generalized doubly connected graph over its external molecules in the box \mathcal{I} .

Lemma 9.12. *Under the assumptions of Lemma 7.3, let \mathcal{G} be a deterministic generalized doubly connected normal regular graph with $2p$ external atoms \mathbf{a}_i , $1 \leq i \leq 2p$. Moreover, suppose \mathcal{G} is a connected graph in the sense that all molecules (including both internal and external molecules) are connected to each other. Finally, suppose all ghost edges are between internal atoms. Then we have that*

$$\frac{1}{(K^d)^{2p}} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{2p} \in \mathcal{I}} |\mathcal{G}(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{2p})| \prec \left(\frac{W^{d-4}}{K^{d-4}} \right)^{2p-1} \cdot \left(\frac{L^2}{W^2} \right)^{k_{gh}(\mathcal{G})} W^{-\text{ord}(\mathcal{G}) \cdot d/2}, \quad (9.20)$$

where recall that $\mathcal{I} = \{y : |y - x_0| \leq K\}$ for some $x_0 \in \mathbb{Z}_L^d$. We emphasize that in calculating $\text{ord}(\mathcal{G})$, \mathbf{a}_i , $1 \leq i \leq 2p$, are still treated as external atoms, regardless of the sum $\sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{2p}}$.

Proof. We can assume that there are no dotted edges in \mathcal{G} . Otherwise, we merge the atoms connected by dotted edges and still get a graph satisfying the assumption of this lemma and with at most $2p$ external atoms (there may be dotted edges between external atoms, so after the merging operation the graph may contain strictly fewer external atoms). Without loss of generality, we assume that the external atoms are \mathbf{a}_i , $1 \leq i \leq q$, for some $1 \leq q \leq 2p$. Moreover, we can simply pick out the $(L^2/W^2)^{k_{\text{gh}}(\mathcal{G})}$ factor in the coefficient of \mathcal{G} and do not keep it in our proof.

Following the argument in the proof of Claim 8.6, we again reduce the problem to bounding a generalized doubly connected auxiliary graph \mathcal{G}_{aux} obtained as follows. \mathcal{G}_{aux} has a set of external atoms, say $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q$, and a set of internal atoms, say x_1, x_2, \dots, x_ℓ , which are the representative atoms of the internal molecules. Every diffusive edge between different molecules of \mathcal{G} is replaced by a double-line edge representing a B factor in \mathcal{G}_{aux} . Every ghost edge in \mathcal{G} is still a ghost edge representing a W^2/L^2 factor in \mathcal{G}_{aux} . To conclude the proof, it suffices to prove that

$$\frac{1}{(K^d)^{2p}} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q \in \mathcal{I}_K} |\mathcal{G}_{aux}(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q)| \prec \left(\frac{W^{d-4}}{K^{d-4}} \right)^{2p-1} W^{-\text{ord}(\mathcal{G}_{aux}) \cdot d/2}, \quad (9.21)$$

where $\text{ord}(\mathcal{G}_{aux})$ is defined by

$$\text{ord}(\mathcal{G}_{aux}) := 2\#\{\text{double-line edges}\} - 2\#\{\text{internal atoms}\}.$$

With the generalized doubly connected property of \mathcal{G}_{aux} , we can choose a collection of blue trees such that every internal atom connects to an external atom through a *unique path* on a blue tree. These blue trees are disjoint, and each of them contains an external atom as the root. Then we sum over the internal atoms from leaves of the blue trees to the roots until each blue tree has only one internal atom that is connected to the root. We bound the summation over each internal atom using estimates

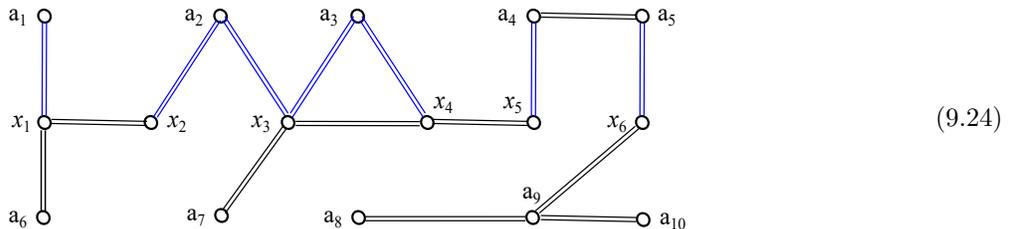
$$\sum_{x_i} B_{x_i \beta} \cdot \prod_{i=1}^k B_{x_i y_i} \prec W^{-d} \Gamma(y_1, \dots, y_k), \quad \sum_{x_i} \frac{W^2}{L^2} \prod_{i=1}^k B_{x_i y_i} \prec \Gamma(y_1, \dots, y_k), \quad (9.22)$$

which follow from (8.10) with $(a, b) = (2, 2)$ and (9.8). Here $B_{x_i \beta}$ and W^2/L^2 respectively represent a double-line edge and a ghost edge in the blue tree, and $B_{x_i y_1}, \dots, B_{x_i y_k}$ are other double-line edges connected to x_i (we always have $k \geq 1$ because of the generalized doubly connected property of \mathcal{G}_{aux}). It is not hard to check that after each summation, we get a sum of new graphs that are generalized doubly connected and whose atoms are all connected to each other. Finally, we will get a linear combination of graphs where each blue tree in them contains only one internal atom that is connected to an external atom through a blue double-line edge.

In sum, using the above argument, we can bound \mathcal{G}_{aux} by a linear combination of deterministic graphs:

$$\mathcal{G}_{aux} \prec \sum_{\omega} W^{-\Delta_{\kappa} d/2} \mathcal{G}_{\omega, aux}, \quad \Delta_{\kappa} := \text{ord}(\mathcal{G}_{aux}) - \text{ord}(\mathcal{G}_{\omega, aux}). \quad (9.23)$$

Every $\mathcal{G}_{\omega, aux}$ satisfies the following properties: (a) $\mathcal{G}_{\omega, aux}$ is a *connected* graph consisting of double-line edges only, (b) $\mathcal{G}_{\omega, aux}$ is generalized doubly connected, and (c) each internal atom in $\mathcal{G}_{\omega, aux}$ is connected with at least one external atom through a double-line edge in the blue net. Here we give such an example with 10 external atoms \mathbf{a}_i , $1 \leq i \leq 10$, and 6 internal atoms x_i , $1 \leq i \leq 6$:



Now we sum over the internal atoms in $\mathcal{G}_{\omega, aux}$. We introduce a new type of purple solid edges: a purple solid edge between atoms α and β represents a $\bar{B}_{\alpha\beta} = W^{-4} \langle \alpha - \beta \rangle^{-(d-4)}$ factor. Purple solid edges are not

included into either the black net or the blue net. We will use the following estimate, which can be proved with basic calculus: if $k \geq 1$ and $r \geq 0$, we have

$$\begin{aligned} \sum_{x_i} \prod_{j=1}^k B_{x_i y_j} \cdot \prod_{s=1}^r \tilde{B}_{x_i z_s} \cdot B_{x_i \mathbf{a}} &\lesssim \prod_{j=2}^k B_{y_j \mathbf{a}} \cdot \left(\tilde{B}_{y_1 \mathbf{a}} \prod_{s=1}^r \tilde{B}_{z_s \mathbf{a}} \right) \\ &+ \sum_{l=1}^k \prod_{j:j \neq l} B_{y_j y_l} \cdot \left(\tilde{B}_{y_l \mathbf{a}} \prod_{s=1}^r \tilde{B}_{z_s y_l} \right) + \sum_{t=1}^r \prod_{j=2}^k B_{y_j z_t} \cdot \left(\tilde{B}_{y_1 z_t} \tilde{B}_{z_t \mathbf{a}} \prod_{s:s \neq t} \tilde{B}_{z_s z_t} \right). \end{aligned} \quad (9.25)$$

Note that the left-hand side is a star graph consisting of $k + 1$ double-line edges and r purple solid edges connected with x_i , while each graph on the right-hand side is a star graph consisting of $k - 1$ double-line edges and $r + 1$ purple solid edges connected with \mathbf{a} , y_l or z_t .

Now we use (9.25) to bound the sums over the internal atoms in $\mathcal{G}_{\omega, aux}$. We choose a collection of black trees such that each internal atom connects to an external atom through a *unique path* on a black tree. These black trees are disjoint, and each of them contains an external atom as the root. Then we sum over the internal atoms from leaves of the black trees to the roots. First, suppose x_1 is a leaf of a black tree. Then using (9.25), we can bound the summation over x_1 by a sum of new graphs, each of which satisfies the following properties:

- (i) it is a connected graph consisting of double-line edges and purple solid edges;
- (ii) it is generalized doubly connected;
- (iii) every internal atom is connected with at least one external atom through a blue double-line edge.

In every new graph, we again find a leaf of a black tree, and bound the sum over it using (9.25). More precisely, when we sum over x_i , x_i is a leaf of a black tree, y_1 is the parent of x_i on this tree, $B_{x_i \mathbf{a}}$ is a blue double-line edge connecting x_i to an external atom \mathbf{a} , $B_{y_j x_i}$, $2 \leq j \leq k$, are the remaining double-line edges connected with x_i , and the purple solid edges connected with z_1, \dots, z_r are the edges coming from previous sums over internal atoms. In this way, we can bound the summation over x_i by a sum of new graphs satisfying the above properties (i)–(iii). Finally, after summing over all internal atoms, we obtain that

$$\mathcal{G}_{\omega, aux} \prec \sum_{\gamma} \mathcal{G}_{\omega, \gamma, aux}, \quad (9.26)$$

where every $\mathcal{G}_{\omega, \gamma, aux}$ is a connected graph consisting of external atoms $\mathbf{a}_1, \dots, \mathbf{a}_q$, and double-line and purple solid edges. Since $\mathcal{G}_{\omega, \gamma, aux}$ only contains external atoms, its scaling order is

$$\text{ord}(\mathcal{G}_{\omega, \gamma, aux}) = 2\#\{\text{diffusive and purple solid edges in } \mathcal{G}_{\omega, \gamma, aux}\} = \text{ord}(\mathcal{G}_{\omega, aux}). \quad (9.27)$$

Finally, it remains to bound

$$\frac{1}{(K^d)^{2p}} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q \in \mathcal{I}} \mathcal{G}_{\omega, \gamma, aux}(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q).$$

We perform the summations according to the order $\sum_{\mathbf{a}_q} \dots \sum_{\mathbf{a}_2} \sum_{\mathbf{a}_1}$, and we use the following estimate to bound each average:

$$\frac{1}{K^d} \sum_{\mathbf{a}_i \in \mathcal{I}} \prod_{j=1}^k \tilde{B}_{y_j \mathbf{a}_i} \lesssim \frac{1}{W^4 K^{d-4}} \sum_{l=1}^k \prod_{j:j \neq l} \tilde{B}_{y_l y_j} = W^{-d} \cdot \frac{W^{d-4}}{K^{d-4}} \sum_{l=1}^k \prod_{j \neq l} \tilde{B}_{y_l y_j}.$$

This estimate shows that we can bound each average by a sum of new connected graphs with one fewer atom and one fewer edge, while gaining an extra factor $W^{-4} K^{-(d-4)}$. After taking averages over $\mathbf{a}_1, \dots, \mathbf{a}_{q-2}$, we obtain a graph $(\tilde{B}_{\mathbf{a}_{q-1} \mathbf{a}_q})^k$ with

$$k := \text{ord}(\mathcal{G}_{\omega, \gamma, aux}) / 2 - (q - 2).$$

Its average over \mathbf{a}_{q-1} can be bounded by

$$\frac{1}{K^d} \sum_{\mathbf{a}_{q-1} \in \mathcal{I}} (\tilde{B}_{\mathbf{a}_{q-1} \mathbf{a}_q})^k \lesssim W^{-kd} \frac{W^{d-4}}{K^{d-4}}.$$

Finally, the average over \mathbf{a}_q is equal to 1. In sum, we get that

$$\frac{1}{(K^d)^{2p}} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q \in \mathcal{I}} \mathcal{G}_{\omega, \gamma, aux}(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q) \prec \left(\frac{1}{K^d}\right)^{2p-q} \left(\frac{W^{d-4}}{K^{d-4}}\right)^{q-1} W^{-\text{ord}(\mathcal{G}_{\omega, \gamma, aux}) \cdot d/2}. \quad (9.28)$$

Plugging this estimate into (9.26) and further into (9.23), we obtain (9.21), which concludes (9.20). \square

9.4 Proof of Lemma 9.1

In this subsection, we complete the proof of Lemma 9.1. Using (9.1), we can expand $\mathbb{E} \text{Tr}(A^{2p})$ as

$$\mathbb{E} \text{Tr}(A^{2p}) = \sum_{\mathbf{a}_1, \dots, \mathbf{a}_{2p} \in \mathcal{I}} \sum_{s_1, \dots, s_{2p} \in \{+, -\}} c(s_1, \dots, s_{2p}) \prod_{i=1}^{2p} G_{\mathbf{a}_i \mathbf{a}_{i+1}}^{s_i}, \quad (9.29)$$

where as a convention we let $\mathbf{a}_{2p+1} := \mathbf{a}_1$, $c(s_1, \dots, s_{2p})$ is a deterministic coefficient of order $O(1)$, and s_i , $i = 1, \dots, 2p$, denote \pm signs. Here we adopted the notations

$$G_{xy}^+ := G_{xy}, \quad G_{xy}^- := \bar{G}_{xy}.$$

Thus to conclude (9.5), it suffices to prove that for any $2p$ -gon graph

$$\mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}} \equiv \mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}(s_1, \dots, s_{2p}) := \prod_{i=1}^{2p} G_{\mathbf{a}_i \mathbf{a}_{i+1}}^{s_i}, \quad (9.30)$$

we have

$$\sum_{\mathbf{a}_1, \dots, \mathbf{a}_{2p} \in \mathcal{I}} \mathbb{E} \mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}} \leq K^d \left(W^\varepsilon \frac{K^4}{W^4} \right)^{2p-1}, \quad (9.31)$$

for any small constant $\varepsilon > 0$. The proof of (9.31) is based on the results in Sections 9.2 and 9.3: we first use Lemma 9.7 to expand $\mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}$ into a sum of deterministic generalized doubly connected graphs, and then use Lemma 9.12 to bound each of them.

Because of the estimates (9.11), (9.12) and (9.15), it is more natural to treat graphs $B^{(\mu)}$, $\tilde{B}^{(\nu)}$, $\hat{B}^{(\mu)}$ and $\mathcal{B}^{(\omega)}$ in Lemma 9.7 as new types of diffusive edges in the following proof. It is not hard to see that Lemma 9.11 and Lemma 9.12 still hold for generalized doubly connected graphs containing these new diffusive edges, as long as we replace the factor $(L^2/W^2)^{k_{\text{gb}}(\mathcal{G})} W^{-\text{ord}(\mathcal{G}) \cdot d/2}$ by $\text{size}(\mathcal{G})$ defined in (9.16).

Corresponding to Definition 9.10, we can extend the generalized SPD property in Definition 9.6 and the globally standard property in Definition 6.2 as follows.

Definition 9.13. (i) A graph \mathcal{G} is said to satisfy the **generalized SPD property with external molecules** if, after merging all external molecules of \mathcal{G} into one single internal molecule, the resulting molecular graph satisfies Definition 9.6.

(ii) A graph \mathcal{G} is said to be **globally standard with external molecules** if it is generalized SPD with external molecules in the above sense, and every proper isolated subgraph with non-deterministic closure is weakly isolated.

It is easy to see that Lemma 9.1 is an immediate consequence of the following lemma.

Lemma 9.14. Suppose the assumptions of Lemma 7.3 hold. Then for any large constant $D > 0$, a $2p$ -gon graph in (9.30) can be expanded as

$$\mathbb{E} \mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}} = \sum_{\omega} \mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}^{(\omega)} + O_{\prec}(W^{-D}), \quad (9.32)$$

where the first term on the right-hand side is a sum of $O(1)$ many deterministic graphs $\mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}^{(\omega)}$ satisfying the assumptions of Lemma 9.12. In particular, they satisfy the estimate

$$\frac{1}{(K^d)^{2p}} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{2p} \in \mathcal{I}} \mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}^{(\omega)} \prec \left(\frac{1}{W^4 K^{d-4}} \right)^{2p-1}. \quad (9.33)$$

Proof. The expansion (9.32) can be obtained by applying Strategy 6.6 with the following modifications:

- (i) we will use the non-universal T -expansion (9.10) instead of the n -th order T -expansion;
- (ii) we will use the globally standard property with external molecules defined in Definition 9.13;
- (iii) we will stop the expansion of a graph if it is deterministic, its size is less than W^{-D} or it is a Q -graph.

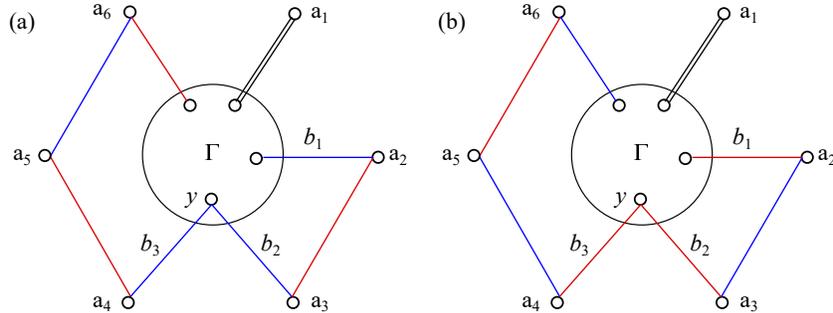
The proof is actually easier than that for Theorem 3.7, because the non-universal T -expansion takes a simpler form with only two types of graphs: graphs with deterministic maximal subgraphs and Q -graphs. Moreover, Q -graphs from the expansion of $\mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}$ will vanish after taking expectation, so we do not need to keep them. We now give more details.

First, we apply local expansions to $\mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}$ to get a linear combination of locally standard graphs without P/Q labels. The new atoms generated in this process are all included into the external molecules around \mathbf{a}_i , $1 \leq i \leq 2p$. Then we pick any $t_{x, y_1 y_2}$ variable in one of the new graphs, say $\tilde{\mathcal{G}}$, and replace it with the non-universal T -expansion (9.10):

$$\begin{aligned}
 t_{x, y_1 y_2} = & m\Theta_{xy_1} \bar{G}_{y_1 y_2} + \sum_{\mu} B_{xy_1}^{(\mu)} \bar{G}_{y_1 y_2} f_{\mu}(G_{y_1 y_1}) + \sum_{\nu} \tilde{B}_{xy_2}^{(\nu)} G_{y_2 y_1} \tilde{f}_{\nu}(G_{y_2 y_2}) \\
 & + \sum_{\mu} \mathcal{B}_{x, y_1 y_2}^{(\mu)} g_{\mu}(G_{y_1 y_1}, G_{y_2 y_2}, \bar{G}_{y_1 y_2}, G_{y_2 y_1}) + \mathcal{Q}_{x, y_1 y_2} + \mathcal{E}rr_{x, y_1 y_2}.
 \end{aligned} \tag{9.34}$$

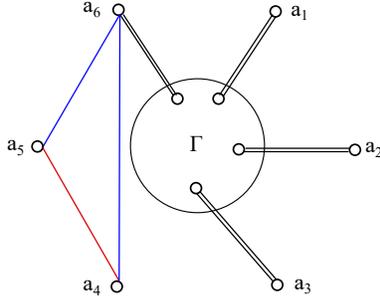
Here we again include the graphs containing $t_{x, y_1 y_2} - T_{x, y_1 y_2}$ into the second and third terms on the right-hand side of (9.34) (where we abuse the notation a little bit). If we replace $t_{x, y_1 y_2}$ with a graph in the first four terms on the right-hand side of (9.34), then we will get a generalized doubly connected graph which either does not contain any internal molecule or has a deterministic maximal subgraph. Moreover, the new graph either has one fewer blue solid edge or is of smaller size than $\text{size}(\tilde{\mathcal{G}})$ by a factor W^{-c_1} . If we replace $t_{x, y_1 y_2}$ with a graph in $\mathcal{E}rr_{x, y_1 y_2}$, then the new graph is of size $\leq W^{-D}$.

Now suppose we replace $t_{x, y_1 y_2}$ in $\tilde{\mathcal{G}}$ with a Q -graph in $\mathcal{Q}_{x, y_1 y_2}$ and apply the Q -expansions. Then by Lemma 6.5, the resulting non- Q graphs are globally standard with external molecules in the sense of Definition 9.13. Here we draw two examples of such molecular graphs with $2p = 6$:



Inside the black circle is a subgraph containing all internal molecules, and y is the atom in the label of the Q -graph (where we used y to label the molecule containing it). Graph (a) does not contain any isolated subgraph with non-deterministic closure and has a pre-deterministic order: internal blue solid edges $\preceq b_1 \preceq b_2 \preceq b_3$. Graph (b) may contain isolated subgraphs with non-deterministic closures, but they are weakly isolated due to the two red solid edges b_2 and b_3 connected with y . Now for each resulting graph from Q -expansions, we either perform local expansions on atoms in the MIS as in Step 1 of Strategy 6.6, or expand the first blue solid edge in a pre-deterministic order of the MIS with non-deterministic closure as in Step 3 of Strategy 6.6 by plugging into the non-universal T -expansion.

Continuing the expansions, we will get a sum of graphs that are generalized doubly connected with external molecules, and whose internal molecules are only connected with deterministic edges. In other words, all the G edges are inside or between external molecules as in the following example:



Now we repeat the previous expansions, that is, we first apply local expansions and then pick any t_{x,y_1y_2} variable to expand using (9.34). This may generate a new subset of internal molecules. Again we will apply Strategy 6.6 to the resulting graphs. Notice that since the old internal molecules are connected only with deterministic edges, they will not be affected in the rest of the expansion process.

After each step of expansion, all non- Q graphs satisfy the following properties: it is generalized doubly connected, all molecules are connected together, and all ghost edges are between internal atoms. Our expansions will stop when every graph is deterministic, of size $\leq W^{-D}$, or a Q -graph. Then taking expectation gives (9.32) with deterministic graphs $\mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}^{(\omega)}$ satisfying the assumptions of Lemma 9.12. Notice that throughout the expansion process, the number of ghost edges in each graph (including $\mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}^{(\omega)}$) are under control due to the conditions (9.13) and (9.14). Now repeating the proof of Lemma 9.12, we can bound that

$$\frac{1}{(K^d)^{2p}} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_{2p} \in \mathcal{I}} \mathcal{G}_{\mathbf{a}_1, \dots, \mathbf{a}_{2p}}^{(\omega)} \prec \frac{1}{(K^d)^{2p}} \sum_{q=1}^{2p} \sum_{\omega, \gamma} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q \in \mathcal{I}} \mathcal{G}_{\omega, \gamma, aux}(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q), \quad (9.35)$$

where we followed the notation in (9.26): $\mathcal{G}_{\omega, \gamma, aux}$ are connected graphs consisting of external atoms $\mathbf{a}_1, \dots, \mathbf{a}_q$, and double-line and purple solid edges. Using (9.28) and the fact

$$\text{ord}(\mathcal{G}_{\omega, \gamma, aux}) = 2\#\{\text{diffusive and purple solid edges in } \mathcal{G}_{\omega, \gamma, aux}\} \geq 2(q-1),$$

we get that

$$\frac{1}{(K^d)^{2p}} \sum_{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q \in \mathcal{I}} \mathcal{G}_{\omega, \gamma, aux}(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_q) \prec \left(\frac{1}{K^d}\right)^{2p-q} \left(\frac{W^{d-4}}{K^{d-4}}\right)^{q-1} W^{-(q-1)d}.$$

Plugging it into (9.35), we conclude (9.33). \square

A PROOF OF LEMMA 5.11 AND LEMMA 5.12

All graphs in this section are *molecular graphs without red solid edges*. We will say a diffusive edge is black (resp. blue) if this edge is used in the black (resp. blue) net. In the proof, whenever we say “we can change a blue solid edge into a diffusive edge”, we actually mean “this edge is redundant and hence we can change it into a diffusive edge”. Thus showing a subgraph is pre-deterministic is equivalent to showing that “we can change the blue solid edges in this subgraph into diffusive edges one by one”.

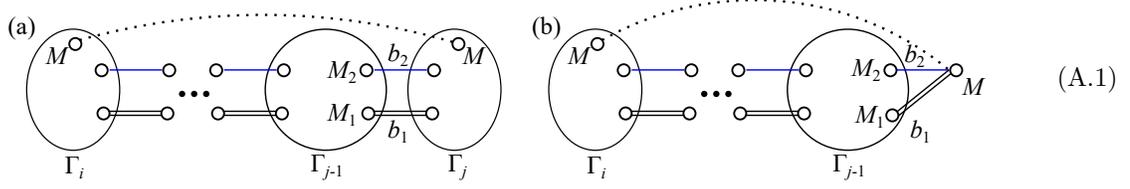
First, we state the following two claims, whose proofs are trivial.

Claim A.1. *Given a graph \mathcal{G} , let \mathcal{S} be a subset of molecules such that the subgraph induced on \mathcal{S} is doubly connected. Then \mathcal{G} is doubly connected if and only if the following quotient graph \mathcal{G}/\mathcal{S} is doubly connected: \mathcal{G}/\mathcal{S} is obtained by treating the subset of molecules \mathcal{S} as one single vertex, and the edges connected with \mathcal{S} in \mathcal{G} are now connected with this vertex \mathcal{S} in \mathcal{G}/\mathcal{S} .*

Claim A.2. *Suppose a blue solid edge b_0 is redundant in a doubly connected graph \mathcal{G} . We replace a diffusive edge b between two molecules \mathcal{M}_1 and \mathcal{M}_2 with a path of two diffusive edges: b_1 from \mathcal{M}_1 to another molecule \mathcal{M} , and b_2 from \mathcal{M} to \mathcal{M}_2 . Then the edge b_0 is still redundant in the new graph.*

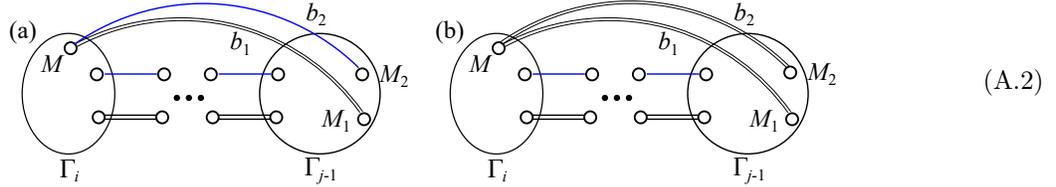
Now Lemma 5.11 follows from repeated applications of the above two claims.

Proof of Lemma 5.11. We replace \mathcal{I}_{j+1} and its two external edges with a black diffusive edge, and get the following graph (a) for \mathcal{I}_i :



Here we keep the names Γ_l , $i \leq l \leq j$, for the subgraph components inside the black circles. We also keep the dotted edge between Γ_i and Γ_j in order to have a clearer comparison with the original graph without this dotted edge. In particular, the ending molecules of this dotted edge should be understood as the same molecule, denoted by \mathcal{M} .

First, by the SPD property of the original graph \mathcal{G} , we know that the component Γ_j in graph (a) of (A.1) is pre-deterministic, and hence we can change the blue solid edges in it into diffusive edges one by one according to a pre-deterministic order. By Claim A.1, graph (a) of (A.1) is equivalent (in the sense of doubly connected property) to graph (b) of (A.1) with Γ_j replaced by a vertex. Furthermore, by merging the molecules connected by the dotted edge, we get the following graph (a):



We claim that b_2 is redundant in graph (a) of (A.1). Due to the doubly connected property of the original graph \mathcal{G} , removing the subgraph \mathcal{I}_j and its two external edges still gives a doubly connected graph. Correspondingly, in graph (a) of (A.2), if we remove the edges b_1 and b_2 , we still get a doubly connected graph, so the edge b_2 is redundant. Then we can change b_2 into a diffusive edge and get graph (b) of (A.2).

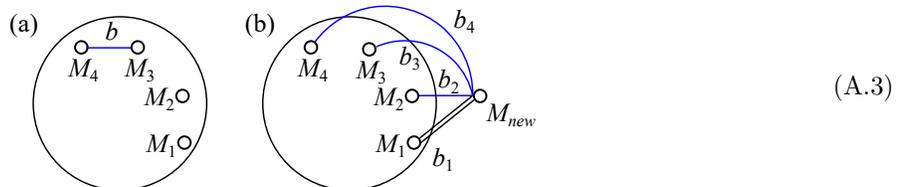
Next, by property (iii) of Definition 5.9, if we replace b_1 and b_2 with a single diffusive edge b between \mathcal{M}_1 and \mathcal{M}_2 in graph (b) of (A.2), the component Γ_{j-1} in the resulting graph becomes pre-deterministic. Then using Claim A.2, we get that the component Γ_{j-1} in graph (b) of (A.2) is pre-deterministic, and we can change the blue solid edges in it into diffusive edges one by one. After that, the subgraph induced on the molecule \mathcal{M} and the molecules in Γ_{j-1} is a doubly connected graph. Thus we can replace this subgraph with a vertex by Claim A.1 and obtain a graph with a similar structure as graph (a) of (A.2). Hence we can repeat exactly the same argument again.

Continuing in this way, we can show that the blue solid edges in \mathcal{I}_i can be changed into diffusive edges one by one according to an order given by the above argument. Hence \mathcal{I}_i is pre-deterministic. \square

The proof of the case (i) of Lemma 5.12 uses Claim A.1 and the following three claims.

Claim A.3. *Given a doubly connected graph \mathcal{G} , we construct a new graph \mathcal{G}_{new} as follows: we create a new molecule \mathcal{M}_{new} ; we add a diffusive edge b_1 between \mathcal{M}_{new} and a molecule \mathcal{M}_1 in \mathcal{G} , and a blue solid edge b_2 between \mathcal{M}_{new} and a molecule \mathcal{M}_2 in \mathcal{G} ; we replace a blue solid edge b between molecules \mathcal{M}_3 and \mathcal{M}_4 in \mathcal{G} with two blue solid edges b_3 between \mathcal{M}_3 and \mathcal{M}_{new} and b_4 between \mathcal{M}_4 and \mathcal{M}_{new} . Then the blue solid edge b_2 is redundant in \mathcal{G}_{new} .*

Proof. We illustrate the setting of this claim with the following figure, where graphs (a) and (b) represent \mathcal{G} and \mathcal{G}_{new} , respectively:



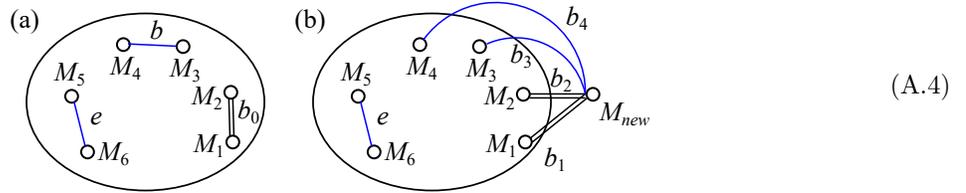
The original graph \mathcal{G} is doubly connected with black and blue nets denoted by \mathcal{B}_{black} and \mathcal{B}_{blue} . In \mathcal{G}_{new} , the edge b_1 connects the new molecule \mathcal{M}_{new} to \mathcal{M}_1 , and hence $\mathcal{B}_{black} \cup \{b_1\}$ is a black net in \mathcal{G}_{new} . Moreover, the path of edges b_3 and b_4 in \mathcal{G}_{new} can replace the role of b in the blue net \mathcal{B}_{blue} , and they also connect \mathcal{M}_{new} to the molecules in \mathcal{G} . Hence $\mathcal{B}_{blue} \cup \{b_3, b_4\} \setminus \{b\}$ is a blue net in \mathcal{G}_{new} . Since b_2 is not used in this blue net, it is redundant in \mathcal{G}_{new} . \square

Claim A.4. *Given a doubly connected graph \mathcal{G} , we construct a new graph \mathcal{G}_{new} as follows: we create a new molecule \mathcal{M}_{new} ; we replace a diffusive edge b_0 between molecules \mathcal{M}_1 and \mathcal{M}_2 in \mathcal{G} with two diffusive edges b_1 between \mathcal{M}_1 and \mathcal{M}_{new} , and b_2 between \mathcal{M}_2 and \mathcal{M}_{new} ; we replace a blue solid edge b between molecules \mathcal{M}_3 and \mathcal{M}_4 in \mathcal{G} with two blue solid edges b_3 between \mathcal{M}_3 and \mathcal{M}_{new} , and b_4 between \mathcal{M}_4 and \mathcal{M}_{new} . Then we have that:*

- (i) *If a blue solid edge is not equal to b and is redundant in \mathcal{G} , then it is also redundant in \mathcal{G}_{new} .*
- (ii) *If the edge b is redundant in \mathcal{G} , then either b_3 or b_4 is redundant. Moreover, if we change one redundant edge of them into a diffusive edge, the other edge also becomes redundant.*

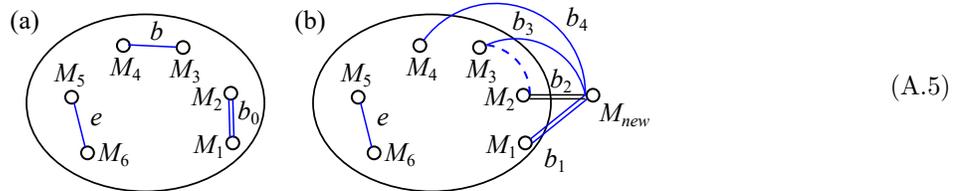
Proof. We first prove the statement (i). Suppose the redundant blue solid edge we are considering is $e = (\mathcal{M}_5, \mathcal{M}_6)$. We consider two cases: (A) the edge b_0 is included in the black net of \mathcal{G} in order for e to be redundant, and (B) the edge b_0 is included in the blue net of \mathcal{G} in order for e to be redundant.

Case (A): The graphs (a) and (b) of the following figure represent \mathcal{G} and \mathcal{G}_{new} , respectively:



In graph \mathcal{G} , the edge $e = (\mathcal{M}_5, \mathcal{M}_6)$ is redundant by putting b_0 into the black net. Let the corresponding black net and blue net be \mathcal{B}_{black} and \mathcal{B}_{blue} , such that $b_0 \in \mathcal{B}_{black}$ and $\mathcal{B}_{blue} \setminus \{e\}$ is still a blue net of \mathcal{G} . Then in \mathcal{G}_{new} , if we put edges b_1 and b_2 into the black net, they can replace the role of b_0 in the black net \mathcal{B}_{black} and also connect \mathcal{M}_{new} to other molecules. Hence $\mathcal{B}_{black} \cup \{b_1, b_2\} \setminus \{b_0\}$ is a black net in \mathcal{G}_{new} . Similarly, the path of edges b_3 and b_4 can replace the role of b in the blue net $\mathcal{B}_{blue} \setminus \{e\}$ and also connect \mathcal{M}_{new} to other molecules. Hence $\mathcal{B}_{blue} \cup \{b_3, b_4\} \setminus \{e, b\}$ is a blue net in \mathcal{G}_{new} . Since e is not used in this blue net, it is redundant in \mathcal{G}_{new} .

Case (B): The graphs (a) and (b) of the following figure represent \mathcal{G} and \mathcal{G}_{new} , respectively:

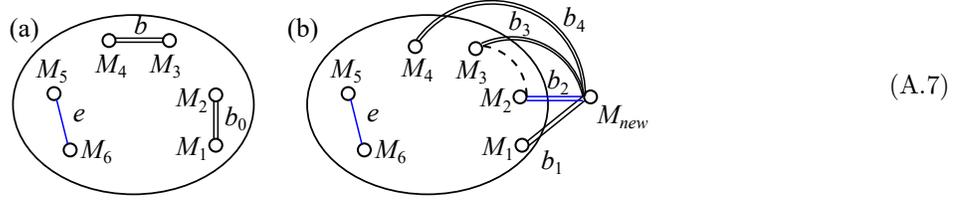


In graph \mathcal{G} , the edge $e = (\mathcal{M}_5, \mathcal{M}_6)$ is redundant by putting b_0 into the blue net. Let the corresponding black net and blue net be \mathcal{B}_{black} and \mathcal{B}_{blue} , such that $b_0 \in \mathcal{B}_{blue}$ and $\mathcal{B}_{blue} \setminus \{e\}$ is still a blue net of \mathcal{G} . Then either \mathcal{M}_1 or \mathcal{M}_2 is connected to molecules \mathcal{M}_3 and \mathcal{M}_4 through a path of edges in $\mathcal{B}_{blue} \setminus \{e, b_0\}$, since otherwise adding back the edge b_0 to $\mathcal{B}_{blue} \setminus \{e, b_0\}$ does not give a blue net, which is a contradiction. Without loss of generality, assume that \mathcal{M}_2 is connected to \mathcal{M}_3 through a path of edges in $\mathcal{B}_{blue} \setminus \{e, b_0, b\}$. In graph (b) of (A.5), the dashed edge represents such a path from \mathcal{M}_2 to \mathcal{M}_3 .

Now in graph (b) of (A.5), we put b_1 into the blue net and b_2 into the black net. Then $\mathcal{B}_{black} \cup \{b_2\}$ is a black net in \mathcal{G}_{new} , because b_2 connects the new molecule \mathcal{M}_{new} to other molecules. On the other hand, we claim that $\mathcal{B}_{blue}^{new} := \mathcal{B}_{blue} \cup \{b_1, b_3, b_4\} \setminus \{e, b_0, b\}$ is a blue net in \mathcal{G}_{new} . This can be derived from the following observations.

net). Notice that b_0 and b play symmetric roles. Hence if b_0 is included into the blue net in order for e to be redundant in \mathcal{G} , we can conclude the proof with the same argument.

It remains to consider the case where both b and b_0 are included into the black net in order for e to be redundant in \mathcal{G} . We have the following figure, where the graphs (a) and (b) respectively represent \mathcal{G} and \mathcal{G}_{new} :



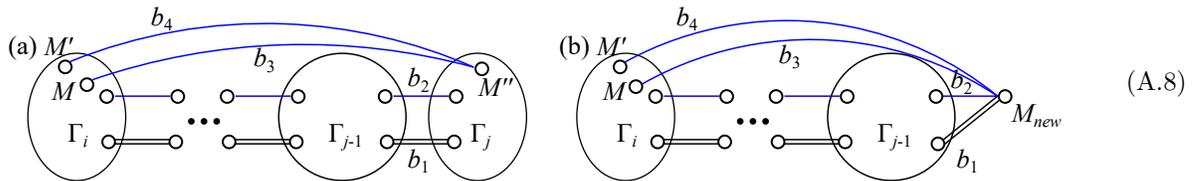
The graph \mathcal{G} has a black net \mathcal{B}_{black} and a blue net \mathcal{B}_{blue} , such that $b_0, b \in \mathcal{B}_{black}$ and $\mathcal{B}_{blue} \setminus \{e\}$ is still a blue net of \mathcal{G} . Then either \mathcal{M}_3 or \mathcal{M}_4 is connected to one of \mathcal{M}_1 and \mathcal{M}_2 through a path of black edges in $\mathcal{B}_{black} \setminus \{b, b_0\}$, since otherwise adding back the edges b and b_0 to $\mathcal{B}_{black} \setminus \{b, b_0\}$ does not give a black net, which is a contradiction. Without loss of generality, assume that \mathcal{M}_3 is connected to \mathcal{M}_2 through a path of edges in $\mathcal{B}_{black} \setminus \{b, b_0\}$, which is represented by the dashed edge in the graph (b) of (A.7). Then in \mathcal{G}_{new} , we put b_2 into the blue net, and put edges b_1, b_3 and b_4 into the black net. First, using the fact that $\mathcal{B}_{blue} \setminus \{e\}$ is a blue net in \mathcal{G} , it is easy to see that $\mathcal{B}_{blue} \cup \{b_2\} \setminus \{e\}$ is a blue net in \mathcal{G}_{new} . Then we claim that $\mathcal{B}_{black}^{new} := \mathcal{B}_{black} \cup \{b_1, b_3, b_4\} \setminus \{b, b_0\}$ is a black net in \mathcal{G}_{new} . This is due to the following observations.

- (1) \mathcal{M}_3 and \mathcal{M}_4 are connected by the path of edges b_3 and b_4 , which replaces the role of edge b in the original black net \mathcal{B}_{black} .
- (2) \mathcal{M}_1 and \mathcal{M}_2 are connected by a path of edges in $\mathcal{B}_{black}^{new}$ consisting of b_1, b_3 and a path of black edges connecting \mathcal{M}_2 to \mathcal{M}_3 in $\mathcal{B}_{black} \setminus \{b, b_0\}$. This shows that the role of edge b_0 in the original black net \mathcal{B}_{black} can be replaced by a path of edges in $\mathcal{B}_{black}^{new}$.
- (3) The new molecule \mathcal{M}_{new} is connected to other molecules through b_1, b_3 and b_4 .

Hence \mathcal{G}_{new} has a black net $\mathcal{B}_{black}^{new}$ and a blue net $\mathcal{B}_{blue} \cup \{b_2\} \setminus \{e\}$. Since e is not used in this blue net, it is redundant. \square

Now we give the proof of the case (i) of Lemma 5.12 using Claims A.3–A.5. Recall that the original graph is denoted by \mathcal{G} , and the new graph is denoted by $\tilde{\mathcal{G}}$.

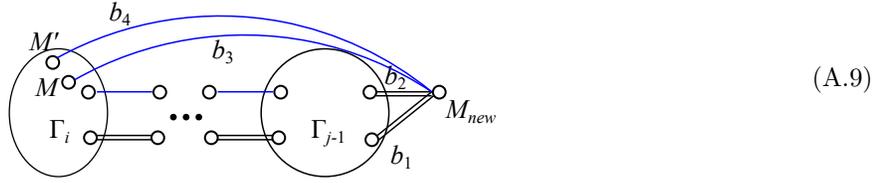
Proof of Lemma 5.12: case (i). The statement that \mathcal{I}_{j+1} is the maximal isolated subgraph of \mathcal{I}_i is trivial. We replace \mathcal{I}_{j+1} and its two external edges with a diffusive edge, and get the following graph (a) for the isolated subgraph \mathcal{I}_i of $\tilde{\mathcal{G}}$:



Here we keep the names Γ_l , $i \leq l \leq j$, for the subgraph components inside the black circles. By the SPD property of \mathcal{G} , we know that the component Γ_j in graph (a) is pre-deterministic, and hence we can change its blue solid edges into diffusive edges one by one according to a pre-deterministic order. Now by Claim A.1, it suffices to show that the graph (b) with Γ_j replaced by a vertex is pre-deterministic.

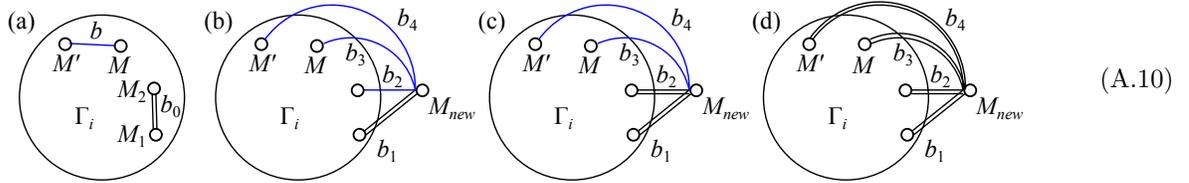
Now we show that the edge b_2 is redundant in the graph (b) of (A.8). By the doubly connected property of \mathcal{G} , removing the subgraph \mathcal{I}_{j+1} and its two external edges still gives a doubly connected graph. Correspondingly, in the graph (b) of (A.8), if we remove the two edges b_1 and b_2 and replace the edges b_3 and b_4 with a single blue solid edge $b = (\mathcal{M}, \mathcal{M}')$, we still get a doubly connected graph. Then by Claim A.3, the

edge b_2 is redundant, so we can change it into a diffusive edge and get the following graph:



By the SPD property of \mathcal{G} , if we replace \mathcal{I}_j and its two external edges with a diffusive edge, then the blue solid edges in Γ_{j-1} can be changed into diffusive edges one by one according to a pre-deterministic order. Now using Claim A.4 (i), we get that the blue solid edges inside Γ_{j-1} in (A.9) can be changed into diffusive edges according to the same pre-deterministic order. After that, since the subgraph induced on the molecules in Γ_{j-1} and the molecule \mathcal{M}_{new} is doubly connected, by Claim A.1 it is equivalent to replace them with a single molecule and get a graph that is similar to graph (b) of (A.8).

Repeating the above argument, we finally reduced the graph to the following graph (b) with component Γ_i only and a new molecule \mathcal{M}_{new} :

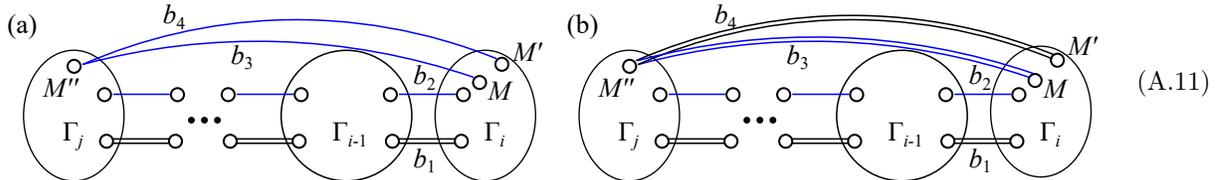


Here the graph (a) is obtained from \mathcal{G} by replacing \mathcal{I}_{i+1} and its two external edges with a diffusive edge b_0 between \mathcal{M}_1 and \mathcal{M}_2 . By the property (iii) of Definition 5.9, the component Γ_i in graph (a) is pre-deterministic. Suppose a pre-deterministic order of the blue solid edges is $e_1 \preceq \dots \preceq e_{\ell-1} \preceq b \preceq e_{\ell+1} \preceq \dots \preceq e_k$. First, by Claim A.3, the edge b_2 in the graph (b) of (A.10) is redundant, so we can change it into a diffusive edge and get the graph (c). Second, by Claim A.4 (i), the blue solid edges $e_1, \dots, e_{\ell-1}$ inside Γ_i can be changed into diffusive edges one by one. Third, by Claim A.4 (ii), the edges b_3 and b_4 can be changed into diffusive edges according to the order $b_3 \preceq b_4$ or $b_4 \preceq b_3$, which gives the graph (d) of (A.10). Finally, by Claim A.5, the blue solid edges $e_{\ell+1}, \dots, e_k$ in Γ_i can be changed into diffusive edges one by one.

In sum, we have shown that the blue solid edges in \mathcal{I}_i can be changed into diffusive edges one by one according to an order given by the above argument. Hence \mathcal{I}_i is pre-deterministic. This concludes the case (i) of Lemma 5.12. \square

The cases (ii)–(v) of Lemma 5.12 are all easier to prove than case (i). We consider them case by case.

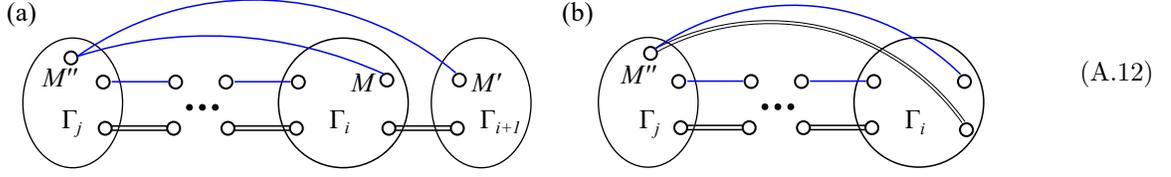
Proof of Lemma 5.12: cases (ii) and (iv). For the case (ii), the statement that \mathcal{I}_{i+1} is the maximal isolated subgraph of \mathcal{I}_j is trivial. We replace \mathcal{I}_{i+1} and its two external edges with a diffusive edge, and get the following graph (a) for the isolated subgraph \mathcal{I}_j of $\tilde{\mathcal{G}}$:



By the SPD property of \mathcal{G} , we know that after replacing the edges b_3 and b_4 in the graph (a) with a blue solid edge $b := (\mathcal{M}, \mathcal{M}')$, the graph component Γ_j becomes pre-deterministic. Suppose a pre-deterministic order of blue solid edges in Γ_i is $e_1 \preceq \dots \preceq e_{\ell-1} \preceq b \preceq e_{\ell+1} \preceq \dots \preceq e_k$. Then it is trivial to observe that in the graph (a), the edges $e_1, \dots, e_{\ell-1}, b_3, b_4, e_{\ell+1}, \dots, e_k$ can be changed into diffusive edges one by one, which gives the graph (b) of (A.11). Now if we put b_3 into the blue net and b_4 into the black net, the subgraph induced on the molecules in Γ_i and the molecule \mathcal{M}'' is doubly connected. By Claim A.1, it is equivalent to look at the quotient graph with this subgraph replaced by a single vertex. The quotient graph has the same

structure as the graph (a) of (A.2), which has been shown to be pre-deterministic. This concludes the case (ii) of Lemma 5.12.

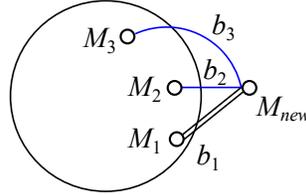
For the case (iv), we replace \mathcal{I}_{i+2} and its two external edges with a diffusive edge, and get the following graph (a) for the isolated subgraph \mathcal{I}_j of $\tilde{\mathcal{G}}$:



The statement that \mathcal{I}_{i+1} is the maximal isolated subgraph of \mathcal{I}_j is trivial. Then we replace \mathcal{I}_{i+1} and its two external edges with a diffusive edge, and get the graph (b) in (A.12). Again this graph has the same structure as the graph (a) of (A.2), which has been shown to be pre-deterministic. Hence we conclude the case (iv) of Lemma 5.12. \square

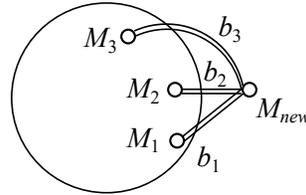
The proofs of cases (iii) and (v) of Lemma 5.12 use the following two claims.

Claim A.6. *Given a doubly connected graph \mathcal{G} , we construct a new graph \mathcal{G}_{new} as follows:*



More precisely, we create a new molecule M_{new} . Given any three molecules M_1, M_2 and M_3 in \mathcal{G} , we add a diffusive edge b_1 between M_{new} and M_1 , a blue solid edge b_2 between M_{new} and M_2 , and a blue solid edge b_3 between M_{new} and M_3 . Then the blue solid edges b_2 and b_3 are both redundant in \mathcal{G}_{new} .

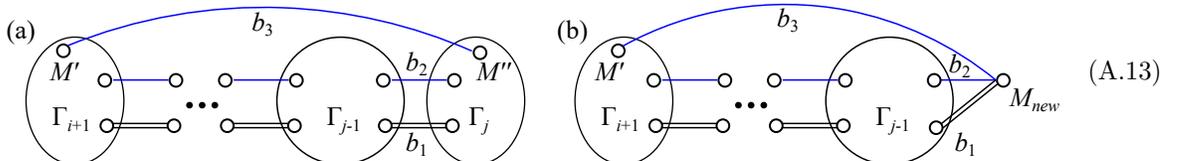
Claim A.7. *Given a doubly connected graph \mathcal{G} , we construct a new graph \mathcal{G}_{new} as follows:*



More precisely, we create a new molecule M_{new} , replace a diffusive edge $b_0 = (M_1, M_2)$ in \mathcal{G} with two diffusive edges b_1 between M_1 and M_{new} and b_2 between M_2 and M_{new} , and add a diffusive edge b_3 between M_{new} and a molecule M_3 in \mathcal{G} . If a blue solid edge is redundant in \mathcal{G} , it is also redundant in \mathcal{G}_{new} .

The proofs of the above two claims are simple, so we omit the details.

Proof of Lemma 5.12: cases (iii) and (v). The case (v) can be regarded as a special case of the case (iii). For the case (iii), it is trivial to show that \mathcal{I}_{i+1} is the maximal isolated subgraph of \mathcal{I}_i , and \mathcal{I}_{j+1} is the maximal isolated subgraph of \mathcal{I}_{i+1} . We replace \mathcal{I}_{j+1} and its two external edges with a diffusive edge and get the following graph (a) for the isolated subgraph \mathcal{I}_{i+1} :



By the SPD property of \mathcal{G} , the component Γ_j in the graph (a) of (A.13) is pre-deterministic, so we can change its blue solid edges into diffusive edges one by one. Then by Claim A.1, we can replace Γ_j with a single molecule and get the graph (b) of (A.13). Now by Claim A.6, both b_2 and b_3 are redundant, so we can change them into diffusive edges. Next by Claim A.7, we can change the blue solid edges in Γ_{j-1} into diffusive edges one by one. In the resulting graph, since the subgraph induced on the molecules in Γ_{j-1} and the molecule \mathcal{M}_{new} is a doubly connected subgraph, by Claim A.1 we can replace them with a single molecule and get a graph that is similar to the graph (b) of (A.13). Repeating the above argument, we can show that the blue solid edges in \mathcal{I}_{i+1} can be changed into diffusive edges one by one according to some order. Hence \mathcal{I}_{i+1} is pre-deterministic, which concludes the case (iii) of Lemma 5.12. \square

B PROOF OF LEMMA 9.7

As discussed below Lemma 9.7, we need to expand the graphs in $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ and $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$. First, we keep applying cases 1 and 2 of Strategy 9.8 until all graphs satisfy the stopping rules (T1)–(T3) or the setting in cases 3 of Strategy 9.8. So far, all the resulting graphs do not contain any ghost edge. Moreover, as shown in Section 6.4, the resulting graphs $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be classified as follows.

- (a) If $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ satisfies (T2), then it can be included into $\mathcal{E}rr_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$.
- (b) If $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ is a Q -graph, then it satisfies the property (v) of Lemma 9.7 with $k_{\text{gh}}(\mathcal{G}) = 0$.
- (c) Suppose $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ satisfies (T1) and is a \oplus/\ominus -recollision graph. Depending on whether each of \oplus and \ominus is connected with a dotted edge or not, we can write $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ as

$$\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_x \Theta_{\mathbf{a}x} \mathcal{D}_{x\mathbf{b}_1} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} f(G_{\mathbf{b}_1 \mathbf{b}_1}), \quad \text{or} \quad \mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_x \Theta_{\mathbf{a}x} \mathcal{D}_{x\mathbf{b}_2} G_{\mathbf{b}_2 \mathbf{b}_1} f(G_{\mathbf{b}_2 \mathbf{b}_2}), \quad (\text{B.1})$$

or

$$\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_x \Theta_{\mathbf{a}x} \mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2} g(G_{\mathbf{b}_1 \mathbf{b}_1}, G_{\mathbf{b}_2 \mathbf{b}_2}, \bar{G}_{\mathbf{b}_1 \mathbf{b}_2}, G_{\mathbf{b}_2 \mathbf{b}_1}), \quad (\text{B.2})$$

where \mathcal{D} are deterministic doubly connected graphs with x , \mathbf{a} , \mathbf{b}_1 and \mathbf{b}_2 regarded as internal atoms, and f and g are monomials satisfying (iv) of Lemma 9.7. If $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ takes the form (B.2), then it can be included into the fourth term on the right-hand side of (9.10). If $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ takes one of the forms in (B.1), using Lemma 8.5 we get that

$$\sum_x |\Theta_{\mathbf{a}x} \mathcal{D}_{x\mathbf{b}_i}| \prec \sum_x B_{\mathbf{a}x} B_{x\mathbf{b}_i}^2 \prec W^{-d} B_{\mathbf{a}\mathbf{b}_i}, \quad i = 1, 2. \quad (\text{B.3})$$

Hence $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be included into the second and third terms on the right-hand side of (9.10).

- (d) If $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ satisfies (T1) and is not a \oplus/\ominus -recollision graph, then we have $\text{ord}(\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}) > n$, because it must come from expansions of a graph in $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$. Then $\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$ can be written as

$$\mathcal{G}_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} = \sum_{x,y} \Theta_{\mathbf{a}x} \mathcal{D}_{xy} t_{y, \mathbf{b}_1 \mathbf{b}_2}, \quad (\text{B.4})$$

where \mathcal{D}_{xy} is a deterministic doubly connected graph of scaling order $> n$.

Now we consider the remaining graphs that satisfy the setting in cases 3 of Strategy 9.8 but not the stopping rules (T1)–(T3). So far, these graphs do not contain any ghost edge. We claim that all these graphs are GGS. First, by Lemma 5.10 and Lemma 6.5, all these graphs are SPD. Then we show that these graphs satisfy (9.17). We have two cases. If a graph comes from expansions of $(\mathcal{A}_T^{(>n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$, then it trivially satisfies (9.17) with $k_{\text{gh}} = 0$. On the other hand, suppose a graph, say \mathcal{G} , comes from expansions of a graph, say \mathcal{G}_0 , in $(\mathcal{R}_T^{(n)})_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2}$. Since \mathcal{G}_0 is globally standard, it has no strongly isolated subgraphs. Furthermore, the only operation to generate a strongly isolated subgraph is to replace a $t_{x, y_1 y_2}$ variable with a graph in $(\mathcal{A}_T^{(>n)})_{x, y_1 y_2}$ in Case 2 of Strategy 9.8. Hence \mathcal{G} is of scaling order $> n$, and satisfies (9.17) with $k_{\text{gh}} = 0$.

In the next few lemmas, we show that Strategy 9.8 preserve the GGS property.

Lemma B.1. Let $\mathcal{G}_{\alpha, b_1 b_2}$ be a GGS graph without P/Q labels and satisfy the setting in Case 3 of Strategy 9.8. Applying Strategy 9.8 to $\mathcal{G}_{\alpha, b_1 b_2}$, the resulting non- Q graphs are still GGS, and the resulting Q -graphs satisfy the property (v) of Lemma 9.7.

Proof. $\mathcal{G}_{\alpha, b_1 b_2}$ satisfies either (A) or (B) of Definition 9.9. If \mathcal{G} satisfies (B), then, by the fact that \mathcal{I}_k is deterministic, there exists a redundant ghost edge in \mathcal{I}_k . We can remove this edge, and get a new graph satisfying (A) of Definition 9.9. Hence without loss of generality, we assume that $\mathcal{G}_{\alpha, b_1 b_2}$ satisfies (9.17). Now we add a ghost edge, denoted by g_0 , between the ending atoms of b_1 , and denote the resulting graph by $\tilde{\mathcal{G}}$. Then we have

$$\text{ord}(\tilde{\mathcal{G}}) \geq (n-1) \cdot k_{\text{gh}}(\tilde{\mathcal{G}}) + 2, \quad (\text{B.5})$$

and b_1 becomes a redundant edge in $\tilde{\mathcal{G}}$. Using the generalized SPD property of $\mathcal{G}_{\alpha, b_1 b_2}$, it is trivial to see that b_1 is the first edge in a pre-deterministic order of the MIS containing \mathcal{I}_k .

Now we apply (4.15) (with $n-1$ replaced by n) to $t_{x, y_1 y_2}$, where $G_{\alpha y_1}$ is the edge b_1 and α is the standard neutral atom in \mathcal{I}_k . By (B.5), all the resulting graphs satisfy (9.18). Moreover, using Lemma 6.5, we get that the resulting Q -graphs satisfy the property (v) of Lemma 9.7, and the resulting non- Q graphs satisfy the generalized SPD property. It remains to prove the property (A) or (B1) of Definition 9.9 for the non- Q graphs. Corresponding to the terms on the right-hand side of (4.15), we have the following four cases.

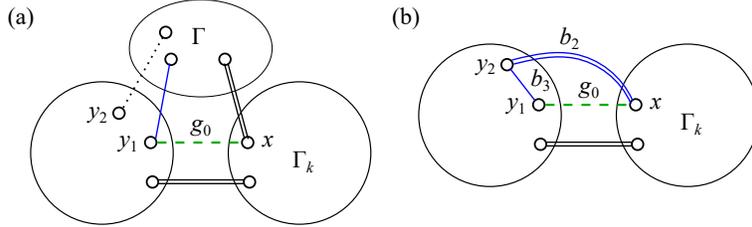
Case I: If we replace $t_{x, y_1 y_2}$ with the first two terms on the right-hand side of (4.15), then it is trivial to see that the edge g_0 is redundant in each resulting graph, so that the property (B1) of Definition 9.9 holds.

Case II: If we replace $t_{x, y_1 y_2}$ with a graph $(\mathcal{G}_A)_{x, y_1 y_2}$ in $(\mathcal{A}_T^{(>n)})_{x, y_1 y_2}$ or $(\mathcal{E}rr_{n, D})_{x, y_1 y_2}$, then every resulting graph, say \mathcal{G}_{new} , satisfies that

$$\text{ord}(\mathcal{G}_{new}) \geq \text{ord}(\tilde{\mathcal{G}}) + (n-1) \geq (n-1) \cdot [k_{\text{gh}}(\tilde{\mathcal{G}}) + 1] + 2 = (n-1) \cdot [k_{\text{gh}}(\mathcal{G}_{new}) + 1] + 2.$$

Hence \mathcal{G}_{new} satisfies the property (A) of Definition 9.9.

Case III: Suppose we replace $t_{x, y_1 y_2}$ with a graph $(\mathcal{G}_R)_{x, y_1 y_2}$ in $(\mathcal{R}_T^{(n)})_{x, y_1 y_2}$, and get the following molecular graph (a) without red solid edges. We only show a case where there is a dotted edge connected with y_2 in $(\mathcal{G}_R)_{x, y_1 y_2}$. All the other cases can be analyzed in a similar way. With a slight abuse of notation, we use x , y_1 and y_2 to denote the molecules that contain atoms x , y_1 and y_2 .



Inside the back circles of graph (a) are some subgraphs, where Γ_k contains the molecules in \mathcal{I}_k of the original graph $\tilde{\mathcal{G}}$, and Γ contains the molecules in $(\mathcal{G}_R)_{x, y_1 y_2}$. We now show that g_0 is redundant in graph (a), which is stronger than the property (B1) of Definition 9.9. By Claim A.1, it is equivalent to consider the graph (b) obtained by merging all molecules in Γ with molecule y_2 . If we include the edges b_2 and b_3 into the blue net, then g_0 becomes redundant.

Case IV: Suppose we replace $t_{x, y_1 y_2}$ with a graph $(\mathcal{G}_Q)_{x, y_1 y_2}$ in $\mathcal{Q}_{x, y_1 y_2}^{(n)}$ and get a graph $(\mathcal{G}_{new})_{\alpha, b_1 b_2}$. Applying Q -expansions, we can expand it into a sum of $O(1)$ many new graphs:

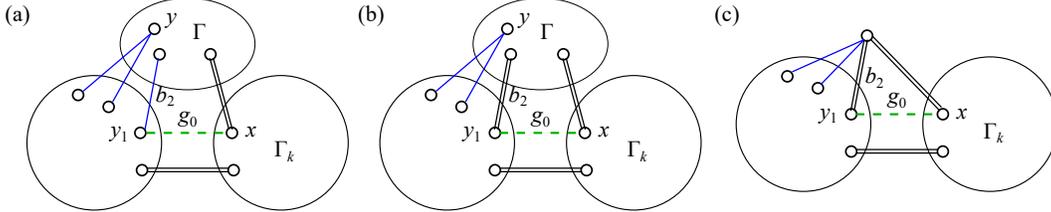
$$(\mathcal{G}_{new})_{\alpha, b_1 b_2} = \sum_{\omega} \mathcal{G}_{\omega} + \mathcal{Q} + \mathcal{G}_{err},$$

where \mathcal{G}_{ω} are graphs without P/Q labels, \mathcal{Q} is a sum of Q -graphs and \mathcal{G}_{err} satisfies $|\mathcal{G}_{err}| \prec W^{-D}$. Now we show that the graphs \mathcal{G}_{ω} are all GGS. Suppose all the solid edges and weights in $(\mathcal{G}_Q)_{x, y_1 y_2}$ have the same Q_y label for an atom y . Let \mathcal{G}' be the complement of \mathcal{I}_k in $\tilde{\mathcal{G}}$. By the property (iv) of Lemma 4.15, \mathcal{G}_{ω} satisfies at least one of the following properties:

- (1) there exist atoms in \mathcal{G}' that have been merged with y due to dotted edges;

- (2) the atoms in \mathcal{G}' connect to y only through red solid edges;
- (3) there exist atoms in \mathcal{G}' that connect to y through blue solid edges.

In the case (1), we can show that g_0 is redundant using the argument in Case III. In the case (2), if $(\mathcal{G}_Q)_{x,y_1,y_2}$ is a \oplus/\ominus -recollision graph, we can again use the argument in Case III to show that g_0 is redundant. Otherwise, $(\mathcal{G}_Q)_{x,y_1,y_2}$ is the closure of a weakly isolated subgraph, and replacing it with a diffusive edge corresponds to replacing the edge b_1 in graph $\tilde{\mathcal{G}}$ with a diffusive edge, in which case the ghost edge g_0 becomes redundant. This shows that \mathcal{G}_ω satisfies the property (B1) of Definition 9.9 in the case (2). Finally, we consider the case (3), where we have the following molecular graph (a) without red solid edges:



We change b_2 to a diffusive edge and get the graph (b). We claim that g_0 is redundant in the graph (b), which implies that \mathcal{G}_ω satisfies the property (B1) of Definition 9.9. By Claim A.1, it is equivalent to show that g_0 is redundant in the graph (c) obtained by merging the molecules in Γ . This follows directly from Claim A.4.

Combining the above four cases, we conclude that the resulting non- Q graphs satisfy either (A) or (B) of Definition 9.9, and hence are GGS. \square

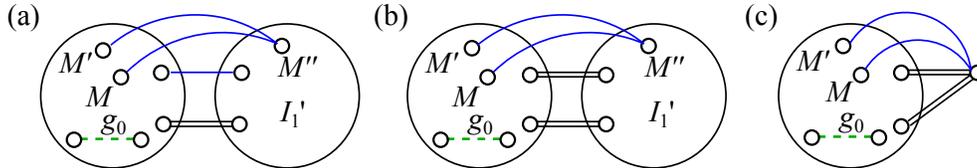
Lemma B.2. *Let \mathcal{G}_{a,b_1,b_2} be a GGS graph without P/Q labels. Applying any expansion in Definitions 4.3, 4.4, 4.5 and 4.6 on an atom in the MIS with non-deterministic closure, the resulting non- Q graphs are still GGS, and the resulting Q -graphs satisfy the property (v) of Lemma 9.7.*

Proof. Using Lemma 6.4, we get that the resulting non- Q graphs satisfy the generalized SPD property, and the resulting Q -graphs satisfy the property (v) of Lemma 9.7. It remains to prove that the new non- Q graphs satisfy the property (A) or (B1) of Definition 9.9. If \mathcal{G} satisfies (9.17) (resp. (9.18)), then the new graphs also satisfy (9.17) (resp. (9.18)), because they have scaling orders $\geq \text{ord}(\mathcal{G})$. Hence we only need to prove that if \mathcal{G}_{a,b_1,b_2} satisfies the property (B1) of Definition 9.9, then the resulting non- Q graphs also satisfy the property (B1).

Similar to the proof of Lemma 5.10, we need to show that the following two operations will preserve the property (B1) of Definition 9.9:

- (I) merging a pair of molecules due to a newly added dotted or waved edge between them;
- (II) replacing a plus G edge between molecules \mathcal{M} and \mathcal{M}' with a path of two plus G edges from $\mathcal{M} \rightarrow \mathcal{M}'' \rightarrow \mathcal{M}'$ for a molecule \mathcal{M}'' in the MIS with non-deterministic closure.

Denote the maximal isolated subgraph of \mathcal{I}' in \mathcal{G}_{a,b_1,b_2} by \mathcal{I}'_1 . The proof of case (I) is non-trivial only when one molecule is inside \mathcal{I}'_1 , while the other is not. The proof is the same as the one for Lemma 5.11 by using Claims A.1 and A.2, so we omit the details. The proof of case (II) is non-trivial only when molecules \mathcal{M} and \mathcal{M}' are not inside \mathcal{I}'_1 , as shown in the graph (a) of the following figure:



We replace the blue solid edges inside \mathcal{I}' with diffusive edges and get the graph (b), where we have drawn a case such that \mathcal{M} or \mathcal{M}' does not belong to \mathcal{I}' . To show that g_0 is redundant in the graph (b), by Claim A.1 it is equivalent to consider the graph (c) obtained by merging the molecules in \mathcal{I}'_1 . Now by Claim A.4, g_0 is redundant in the graph (c). This implies that the graph (a) satisfies the property (B1) of Definition 9.9. Finally, for the case where \mathcal{M} and \mathcal{M}' belong to \mathcal{I}' , we can conclude the proof with a similar argument by using Claim A.5. \square

Lemma B.3. *Let \mathcal{G}_{a,b_1b_2} be a GGS graph without P/Q labels. Applying the expansion in Case 2 of Strategy 9.8, the resulting non- Q graphs are still GGS, and the resulting Q -graphs satisfy the property (v) of Lemma 9.7.*

Proof. This lemma can be proved using similar arguments as in the proofs of Lemmas B.1 and B.2. We do not repeat them again. \square

In sum, Lemmas B.1–B.3 show that applying Strategy 9.8 to any GGS input graph once, all the resulting non- Q graphs are still GGS and all the Q -graphs satisfy the property (v) of Lemma 9.7. Hence we can apply Strategy 9.8 repeatedly until all graphs satisfy the stopping rules (T1)–(T3). Now we claim that the expansion process will stop after $O(1)$ many iterations of Strategy 9.8. The proof of this claim is similar to the one for Lemma 6.8, so we will not write down all the details.

If we only apply the Cases 1 and 2 of Strategy 9.8, then the expansions will stop after $O(1)$ many steps by Lemma 6.8. To complete the proof, it suffices to show that the Case 3 of Strategy 9.8 is applied at most for $O(1)$ many times when all graphs satisfy the stopping rules (T1)–(T3). Suppose a graph \mathcal{G} satisfies the setting in the Case 3 of Strategy 9.8. As explained in the proof of Lemma B.1, we can remove a redundant ghost edge from \mathcal{G} if necessary so that \mathcal{G} satisfies the property (A) of Definition 9.9. We expand \mathcal{G} by applying Strategy 9.8 repeatedly, and construct correspondingly a tree diagram of graphs as in the proof of Lemma 6.8. Suppose \mathcal{G}_1 is a graph on the tree so that it satisfies the setting in Case 3 of Strategy 9.8, but all the other graphs on the unique path between \mathcal{G} and \mathcal{G}_1 do not. Following the expansion process, we find that at least one of the following properties holds for \mathcal{G}_1 .

- \mathcal{G}_1 contains strictly fewer blue solid edges than \mathcal{G} , and $\text{size}(\mathcal{G}_1) \leq \text{size}(\mathcal{G})$.
- \mathcal{G}_1 has a strictly higher scaling order than \mathcal{G} , but not more ghost edges. Hence we have

$$\text{size}(\mathcal{G}_1) \leq W^{-d/2} \text{size}(\mathcal{G}).$$

- \mathcal{G}_1 has one more ghost edge than \mathcal{G} , and is of scaling order

$$\text{ord}(\mathcal{G}_1) \geq \text{ord}(\mathcal{G}) + (n - 1). \quad (\text{B.6})$$

Here the extra ghost edge appears when we apply the Case 3 of Strategy 9.8 to \mathcal{G} . Furthermore, in order for this ghost edge to be pivotal in \mathcal{G}_1 , we must have replaced a t_{x,y_1y_2} variable with a graph in $(\mathcal{A}_T^{(>n)})_{x,y_1y_2}$ at some step. This gives the condition (B.6). Using (3.15) and (9.16), we get that

$$\text{size}(\mathcal{G}_1) \leq W^{-c_0} \text{size}(\mathcal{G}).$$

With the above facts, it is easy to show that the Case 3 of Strategy 9.8 are applied at most for $O(1)$ many times when the expansion process stops.

Applying Strategy 9.8 repeatedly until all graphs satisfy the stopping rules (T1)–(T3), we can expand T_{a,b_1b_2} into a sum of $O(1)$ many graphs. If a graph satisfies the stopping rule (T2), then it can be included into $\mathcal{E}rr_{a,b_1b_2}$ in (9.10). If a graph satisfies the stopping rule (T3), then it can be included into \mathcal{Q}_{a,b_1b_2} in (9.10). If a graph \mathcal{G}_{a,b_1b_2} satisfies the stopping rule (T1) and is a \oplus/\ominus -recollision graph, then it can be written into one of the forms in (B.1) and (B.2), where \mathcal{D}_{xb_1} , \mathcal{D}_{xb_2} and \mathcal{D}_{x,b_1b_2} are deterministic doubly connected graphs satisfying (9.18). Then using Lemma 9.5 and a similar calculation as in (B.3), we get that \mathcal{G}_{a,b_1b_2} can be included into the second to fourth terms in (9.10). If a graph \mathcal{G}_{a,b_1b_2} satisfies the stopping rule (T1) and is *not* a \oplus/\ominus -recollision graph, then it is GGS and can be written into

$$\mathcal{G}_{a,b_1b_2} = \sum_{x,y} \Theta_{ax} \tilde{\mathcal{D}}_{xy} t_{y,b_1b_2} = \sum_{x,y} \Theta_{ax} \tilde{\mathcal{D}}_{xy} T_{y,b_1b_2} - \sum_{x,y} \Theta_{ax} \tilde{\mathcal{D}}_{xy} |m|^2 \sum_{\alpha} s_{y\alpha} G_{\alpha b_1} \bar{G}_{\alpha b_2} (1 - \mathbf{1}_{\alpha \neq b_1} \mathbf{1}_{\alpha \neq b_2}),$$

where $\tilde{\mathcal{D}}_{xy}$ is a deterministic doubly connected graph satisfying (9.17) (by removing a redundant ghost edge if necessary). We include the second term of the above equation into the second to fourth terms in (9.10). In sum, we have obtained the following expansion:

$$\begin{aligned} T_{a,b_1b_2} &= m \Theta_{ab_1} \bar{G}_{b_1b_2} + \sum_{\mu} B_{ab_1}^{(\mu)} \bar{G}_{b_1b_2} f_{\mu}(G_{b_1b_1}) + \sum_{\nu} \tilde{B}_{ab_2}^{(\nu)} G_{b_2b_1} \tilde{f}_{\nu}(G_{b_2b_2}) \\ &+ \sum_{\mu} \sum_x \Theta_{ax} \mathcal{D}_{x,b_1b_2}^{(\mu)} g_{\mu}(G_{b_1b_1}, G_{b_2b_2}, \bar{G}_{b_1b_2}, G_{b_2b_1}) + \sum_{\mu} \sum_{x,y} \Theta_{ax} \tilde{\mathcal{D}}_{xy}^{(\mu)} T_{y,b_1b_2} + \mathcal{Q}_{a,b_1b_2} + \mathcal{E}rr_{a,b_1b_2}, \end{aligned} \quad (\text{B.7})$$

where $\mathcal{D}_{x, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)}$ are deterministic doubly connected graphs satisfying (9.18), and $\tilde{\mathcal{D}}_{xy}^{(\mu)}$ are deterministic doubly connected graphs satisfying (9.17).

Now similar to the proof of Corollary 3.8 in Section 6.1, we solve (B.7) to get that

$$\begin{aligned} T_{\mathbf{a}, \mathbf{b}_1 \mathbf{b}_2} &= \sum_x \left(1 - \Theta \tilde{\mathcal{D}}^{(\mu)}\right)_{\mathbf{a}x}^{-1} \left[m \Theta_{x \mathbf{b}_1} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} + \sum_{\mu} B_{x \mathbf{b}_1}^{(\mu)} \bar{G}_{\mathbf{b}_1 \mathbf{b}_2} f_{\mu}(G_{\mathbf{b}_1 \mathbf{b}_1}) + \sum_{\nu} \tilde{B}_{x \mathbf{b}_2}^{(\nu)} G_{\mathbf{b}_2 \mathbf{b}_1} \tilde{f}_{\nu}(G_{\mathbf{b}_2 \mathbf{b}_2}) \right] \\ &+ \sum_x \left(1 - \Theta \tilde{\mathcal{D}}^{(\mu)}\right)_{\mathbf{a}x}^{-1} \left[\sum_{\mu} \sum_y \Theta_{xy} \mathcal{D}_{y, \mathbf{b}_1 \mathbf{b}_2}^{(\mu)} g_{\mu}(G_{\mathbf{b}_1 \mathbf{b}_1}, G_{\mathbf{b}_2 \mathbf{b}_2}, \bar{G}_{\mathbf{b}_1 \mathbf{b}_2}, G_{\mathbf{b}_2 \mathbf{b}_1}) \right] \\ &+ \sum_x \left(1 - \Theta \tilde{\mathcal{D}}^{(\mu)}\right)_{\mathbf{a}x}^{-1} \left[\mathcal{Q}_{x, \mathbf{b}_1 \mathbf{b}_2} + \mathcal{E}rr_{x, \mathbf{b}_1 \mathbf{b}_2} \right]. \end{aligned} \quad (\text{B.8})$$

Using (9.9), we can get that

$$\sum_{\alpha} \Theta_{x\alpha} \tilde{\mathcal{D}}_{\alpha y}^{(\mu)} \prec \left(\frac{L^2}{W^2} \right)^{k_{\text{gh}}(\tilde{\mathcal{D}}_{\alpha y}^{(\mu)})} W^{-[\text{ord}(\tilde{\mathcal{D}}_{\alpha y}^{(\mu)})-2]d/2} B_{xy} \leq \frac{W^{-c_0}}{\langle x-y \rangle^d},$$

where we used (9.17), (3.15) and $W^2/L^2 \cdot B_{xy} \leq \langle x-y \rangle^d$ in the second step. Using this estimate and the Taylor expansion of $(1 - \Theta \tilde{\mathcal{D}}^{(\mu)})^{-1}$, we can get that

$$\left| (1 - \Theta \tilde{\mathcal{D}}^{(\mu)})_{xy}^{-1} - \delta_{xy} \right| \prec \frac{W^{-c_0}}{\langle x-y \rangle^d} + W^{-D}, \quad (\text{B.9})$$

for any large constant $D > 0$. By (B.9), we see that

- matrix products of (labelled) diffusive edges with $(1 - \Theta \tilde{\mathcal{D}}^{(\mu)})^{-1}$ give deterministic graphs $\widehat{B}^{(\mu)}$ and $\mathcal{B}^{(\omega)}$ satisfying (9.12) and (9.15);
- matrix products of $B^{(\mu)}$ and $\tilde{B}^{(\nu)}$ in (B.8) with $(1 - \Theta \tilde{\mathcal{D}}^{(\mu)})^{-1}$ give deterministic graphs satisfying (9.11) (where we have used the same notations $B^{(\mu)}$ and $\tilde{B}^{(\nu)}$ for convenience);
- $[(1 - \Theta \tilde{\mathcal{D}}^{(\mu)})^{-1} \Theta]_{xy} = \Theta_{xy} + B_{x \mathbf{b}_1}^{(\mu)}$ for a deterministic graph $B_{x \mathbf{b}_1}^{(\mu)}$ satisfying (9.11).

Hence (B.8) can be written into (9.10), which concludes the proof of Lemma 9.7.

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