Quantum Factor Graphs: Closing-the-Box Operation and Variational Approaches

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Abstract

Factor graph model is a popular statistical graphical model, where a number of practical problems can be abstracted as marginal problems on factor graphs, including problems from the fields of statistical physics, machine learning, coding theory, and signal processing. The sum-product algorithm is a powerful algorithm to solve the marginal problems on factor graphs. The algorithm has been justified using a number of different approaches which include the closing-the-box notion and the variational approach. In this report, we consider a generalization of factor graphs known as quantum factor graphs, along with a generalization of the sum-product algorithm known as the quantum sum-product algorithm. Our work is to migrate the notion of the closing-the-box operation and the method of the variational approach to the new quantum setup. In particular, we consider a generalization of the Bethe free energy and the related concepts on quantum factor graphs. Some expressions that hold exactly in the classical case hold only approximately in the quantum case; we give some analytical and numerical characterizations of these approximations.

I. INTRODUCTION

Factor graph [1], [2], or more often referred to as the classical factor graph (CFG) in this report, is a graphical model representing factorizations of functions with multiple variables in real or complex domain. In particular, serving as a popular variant of probabilistic graphical models [3], factor graphs have been proven useful in describing probability factorizations and solving the related marginal problems. The latter problem represents the essence of many practical problems in a number of scientific/engineering fields including statistical physics, machine learning, coding theory, and signal processing. Famous applications include the Ising model [4] and LDPC codes [5].

As a brief introduction to CFGs, we associate the factorization below

\[ g(x) \triangleq \prod_{a \in F} f_a(x_a) \]  

to the CFG with variable node set \( \mathcal{V} \), function node set \( \mathcal{F} \), and edge set \( \mathcal{E} \subseteq \mathcal{V} \times \mathcal{F} \) given by

\[ \mathcal{E} = \{(i,a) \in \mathcal{V} \times \mathcal{F} : i \in \partial a\} \].  

(2)

Here, \( x \triangleq (x_i)_{i \in \mathcal{V}} \), \( x_a \triangleq (x_i)_{i \in \partial a} \), \( \partial a \subseteq \mathcal{V} \), and \( x_i \in \mathcal{X}_i \). A fundamental problem is to calculate the so called partition sum of the CFG, which is defined as

\[ Z \triangleq \left\{ \begin{array}{ll} \sum_x g(x) & \mathcal{X}_\mathcal{V} \text{ is finite;} \\ \int g(x)dx & \mathcal{X}_\mathcal{V} \text{ is continuous}. \end{array} \right. \]  

(3)

In this report, we only consider the finite case with non-negative local functions, i.e., \( f_a(x_a) \in \mathbb{R}_{\geq 0} \) for all \( a \in \mathcal{F} \). In this case, the global function \( g \) is always a measure function of \( x \).

In general, calculation of the partition sum is an NP hard problem. However, in the case of acyclic CFGs, \( Z \) can always be computed efficiently by the so called sum-product algorithm (SPA). The main idea is to take advantage of the distributive law of multiplication over addition in the filed of real numbers (\( \mathbb{R} \)). In the following examples, we use rectangle and circle nodes to represent factor nodes and variable nodes in CFGs. Here, we also introduce the notion of normal CFGs where variables are represented by edges [1], [6], [7]. For example, in Fig. 1, CFGs (b) and (d) are the normal versions of CFGs (a) and (c), respectively.

Example 1. Consider the CFG (a) (or (b)) in Fig. 1 with variable node set \( \mathcal{V} = \{1, 2, 3, 4\} \) and function node set \( \mathcal{F} = \{A, B, C\} \). This CFG depicts a global function factorized as

\[ g(x_1, x_2, x_3, x_4) = f_A(x_1) \cdot f_B(x_1, x_2, x_3) \cdot f_C(x_3, x_4). \]  

(4)

With respect to the above factorization, the corresponding partition sum is given as

\[ Z = \sum_{x_1, x_2, x_3, x_4} f_A(x_1) \cdot f_B(x_1, x_2, x_3) \cdot f_C(x_3, x_4) \]  

(5)

\[ = \sum_{x_3} \left( \sum_{x_1} \left( f_A(x_1) \cdot \left( \sum_{x_2} f_B(x_1, x_2, x_3) \right) \right) \right) \cdot \sum_{x_4} f_C(x_3, x_4). \]  

(6)

Assuming each alphabet \( \mathcal{X}_i \) (\( i = 1, \ldots, 4 \)) to be binary, it will take 16 steps of summation in evaluating (5). Whereas, evaluating (6) takes 8 steps of summation, which is clearly more efficient than the direct evaluation of (5).
The process of the above reformulation ((5) to (6)) can be easier understood in terms of the closing-the-box notation [1], where we always “close” the most inner boxes by replacing it with the result of the summing over the interior variable(s). The process ends when the most outer box gets closed, which yields the partition sum $Z$. (We refer to [1] for details.) Interestingly, such notation can also be applied to graph with cycles. This allows the method of the SPA to be applied to more general setups.

**Example 2.** The CFG (c) (or (d)) in Fig. 1 is not acyclic, and has the global function

$$g(x) = f_A(x_1, x_3) \cdot f_B(x_1, x_2, x_3) \cdot f_C(x_3, x_4).$$

(7)

However, we can still simplify the expression of the partition sum using the same technique.

$$Z = \sum_{x_1, x_2, x_3, x_4} f_A(x_1, x_3) \cdot f_B(x_1, x_2, x_3) \cdot f_C(x_3, x_4)$$

(8)

$$= \sum_{x_3} \left( \sum_{x_1} f_A(x_1, x_3) \cdot \sum_{x_2} f_B(x_1, x_2, x_3) \right) \cdot \sum_{x_4} f_C(x_3, x_4).$$

(9)

It seems that the closing-the-box notation helps to generalize the SPA such that we can apply the algorithm to CFGs with cycles. However, such technique fails in more general settings, especially in large-scale setups. (Just consider a (nearly) fully connected normal CFG with $n$ factors.)

On the other hand, however, the SPA can also be interpreted as a message-passing algorithm, where the partial results in each step are represented as messages sent along the edges of the CFGs. The rules according to which the messages (i.e., partial results) are combined are called the SPA message update rules. Since the update rules are applied locally in CFGs, such rules can also be applied to a CFG with cycles, yielding a straightforward generalization of the SPA. Despite that the original justification of the algorithm as illustrated in Example 1 and 2 is no longer valid, the SPA and its variations still yield rather promising results in a number of real-life applications including the decoding of LDPC codes. Thus, it has become a focus of research to understand (and possibly improve) such algorithms. Related work includes the variational approach [8], the loop calculus [9], [10] and the graph covers.

In this report we are interested in a generalization of CFGs called quantum factor graphs (QFGs) [11]. In QFGs, we consider “factorizations” in the following sense

$$\rho \triangleq \bigotimes_{a \in \mathcal{F}} \rho_a = \exp \left[ \sum_{a \in \mathcal{F}} \log(\rho_a) \right],$$

(10)

where $\{\rho_a\}_{a \in \mathcal{F}}$ are positive definite operators. Whereas the concept of the partial sum is generalized as

$$Z = \text{Tr}(\rho).$$

(11)

(The formal definition of $\otimes$ and $\rho_a$ in (10) will be given later in (12).) In this sense, one can treat the CFGs as a special case of the QFGs where all the involved local operators $\{\rho_a\}_{a \in \mathcal{F}}$ are diagonal. We are especially interested in suitable generalizations of the aforementioned CFG techniques to QFGs. In particular, we study the closing-the-box notion and the variational approach in QFG setup. Although there are potentially interesting quantum mechanical uses for these findings, we are more broadly interested in exploring the power of generalizations of CFGs and the sum-product algorithm. Let us note that some other quantum-mechanics-inspired generalizations of factor graphs were studied in [12], [13], [14].

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Fig. 1. CFGs appeared in Examples 1 and 2.
The rest of this report is organized as follows. Section II introduces QFGs and studies the corresponding closing-the-box operations. Section III defines the quantum Bethe approximation and derives the quantum sum-product algorithm (QSPA). Section IV presents a numerical example illustrating the performance of QSPA. Section V concludes the report.

Throughout this report, we use the notations $\mathcal{L}(\mathcal{H})$, $\mathcal{L}^+(\mathcal{H})$, $\mathcal{L}^+_{++}(\mathcal{H})$ to denote the set of linear operators, Hermitian operators, positive semi-definite (PSD), and strict positive definite operators on the Hilbert space $\mathcal{H}$, respectively. Additionally, the set of density operators and strictly positive definite density operators on $\mathcal{H}$ are denoted as $\mathcal{L}^+_{++}(\mathcal{H})$, where the subscript ‘1’ indicates the trace-1 requirement.

The trace of $\rho \in \mathcal{L}^+_{++}(\mathcal{H})$ is defined in the standard way. The partial trace of $\rho \in \mathcal{L}^+_{++} (\mathcal{H}_1 \otimes \mathcal{H}_2)$ over $\mathcal{H}_1$ will be denoted by $\text{Tr}_1(\rho)$, with an analogous notation for the partial trace over $\mathcal{H}_2$. Note that $\text{Tr}(\rho) = \text{Tr}_1 (\text{Tr}_2(\rho)) = \text{Tr}_2 (\text{Tr}_1(\rho))$.

The inner product on operators is defined as $\langle A, B \rangle \triangleq \text{Tr}(AH)$, where $A^H$ stands for the adjoint/Hermitian of the operator $A$. Moreover, $S(\rho) \triangleq -\langle \rho, \log \rho \rangle$ and $S(\sigma \mid \rho) \triangleq \langle \sigma, \log \sigma \rangle - \langle \sigma, \log \rho \rangle$ denote the von Neumann entropy and the quantum relative entropy, respectively.

Equation (13) generalizes the formula [17], one can rewrite (12) as

$$\rho_A \circ \rho_B = \exp \left( \frac{1}{n} \right) \left( \rho_A \rho_B \right)^n,$$

Equation (13) generalizes the $\circ$ product to operators $\rho_A, \rho_B \in \mathcal{L}^+_{++} (\mathcal{H})$. Notice that the $\circ$ product is both associative and commutative, i.e.,

$$\rho_A \circ (\rho_B \circ \rho_C) = (\rho_A \circ \rho_B) \circ \rho_C \quad \forall \rho_A, \rho_B, \rho_C \in \mathcal{L}^+_{++} (\mathcal{H}),$$

In the following text, we will also use the notation $\rho_A \circ \rho_B$ when $\rho_A$ and $\rho_B$ are defined on different Hilbert spaces. For example, if $\rho_A \in \mathcal{L}^+_{++} (\mathcal{H}_1 \otimes \mathcal{H}_2)$ and $\rho_B \in \mathcal{L}^+_{++} (\mathcal{H}_2 \otimes \mathcal{H}_3)$, then

$$\rho_A \circ \rho_B \triangleq \left( \rho_A \otimes I_3 \right) \circ (I_1 \otimes \rho_B),$$

where $I_1$ and $I_3$ are the identity operators on $\mathcal{H}_1$ and $\mathcal{H}_3$, respectively. Note that $\rho_A \circ \rho_B$ is an operator on the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$. Similarly, we also adopt such a convention to expressions like $\bigodot_{a \in \mathcal{F}} \rho_a$, where equation (16) is applied repeatedly. In this case, one should note that $\log (\rho \circ I) = \log (\rho) \circ I$.

**Definition 3.** A QFG [11] is a bipartite graph with variable node set $\mathcal{V}$, function node set $\mathcal{F}$, and edge set $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{F}$, where with every $i \in \mathcal{V}$ we associate a Hilbert space $\mathcal{H}_i$, and with every $a \in \mathcal{F}$ we associate the Hilbert space $\mathcal{H}_a \triangleq \bigotimes_{i \in \partial a} \mathcal{H}_i$ and some local operator $\rho_a \in \mathcal{L}^+ (\mathcal{H}_a)$. The QFG’s global function is then defined to be

$$\rho \triangleq \bigodot_{a \in \mathcal{F}} \rho_a = \exp \left( \sum_{a \in \mathcal{F}} \log (\rho_a) \right),$$

and its partition sum is defined to be

$$Z \triangleq \text{Tr}(\rho).$$

Note that the global operator $\rho$ is always a PSD operator on $\bigotimes_{i \in \mathcal{V}} \mathcal{H}_i$, i.e., $\rho \in \mathcal{L}^+ (\bigotimes_{i \in \mathcal{V}} \mathcal{H}_i)$. Moreover, if all the local operators are strictly positive definite (i.e., $\rho_a \in \mathcal{L}^+_{++} (\mathcal{H}_a)$), we can further conclude $\rho \in \mathcal{L}^+_{++} (\bigotimes_{i \in \mathcal{V}} \mathcal{H}_i)$. In the remaining of this report, all Hilbert spaces $\mathcal{H}_i, i \in \mathcal{V}$, will be considered to be finite-dimensional.

\footnote{To be rigorous, one still need to check the convergence of the limit on the right-hand-side of (13). For such details, we refer the readers to [17] and Theorem 1.2 in [18].}
Example 4. Consider the QFG in Fig. 2 with variable node set \( V = \{1, 2\} \), function node set \( \mathcal{F} = \{A, B, C\} \), and local operators \( \rho_A \in \mathcal{L}^+(H_1) \), \( \rho_B \in \mathcal{L}^+(H_1 \otimes H_2) \), and \( \rho_C \in \mathcal{L}^+(H_2) \). This QFG has the global function \( \rho = \rho_A \odot \rho_B \odot \rho_C \) and the partition sum \( Z = \text{Tr}(\rho_A \odot \rho_B \odot \rho_C) \). Notice that we have adopted the notion of the normal factor graphs in Fig. 2.

The price that we pay for going from CFGs to QFGs is that the operation \( \odot \) does in general not distribute over the partial trace. In terms of the QFG in Example 4, this means that in general
\[
\text{Tr}(\rho_A \odot \rho_B \odot \rho_C) = \text{Tr}(\text{Tr}_2(\rho_A \odot \rho_B \odot \rho_C)) \neq \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)).
\] (19)

Example 5. Consider the Hilbert spaces \( H_1 = H_2 = \mathbb{C}^2 \) and the operators \( X \) and \( Y \) acting on \( H_1 \) and \( H_1 \otimes H_2 \), respectively, where
\[
X \triangleq \frac{1}{2} \left[ \begin{array}{cc} +1 & -1 \\ -1 & +1 \end{array} \right], \quad Y \triangleq \left[ \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right].
\]
In this case, \( \text{Tr}_1(\text{Tr}_2(X \otimes Y)) = 0 \) and \( \text{Tr}_1(\text{Tr}_2(Y)) = 1 \). Apparently, they are far from being equal.

Oftentimes, however, \( \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)) \) approximates \( \text{Tr}_1(\text{Tr}_2(\rho_A \odot \rho_B \odot \rho_C)) \) reasonably well. A central topic of this report is to understand the cases where this happens, so that an approximate notion of closing-the-box can be salvaged.

Lemma 6. Given \( \rho_A \in \mathcal{L}^{++}(H_1) \), \( \rho_B \in \mathcal{L}^{++}(H_1 \otimes H_2) \) and \( \rho_C \in \mathcal{L}^{++}(H_2) \), the quantities appearing in (19) satisfy
\[
S(\kappa(\rho_A))^{-1} \leq \frac{\text{Tr}(\rho_A \odot \rho_B \odot \rho_C)}{\text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C))} \leq S(\kappa(\rho_A)),
\] (20)
where \( \kappa(\rho_A) \geq 1 \) is the condition number of the operator \( \rho_A \), and \( S(\cdot) \) is the Specht ratio function defined as
\[
S(r) \triangleq \frac{(r - 1) \cdot e^{-r}}{r \cdot \log r}.
\] (21)

Proof. Consider the Golden–Thompson inequality and its reverse [19], namely,
\[
\text{Tr}(e^{V+W}) \leq \text{Tr}(e^V e^W) \leq S(\alpha) \cdot \text{Tr}(e^{V+W}),
\] (22)
where \( V \) and \( W \) are Hermitian operators, and \( \alpha \) is the condition number of \( e^V \). Notice that for (strict) positive definite operators \( \rho_1, \rho_2 \), operators \( \log \rho_1 \) and \( \log \rho_2 \) are Hermitian. Thus, by substituting \( V \triangleq \log \rho_1, \ W \triangleq \log \rho_2 \) into (22), we obtain
\[
\text{Tr}(\rho_1 \odot \rho_2) \leq \text{Tr}(\rho_1 \rho_2) \leq S(\kappa(\rho_1)) \cdot \text{Tr}(\rho_1 \odot \rho_2).
\] (23)

The first inequality in (20) follows from
\[
\text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)) \leq \text{Tr}_1(\rho_A \cdot \text{Tr}_2(\rho_B \odot \rho_C)) \quad (24)
\]
\[
= \text{Tr}(\rho_A \cdot (\rho_B \odot \rho_C)) \leq S(\kappa(\rho_A)) \cdot \text{Tr}(\rho_A \odot (\rho_B \odot \rho_C)) \quad (25)
\]
\[
\leq S(\kappa(\rho_A)) \cdot \text{Tr}(\rho_A \odot \rho_B \odot \rho_C), \quad (26)
\]
where we apply the left inequality of (23) in (24) by substituting \( \rho_1 = \rho_A, \rho_2 = \rho_B \odot \rho_C \), and the right inequality in (26) by substituting \( \rho_1 = \rho_A, \rho_2 = \rho_B \odot \rho_C \). Similarly, the second inequality in (20) can be justified via
\[
\text{Tr}(\rho_A \odot \rho_B \odot \rho_C) \leq \text{Tr}(\rho_A \cdot (\rho_B \odot \rho_C)) \leq \text{Tr}(\rho_A \cdot \text{Tr}_2(\rho_B \odot \rho_C)) \leq S(\kappa(\rho_A)) \cdot \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)),
\] (27)
which the use of (23) appears in (28) and (30), respectively.

Finally, equation (22) can be obtained by taking divisions on both sides of inequality (27) and (30) w.r.t.
\[
\text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)) \cdot \text{Tr}(\rho_A \odot \rho_B \odot \rho_C).
\]
Note that \( \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)) > 0 \) since \( \rho_A, \rho_B, \) and \( \rho_C \) are strictly positive definite.
Lemma 6 indicates that $\text{Tr}_{a}(\rho_{A} \circ \text{Tr}_{2}(\rho_{B} \circ \rho_{C}))$ should approximate $\text{Tr}(\rho_{A} \circ \rho_{B} \circ \rho_{C})$ reasonably well when $\rho_{A}$ (or $\rho_{B} \circ \rho_{C}$) is close to the identity matrix. Following theorem identifies such approximation given that $\rho_{A}$ (or $\rho_{B} \circ \rho_{C}$) is close to the identity matrix in a linear fashion, i.e., $\rho_{A} = I + tX$ and $\rho_{B} \circ \rho_{C} = I + tY$ for some number $t$ close to 0. Another approach to study such approximation is to assume $\rho_{A} = e^{tX}$ and $\rho_{B} \circ \rho_{C} = e^{tY}$. We present the second approach in Appendix B.

**Theorem 7.** Consider finite-dimensional Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. Given $X \in \mathcal{L}^{	ext{II}}(\mathcal{H}_1)$, and $Y \in \mathcal{L}^{	ext{II}}(\mathcal{H}_1 \otimes \mathcal{H}_2)$, it holds that

$$\text{Tr}[(I + tX) \otimes (I + tY)] = \text{Tr}_{1}[(I + tX) \otimes \text{Tr}_{2}(I + tY)] + O(t^4),$$

where the real number $t$ is in a neighborhood of 0 such that $I + tX$ and $I + tY$ are always positive definite. In other words, $\text{Tr}_{1}[(I + tX) \otimes \text{Tr}_{2}(I + tY)]$ approximates $\text{Tr}[(I + tX) \otimes (I + tY)]$ when $t$ is small, and the error is of 4-th order of $t$.

**Proof.** The theorem statement can be justified by the Taylor series expansion. Due to the tediousness and the calculation nature of the proof, we skip the proof here. Interested readers may find the detailed proof in Appendix A. \hfill \Box

Similarly, we also have the following approximation.

**Corollary 8.** Following the same setup as in Theorem 7, we have

$$\text{Tr}_{2}[(I + tX) \otimes (I + tY)] = (I + tX) \otimes \text{Tr}_{2}(I + tY) + O(t^3).$$

The proof of Corollary 8 can also be found in Appendix A.

**Corollary 9.** Let $N \geq 3$. Consider a chain QFG as in Fig. 3 where $\rho_{1} \in \mathcal{L}^{++}(\mathcal{H}_1)$, $\rho_{N} \in \mathcal{L}^{++}(\mathcal{H}_{N-1})$ and $\rho_{k} \in \mathcal{L}^{++}(\mathcal{H}_{k-1} \otimes \mathcal{H}_k)$ for each $k = 2, \ldots, N - 1$. Suppose all $\{\rho_{k}\}_{k=1}^{N}$ are close to the identity matrix $I$ in the sense that $\rho_{k} = I + t \cdot \chi_{k}$ for some real number $t$ close to 0 and some Hermitian operator $\chi_{k}$, then Theorem 7 implies the following estimation:

$$\text{Tr}[ho_{1} \circ \rho_{2} \circ \cdots \circ \rho_{N-1} \circ \rho_{N}] = \text{Tr}_{N-1} \{\text{Tr}_{N-2} \{\cdots \text{Tr}_{2} \{\text{Tr}_{1} (\rho_{1} \circ \rho_{2} \cdots ) \circ \rho_{N-1} \} \circ \rho_{N} \} + O(t^4).$$

**Proof.** We can justify (33) by mathematical induction w.r.t. $N$. Note that for $N = 3$, (33) is nothing but an instance of (31). Now, suppose (33) is true for $N = K + 1$, we have

$$\text{Tr}[ho_{1} \circ \cdots \circ \rho_{K+1}] = \text{Tr}_{1} \{\text{Tr}_{2} (\rho_{1} \circ \rho_{2} \circ \cdots \circ \rho_{K+1})\} + O(t^4)$$

$$= \text{Tr}_{K} \{\text{Tr}_{K-1} \{\cdots \text{Tr}_{2}(\text{Tr}_{1} (\rho_{1} \circ \rho_{2} \circ \cdots ) \circ \rho_{K} \} \circ \rho_{K+1} \} + O(t^4),$$

where (34) is due to Theorem 7 and (35) is due to the induction hypothesis. Thus, the corollary is proven. \hfill \Box

Theorem 7 and Corollary 8 establish the following approximate distributive laws of the $\circ$ operation over the (partial) trace functions:

$$\text{Tr} (A \circ B) \approx \text{Tr}_{\partial b \setminus \partial a} (A \circ \text{Tr}_{\partial a} (B)),$$

$$\text{Tr}_{\partial a} (A \circ B) \approx A \circ \text{Tr}_{\partial b} (B),$$

where $A \in \mathcal{L}^{+} (\bigotimes_{i \in \partial a} \mathcal{H}_i)$, $B \in \mathcal{L}^{+} (\bigotimes_{i \in \partial b} \mathcal{H}_i)$ are close to the identity matrix $I$; and the index sets $\mathcal{I} \subseteq \partial b \setminus \partial a$, $\partial a \subseteq \partial b$. For the rest of this report, we shall use the notation “$\approx X$” or “$\sim X$” whenever (36) or (37) is used to derive an approximate equality or an approximate proportionality result, respectively.

It is worthwhile to do a brief numerical comparison between $\text{Tr}_{1}(\rho_{A} \circ \text{Tr}_{2}(\rho_{B}))$ and $\text{Tr}_{1}(\text{Tr}_{2}(\rho_{A} \circ \rho_{B}))$. Namely, we randomly generate $\rho_{A} \in \mathcal{L}^{+}(C^4)$ and $\rho_{B} \in \mathcal{L}^{+}(C^4)$ and plot in Fig. 4 the statistical distribution of

$$\eta \triangleq \frac{\text{Tr}_{1}[\rho_{A} \circ \text{Tr}_{2}(\rho_{B})] - \text{Tr}_{1}[\text{Tr}_{2}(\rho_{A} \circ \rho_{B})]}{\text{Tr}_{1}[\text{Tr}_{2}(\rho_{A} \circ \rho_{B})]}.$$

Here, $\rho_{A} \triangleq U_{A}^{H} \Lambda_{A} U_{A}$ and $\rho_{B} \triangleq U_{B}^{H} \Lambda_{B} U_{B}$, where the unitary matrices $U_{A}$ and $U_{B}$ contain random orthonormal vectors uniformly distributed on the corresponding complex unit spheres, and each of the diagonal entries of the diagonal matrices.
Lemma 10. Consider a QFG with no cycles. Assume that some density operators \( \{ \sigma_a \in \mathcal{L}_1^+(\mathcal{H}_a) \}_{a \in \mathcal{F}} \) and \( \{ \sigma_i \in \mathcal{L}_1^+(\mathcal{H}_i) \}_{i \in \mathcal{V}} \) satisfy the local marginal conditions

\[
\sigma_i = \text{Tr}_{\partial \setminus \{i\}} (\sigma_a) \quad \forall (i, a) \in \mathcal{E}.
\] (39)

Then, there exists a global density operator \( \sigma \) such that

\[
\text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} (\sigma) \approx \sigma_a \quad \forall a \in \mathcal{F},
\] (40)

\[
\text{Tr}_{\mathcal{V} \setminus \{i\}} (\sigma) \approx \sigma_i \quad \forall i \in \mathcal{V}.
\] (41)

Proof. Define the density operator \( \sigma \in \mathcal{L}_1^+ \left( \bigotimes_{i \in \mathcal{V}} \mathcal{H}_i \right) \) by letting

\[
\sigma \propto \exp \left[ \sum_{a \in \mathcal{F}} \log(\sigma_a) - \sum_{i \in \mathcal{V}} (d_i - 1) \log(\sigma_i) \right],
\] (42)

where \( d_i \) is the degree of variable node \( i \in \mathcal{V} \). To prove (40), we have

\[
\text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} (\sigma) \propto \text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} \left\{ \exp \left[ \sum_{a \in \mathcal{F}} \log(\sigma_a) - \sum_{i \in \mathcal{V}} (d_i - 1) \log(\sigma_i) \right] \right\}
\] (43)

\[
= \text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} \left\{ \exp \left[ \log(\sigma_a) + \sum_{n=0}^{N} \sum_{a \in \mathcal{F}} \sum_{c \in \mathcal{H}_a} \log \left( \sigma_c \right) - \log \left( \sigma_i \right) \right] \right\}
\] (44)

\[
= \text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} \left\{ \exp \left[ \log(\sigma_a) + \sum_{n=0}^{N} \sum_{a \in \mathcal{F}} \sum_{c \in \mathcal{H}_a} \log \left( \sigma_c \right) - \log \left( \sigma_i \right) \right] \odot \odot_{i \in \partial \setminus \partial \setminus \{i\}} \left( \sigma_c \odot \sigma_i^{-1} \right) \right\}
\] (45)

\[
\approx \text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} \left\{ \exp \left[ \log(\sigma_a) + \sum_{n=0}^{N-1} \sum_{a \in \mathcal{F}} \sum_{c \in \mathcal{H}_a} \log \left( \sigma_c \right) - \log \left( \sigma_i \right) \right] \odot \odot_{i \in \partial \setminus \partial \setminus \{i\}} \left( \text{Tr}_{\partial \setminus \{i\}} (\sigma_c) \odot \sigma_i^{-1} \right) \right\}
\] (46)

\[
= \text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} \left\{ \exp \left[ \log(\sigma_a) + \sum_{n=0}^{N-1} \sum_{a \in \mathcal{F}} \sum_{c \in \mathcal{H}_a} \log \left( \sigma_c \right) - \log \left( \sigma_i \right) \right] \right\}
\] (47)

\[
\approx \cdots \approx \text{Tr}_{\mathcal{V} \setminus \partial \setminus \{i\}} \left\{ \exp \left[ \log(\sigma_a) \right] \right\} = \sigma_a
\] (48)
where $\partial^a \sigma$ denotes the set of variables reachable from $a$ after walking through $n$ factors, and $\partial^i$ denotes the neighbor set of $i$ excluding the factor through which $a$ reaches $i$. The expansion (44) is due to the tree structure of the QFG, and (46) follows directly from Corollary 8. Here, the number $N$ in (44) is the depth/height of the tree rooting from the factor node $a$.

The justification for (41) is similar, and is omitted.

Notice that if we consider

$$
\sigma \triangleq \exp \left[ \sum_{a \in F} \log(\sigma_a) - \sum_{i \in V} (d_i - 1) \log(\sigma_i) \right],
$$

we may not have $\text{Tr} (\sigma) = 1$; even though a similar results holds on acyclic CFGs, namely

$$
\sum_{\mathbf{x}} \left\{ \prod_{a \in F} b_a(\mathbf{x}_{\partial a}) \prod_{i \in V} b_i(x_i) \right\} = 1,
$$

where $b_a, b_i$ are marginal distributions on $\mathbf{x}_{\partial a}$ and $x_i$, respectively, which satisfy the local marginal constrains, i.e.,

$$
\sum_{\mathbf{x}_{\partial a} \setminus \{i\}} b_a(\mathbf{x}_{\partial a}) = b_i(x_i) \quad \forall i \in X_i, \forall (i, a) \in E.
$$

However, by (48), we can still conclude

$$
\text{Tr} (\bar{\sigma}) = \text{Tr}_{\partial a} \left\{ \text{Tr}_{V \setminus \partial a} \left\{ \exp \left[ \sum_{a \in F} \log(\sigma_a) - \sum_{i \in V} (d_i - 1) \log(\sigma_i) \right] \right\} \right\} \approx \text{Tr}_{\partial a} \{ \sigma_a \} = 1.
$$

In this case, we often regard $\bar{\sigma}$ as an approximation of the corresponding global density operator.

III. VARIATIONAL APPROACHES

In the case of CFGs, the negative log partition sum can be written as the minimum of the so-called Gibbs free energy function [8]. Although this reformulation does not generalize to any similar optimization problem, it suggests the introduction of other free energy functions (like the Bethe free energy function) which approximate the Gibbs free energy function. The Bethe free energy function is particularly interesting because stationary points of the Bethe free energy function correspond to fixed points of the SPA [8]. The minimum of the Bethe free energy function can be used as an approximation of the negative log partition function.

In this section, we present a QFG analog of the Bethe free energy function and use it then to derive the quantum SPA (QSPA), called quantum belief propagation in [11]. We start by defining a quantum analog of the Gibbs free energy function.

**Definition 11.** Given a QFG $\mathcal{G}$ with variable set $V$, factor operators $\{\rho_a\}_{a \in F}$, and global Hilbert space $\mathcal{H} = \bigotimes_{x \in V} \mathcal{H}_x$, we define the quantum Helmholtz free energy and the quantum Gibbs free energy function w.r.t. the density operator $\sigma \in L_1^+(\mathcal{H})$ to be, respectively,\(^2\)

$$
F_H \triangleq -\log(Z),
$$

$$
F_{\text{Gibbs}}(\sigma) \triangleq -\sum_{a \in F} \langle \sigma, \log \rho_a \rangle - S(\sigma)
$$

$$
= -\sum_{a \in F} \langle \text{Tr}_{V \setminus \partial a}(\sigma), \log \rho_a \rangle - S(\sigma).
$$

Here, we recall the definition of $S(\cdot)$ and the operator inner product $\langle \cdot, \cdot \rangle$ from the end of Section I.

**Theorem 12.** We have the following relationship between the quantum Gibbs free energy function and the quantum Helmholtz free energy, namely,

$$
F_{\text{Gibbs}}(\sigma) = F_H + S(\sigma \parallel \bar{\rho}),
$$

where $\sigma$ and $\bar{\rho} \triangleq \rho/Z = Z^{-1} \cdot \exp(\sum_{a \in F} \log \rho_a)$ are density operators.

\(^2\)If $\rho_A$ and $\rho_B$ in $\langle \rho_A, \rho_B \rangle$ are over different Hilbert spaces, then both $\rho_A$ and $\rho_B$ are implicitly embedded in the smallest Hilbert space that contains both Hilbert spaces.
Proof. The proof is straightforward. Namely, we have
\[
F_{\text{Gibbs}}(\sigma) - F_{\text{H}} = - \sum_{a \in F} \langle \sigma, \log \rho_a \rangle + \langle \sigma, \log \sigma \rangle + \log(Z)
\]
\[
= \langle \sigma, \log \sigma \rangle - \left( \sum_{a \in F} \log \rho_a \right) - \langle \sigma, - \log(Z) \cdot I \rangle
\]
\[
= \langle \sigma, \log \sigma \rangle - \langle \sigma, \log \rho - \log(Z) \cdot I \rangle
\]
\[
= \langle \sigma, \log \sigma \rangle - \langle \sigma, \log(\rho/Z) \rangle
\]
\[
= \langle \sigma, \log \sigma \rangle - \langle \sigma, \log \tilde{\rho} \rangle = S(\sigma \| \tilde{\rho}).
\]
\[
\square
\]

It is a well-known result [20] that for density operators \(\rho_A, \rho_B \in \mathcal{L}_1^+ (\mathcal{H})\), the quantum relative entropy satisfies
\[
S(\rho_A \parallel \rho_B) \geq 0,
\]
where equality holds if and only if \(\rho_A = \rho_B\). In this case, the optimization problem
\[
\min_{\sigma} F_{\text{Gibbs}}(\sigma)
\]
\[
s.t. \quad \sigma \in \mathcal{L}_1^+ (\mathcal{H})
\]
has a unique minimizer \(\sigma^* = \tilde{\rho}\), and the minimum value turns out to be \(F_{\text{Gibbs}}(\sigma^*) = F_{\text{H}}\). Thus, (58) can be viewed as a re-formulation of the partition sum as defined in (18). However, such a reformulation does in general not yield a tractable minimization problem because of the number of involved dimensions.

Therefore, we introduce the following quantum Bethe free energy function as an approximation to the Gibbs free energy function.

**Definition 13.** We define the quantum Bethe free energy function of a QFG to be
\[
F_{\text{Bethe}}((\sigma_a)_{a \in F}, (\sigma_i)_{i \in V}) \triangleq - \sum_{a \in F} \langle \sigma_a, \log \rho_a \rangle - \sum_{a \in F} S(\sigma_a) + \sum_{i \in V} (d_i - 1) \cdot S(\sigma_i),
\]
where \((\sigma_a)_{a \in F}\) and \((\sigma_i)_{i \in V}\) are density operators. \(\square\)

Indeed, the Bethe free energy function can be viewed as an approximation of the Gibbs free energy function as shown in next theorem.

**Theorem 14.** Consider a QFG with no cycles. For some global density operator \(\sigma\), let \(\sigma_a \triangleq \text{Tr}_{\mathcal{V} \backslash \partial a}(\sigma)\) for all \(a \in F\), and \(\sigma_i = \text{Tr}_{\partial i}(\sigma)\) for all \(i \in V\). Then, using the approximation notation as in (36), we have
\[
F_{\text{Gibbs}}(\sigma) \approx F_{\text{Bethe}}((\sigma_a)_{a \in F}, (\sigma_i)_{i \in V}).
\]
Or, to be precise, if \(\sigma\) is \(t\)-close to the identity matrix \(I\) in a linear fashion, i.e., \(\sigma = I + t \cdot \chi\) for some real number \(t\) close to 0 and some Hermitian operator \(\chi\), then
\[
F_{\text{Gibbs}}(\sigma) = F_{\text{Bethe}}((\sigma_a)_{a \in F}, (\sigma_i)_{i \in V}) + O(t^3).
\]

**Proof.** Consider the definition of \(F_{\text{Gibbs}}\). Firstly, we have
\[
\sum_{a \in F} \langle \sigma_a, \log \rho_a \rangle = \sum_{a \in F} \langle \text{Tr}_{\mathcal{V} \backslash \partial a} \sigma, \log \rho_a \rangle = \sum_{a \in F} \langle \sigma, \log \rho_a \rangle.
\]
Now, let
\[
\tilde{\sigma} \triangleq \exp \left[ \sum_{a \in F} \log(\sigma_a) - \sum_{i \in V} (d_i - 1) \log(\sigma_i) \right].
\]
Rearranging the terms, we have
\[
\sum_{a \in \mathcal{F}} \mathcal{S}(\sigma_a) - \sum_{i \in \mathcal{V}} (d_i - 1) \cdot \mathcal{S}(\sigma_i) = - \sum_{a \in \mathcal{F}} \text{Tr} (\sigma_a \log (\sigma_a)) + \sum_{i \in \mathcal{V}} (d_i - 1) \cdot \text{Tr} (\sigma, \log (\sigma_i))
\]
\[
= - \text{Tr} \left( \sigma \cdot \left[ \sum_{a \in \mathcal{F}} \log (\sigma_a) - \sum_{i \in \mathcal{V}} (d_i - 1) \log (\sigma_i) \right] \right)
\]
\[
= - \text{Tr} \left( \sigma \cdot \log (\sigma_a) \right)
\]
\[
= - \text{Tr} \left( \sigma \cdot \log \left( \frac{\sigma}{\text{Tr} (\sigma)} \right) \right) - \log (\text{Tr} (\sigma))
\]
\[
= - \text{Tr} \left( \sigma \cdot \log \left( \frac{\sigma}{\text{Tr} (\sigma)} \right) \right) + O(t^3),
\]
where we applied (52) in deriving (68). On the other hand, Lemma 10 indicates \( \text{Tr} \sigma \sigma \approx \sigma \) and \( \text{Tr} \partial_a \sigma \approx \sigma_a \) for each \( i \in \mathcal{V} \) and \( a \in \mathcal{F} \). In terms of their dual variables, this can be denoted as \( \eta(\sigma) = \eta(\sigma) + O(t^3) = \eta(\sigma) + t^3 \cdot \Delta \eta + O(t^4) \) for some real vector \( \Delta \eta \) (see Appendix C). In this case, denoting the function \( f(\eta) \triangleq - \text{Tr} \left( \sigma \cdot \log (\rho(\eta)) \right) \), we can further conclude,
\[
\lim_{t \to 0} \frac{\text{Tr} \left( \sigma \cdot \log \left( \frac{\sigma}{\text{Tr} (\sigma)} \right) \right) - (- \text{Tr} (\sigma \cdot \log (\sigma)))}{t^3} = \lim_{t \to 0} \frac{f(\eta) - f(\eta)}{t^3} = \lim_{t \to 0} \frac{f(\eta + t^3 \cdot \Delta \eta + O(t^4)) - f(\eta)}{t^3} = \nabla f^T \cdot \Delta \eta < \infty.
\]
Here, we assume \( f \) to be differentiable, which is justified in Appendix D. Thus, we can write
\[
- \text{Tr} \left( \sigma \cdot \log \left( \frac{\sigma}{\text{Tr} (\sigma)} \right) \right) = - \text{Tr} (\sigma \cdot \log (\sigma)) + O(t^3) = \mathcal{S}(\sigma) + O(t^3).
\]

Therefore, combining (62), (68) and (71), we have
\[
F_{\text{Bethe}} \left( (\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}} \right) = - \sum_{a \in \mathcal{F}} \langle \sigma_a, \log \rho_a \rangle - \sum_{a \in \mathcal{F}} \mathcal{S}(\sigma_a) + \sum_{i \in \mathcal{V}} (d_i - 1) \cdot \mathcal{S}(\sigma_i)
\]
\[
= - \sum_{a \in \mathcal{F}} \langle \sigma_a, \log \rho_a \rangle - \mathcal{S}(\sigma) + O(t^3)
\]
\[
= F_{\text{Gibbs}} (\sigma) + O(t^3).
\]
Theorem 14 allows us to treat the Bethe free energy \( F_{\text{Bethe}} \) as an approximation to the Gibbs free energy \( F_{\text{Gibbs}} \). This motivates us to define the following optimization problem as an “approximated” version of the optimization problem (58).

**Definition 15.** We call the optimization problem
\[
\min_{(\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}}} F_{\text{Bethe}} \left( (\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}} \right)
\]
\[
\text{s.t.} \quad \sigma_a \in \mathcal{L}_+^1 (H_a) \quad \forall a \in \mathcal{F}
\]
\[
\sigma_i \in \mathcal{L}_+^1 (H_i) \quad \forall i \in \mathcal{V}
\]
\[
\sigma_i = \text{Tr}_{\partial a \setminus i} (\sigma_a) \quad \forall (i, a) \in \mathcal{E}
\]
the **constrained quantum Bethe free energy minimization problem.**

In the case of CFGs without cycles, the minimum of the Bethe free energy function equals the minimum of the Gibbs free energy function, and with that the Bethe approximation of the partition sum is exact. However, in the case of QFGs without cycles, the Bethe approximation of the partition sum is in general only approximately equal to the partition sum.

In the rest of this section, we derive the QSPA from the constrained quantum Bethe free energy minimization problem.

**Theorem 16.** The positive definite density operators \( \{ (\sigma_a^*)_{a \in \mathcal{F}}, (\sigma_i^*)_{i \in \mathcal{V}} \} \) represent an internal stationary point for the constrained Bethe approximation if and only if for each \( a \in \mathcal{F} \) and \( i \in \mathcal{V} \), we have
\[
\sigma_a^* \propto \exp \left[ \log (\rho_a) + \sum_{i \in \partial a} \log (m_{i \rightarrow a}) \right],
\]
\[
\sigma_i^* \propto \exp \left[ \sum_{a \in \partial i} \log (m_{a \rightarrow i}) \right].
\]
where \( \{m_{i \rightarrow a}, m_{a \rightarrow i}\}_{(i,a) \in \mathcal{E}} \) are some positive definite operators satisfying

\[
m_{i \rightarrow a} \propto \exp \left[ \sum_{e \in \partial \setminus a} \log (m_{e \rightarrow i}) \right],
\]

\[
m_{a \rightarrow i} \propto \text{Tr}_{\partial \setminus a} \left\{ \exp \left[ \log (\rho_a) + \sum_{j \in \partial a} \log (m_{j \rightarrow a}) \right] \right\} \circ m_{i \rightarrow a}^{-1},
\]

for all \((i, a) \in \mathcal{E}\).

**Proof.** This theorem is a quantum analog to its classical version in [8], which provides part of the ideas in this proof.

Suppose \(\{(\sigma^*_a)_{a \in \mathcal{F}}, (\gamma^i)_{i \in \mathcal{V}}\}\) is an interior stationary point of the constrained quantum Bethe approximation problem. Since we only consider interior points, the Lagrangian can be written as

\[
L = F_{\text{Bethe}} + \sum_{a \in \mathcal{F}} \gamma_a \cdot (\text{Tr} (\sigma_a) - 1) + \sum_{i \in \mathcal{V}} \gamma_i \cdot (\text{Tr} (\sigma_i) - 1) + \sum_{(i,a) \in \mathcal{E}} \text{Tr} (\lambda_{a,i} \cdot (\sigma_i - \text{Tr}_{\partial a \setminus i} (\sigma_a))),
\]

with the dual variables \(\{\gamma_a\}_{a \in \mathcal{F}}, \{\gamma_i\}_{i \in \mathcal{V}} \in \mathbb{R}, \{\lambda_{a,i}\}_{(i,a) \in \mathcal{E}} \in \mathcal{L}(\mathcal{H}_i)\). Thus, there must exist some \(\{\gamma^*_a\}_{a \in \mathcal{F}}, \{\gamma^*_i\}_{i \in \mathcal{V}}\) and \(\{\lambda^*_{a,i}\}_{(i,a) \in \mathcal{E}}\) such that \(L\) satisfies the following conditions

\[
\frac{\partial L}{\partial \gamma_a} = 0, \quad \forall a \in \mathcal{F};
\]

\[
\frac{\partial L}{\partial \gamma_i} = 0, \quad \forall i \in \mathcal{V};
\]

\[
\frac{d}{dt} L(\lambda^*_{a,i} + tC) = 0, \quad \forall C \in \mathcal{L}^H(\mathcal{H}_i), \quad \forall (i, a) \in \mathcal{E};
\]

\[
\frac{d}{dt} L(\sigma^*_a + tC) = 0, \quad \forall C \in \mathcal{L}^H(\mathcal{H}_a), \quad \forall a \in \mathcal{F};
\]

\[
\frac{d}{dt} L(\sigma^*_i + tC) = 0, \quad \forall C \in \mathcal{L}^H(\mathcal{H}_i), \quad \forall i \in \mathcal{V}.
\]

Notice that (80), (81), and (82) are equivalent to (72), (73), and (74). Also, by the Spectral Theorem and first-order perturbation theory [21], Equations (83) and (84) can be expanded as

\[
- \text{Tr}(C \cdot \log \rho_a) + \text{Tr}(C \cdot (I + \log \sigma^*_a)) + \text{Tr}(C \cdot \gamma_i^* I) - \sum_{i \in \partial a} \text{Tr}(\lambda^*_{a,i} \cdot \text{Tr}_{\partial a \setminus i} C) = 0,
\]

\[
(1 - d_i) \cdot \text{Tr}(C \cdot (I + \log \sigma^*_i)) + \text{Tr}(C \cdot \gamma^*_i I) + \sum_{a \in \partial i} \text{Tr}(C \cdot \lambda^*_{a,i}) = 0.
\]

Solving the above equations for \(\{(\sigma^*_a)_{a \in \mathcal{F}}, (\gamma^*_i)_{i \in \mathcal{V}}\}\), respectively, we have

\[
\sigma^*_a = \exp \left[ \log \rho_a + \sum_{i \in \partial a} \lambda^*_{a,i} - (1 + \gamma_a^* I) \right], \quad \forall a \in \mathcal{F},
\]

\[
\sigma^*_i = \exp \left[ \frac{1}{d_i - 1} \cdot (1 + \gamma_i^* I + \sum_{a \in \partial i} \lambda^*_{a,i}) \right], \quad \forall i \in \mathcal{V}.
\]

Now, define \(\{m_{i \rightarrow a}\}_{(i,a) \in \mathcal{E}}\) and \(\{m_{a \rightarrow i}\}_{(i,a) \in \mathcal{E}}\) in explicit by satisfying

\[
\lambda^*_{a,i} = \log m_{i \rightarrow a},
\]

\[
\lambda^*_{a,i} = \sum_{e \in \partial \setminus a} \log m_{e \rightarrow i} \quad \forall (i, a) \in \mathcal{E}.
\]

In this case, (75) and (76) are direct results of (87) and (88), respectively; and (78) follows from (74). Additionally the positive definite properties of \(\{m_{i \rightarrow a}\}_{(i,a) \in \mathcal{E}}\) and \(\{m_{a \rightarrow i}\}_{(i,a) \in \mathcal{E}}\) follow form the same properties of \(\{\sigma^*_a\}_{a \in \mathcal{F}}\) and \(\{\gamma^*_i\}_{i \in \mathcal{V}}\).

As the reverse part of the proof, suppose there exists some \(\{m_{i \rightarrow a}\}_{(i,a) \in \mathcal{E}}\) and \(\{m_{a \rightarrow i}\}_{(i,a) \in \mathcal{E}}\) satisfying (75), (76), (77), and (78). By choosing \(\{\gamma^*_a\}_{a \in \mathcal{F}}, \{\gamma^*_i\}_{i \in \mathcal{V}},\) and \(\{\lambda^*_{a,i}\}_{(i,a) \in \mathcal{E}}\) satisfying (87), (88), and (89), respectively, one can easily check (85) and (86) (or (83) and (84)). Given that (80), (81), and (82) are equivalent to (72), (73), and (74), we have verified that the chosen \(\{(\sigma^*_a)_{a \in \mathcal{F}}, (\gamma^*_i)_{i \in \mathcal{V}}\}\) is a stationary point. \qed
Notice that, by Theorem 7, Eq. (78) can be approximated by
\[
m_{a \rightarrow i}^{(t+1)} \propto \exp \left[ \sum_{c \in \partial_i \setminus a} \log(m_{c \rightarrow i}^{(t)}) \right],
\]
and
\[
m_{a \rightarrow i}^{(t+1)} \propto \exp \left[ \log(\rho_a) + \sum_{j \in \partial_i \setminus a} \log(m_{j \rightarrow a}^{(t)}) \right].
\]
Thus, the QSPA is defined as follows.

**Definition 17.** The Quantum Sum-Product Algorithm (QSPA) [11] is an iterative method defined by the following message update rules:

\[
m_{i \rightarrow a}^{(t+1)} \propto \exp \left[ \sum_{c \in \partial_i \setminus a} \log(\rho_{c \rightarrow i}) \right],
\]

\[
m_{a \rightarrow i}^{(t+1)} \propto \exp \left[ \log(\rho_a) + \sum_{j \in \partial_i \setminus a} \log(m_{j \rightarrow a}^{(t)}) \right].
\]

Here, we assume the initial messages \( \{m_{i \rightarrow a}^{(0)}, m_{a \rightarrow i}^{(0)}\}_{(i,a) \in E} \) to be the identity matrices on the corresponding Hilbert spaces.

It may seem that Theorem 16 provides a good lead in solving the constrained Bethe approximation problem, but the situation is more complicated. On the one hand, solving Equations (77) and (78) for messages \( \{m_{i \rightarrow a}, m_{a \rightarrow i}\}_{(i,a) \in E} \) is intrinsically of the same complexity as the original problem. By the time of this writing, we know of no explicit solution/practical algorithm in solving (77) and (78) with exact, which is also the case for CFGs. Though the QSPA given by Definition 17 provides an iterative method to estimate \( \{m_{i \rightarrow a}, m_{a \rightarrow i}\}_{(i,a) \in E} \), there is no guarantee of convergence of such algorithm. On the other hand, even if we can find such messages, the obtained density operators \( \{\sigma_{a \rightarrow i}^{*}, \sigma_{i \rightarrow a}^{*}\}_{a \in F, i \in V} \) are merely an approximate stationary point of the constrained Bethe approximation problem, which is not necessarily a minimizer or an approximate minimizer of the problem. Despite such concerns, as illustrated in next section, the QSPA still shows rather promising performance in a number of the numerical applications.

**IV. Numerical Example**

In this section, we apply the QSPA on the QFG in Fig. 5, and consider the relative error between the QSPA-based estimate and the true partition sum, i.e.,
\[
\eta \triangleq \frac{Z_{\text{QSPA}}}{Z} - 1,
\]
where \( Z_{\text{QSPA}} \) is calculated via the Bethe free energy function (59) at the estimated density operators \( \{\sigma_{a \rightarrow i}^{*}, \sigma_{i \rightarrow a}^{*}\}_{a \in F, i \in V} \) given by (75) and (76). Here, for each test, the factors \( \{\rho_a\}_{a=1,...,6} \) are generated randomly in a similar fashion as described in the example depicted in Fig. 4. Fig. 6 plots the statistics of \( \eta \) based on \( 10^4 \) simulated cases for different eigenvalue distributions. Note that the y-axis in Fig. 6 is scaled to match the definition of a density function (i.e., the area under each curve is 1).

**V. Conclusions and Outlook**

In this report, we have considered the generalization of the closing-the-box notion and the variational approach under a quantum setup known as quantum factor graphs (QFGs). In particular, we justified the closing-the-box operations on QFGs as an approximate method to calculate the quantum partition sum. We also studied the relationship between the Bethe free energy minimization problem and the quantum sum-product algorithm (QSPA). It turns out that the fixed-points of the QSPA are the interior stationary point of the Bethe free energy minimization problem.
Currently, we are also considering the generalization of the method of loop calculus to the QFGs. As an example, Theorem 7 is also useful in deriving a quantum version of the Holant Theorem [22], [23], namely:

**Theorem 18 (Holant Theorem for QFGs).** Consider a QFG with variable node set $\mathcal{V}$, function node set $\mathcal{F}$, edge set $\mathcal{E}$ and local operators $\rho_a \in \mathcal{L}^{++}(\bigotimes_{i \in \partial a} \mathcal{H}_i)$ for each $a \in \mathcal{F}$, $\tau_i \in \mathcal{L}^{++}(\mathcal{H}_i)$ for each $i \in \mathcal{V}$. Suppose for each $(i, a) \in \mathcal{E}$, there exist some Hilbert spaces $\mathcal{J}_{i,a}$, $\mathcal{K}_i(= \mathcal{H}_i)$, and some operators $\phi_{i,a} \in \mathcal{L}(\mathcal{H}_i \otimes \mathcal{J}_{i,a})$ and $\hat{\phi}_{i,a} \in \mathcal{L}(\mathcal{J}_{i,a} \otimes \mathcal{K}_i)$ satisfying

$$\text{Tr}_{\mathcal{J}_{i,a}}\left(\phi_{i,a} \odot \hat{\phi}_{i,a}\right) = \iota_i,$$  \hspace{1cm} (94)

where $\iota_i$ is the identification mapping from $\mathcal{H}_i$ to $\mathcal{K}_i$. Furthermore, define operators

$$\hat{\rho}_a = \text{Tr}_{\mathcal{J}_{i,a}}\left[\rho_a \otimes \bigotimes_{i \in \partial a} \hat{\phi}_{i,a}\right] \in \mathcal{L}\left(\bigotimes_{i \in \partial a} \mathcal{J}_{i,a}\right) \hspace{1cm} \forall a \in \mathcal{F},$$  \hspace{1cm} (95)

$$\hat{\tau}_i = \text{Tr}_{\mathcal{J}_{i,a}}\left[\tau_i \otimes \bigotimes_{a \in \partial i} \phi_{i,a}\right] \in \mathcal{L}\left(\bigotimes_{a \in \partial i} \mathcal{J}_{i,a}\right) \hspace{1cm} \forall i \in \mathcal{V},$$  \hspace{1cm} (96)

where we treat $\rho_a$ as an operator on $\bigotimes_{i \in \partial a} \mathcal{K}_i$ in (95). In this case, we have,

$$Z \triangleq \text{Tr}\left(\bigotimes_{a \in \mathcal{F}} \rho_a \odot \bigotimes_{i \in \mathcal{V}} \tau_i\right) \approx \text{Tr}\left(\bigotimes_{a \in \mathcal{F}} \hat{\rho}_a \odot \bigotimes_{i \in \mathcal{V}} \hat{\tau}_i\right).$$  \hspace{1cm} (97)

Proof of above theorem is beyond the scope of this report, and we do not list it here. For the future work, it will be interesting to see more techniques from classical factor graphs to be generalized to quantum factor graphs in order to better understand the obtained approximations. Also, we are happy to see further studies on practical applications based on our work.

**References**


Given such notations, it is straightforward to see that (31) can be rewritten as

\[
\text{Tr}\left[ (I + tX) \odot (I + tY) \right] = \text{Tr}_1 \left[ (I + tX) \odot \text{Tr}_2 (I + tY) \right] + O(t^4).
\]  

Now consider the Taylor series expansion of the both sides of (101). Let \( \bar{X} \triangleq X \otimes I \in L^H(\mathcal{H}_1 \otimes \mathcal{H}_2) \). We have,

\[
\text{Tr}\left[ (I + tX) \odot (I + tY) \right] = \text{Tr}(I) + t \cdot \text{Tr}(\bar{X} + Y) + t^2 \cdot \frac{\text{Tr}(\bar{XY} + Y\bar{X})}{2} + t^3 \cdot \frac{\text{Tr} \left[ 2\bar{XY} + 2Y\bar{XY} - \bar{X}^2Y - Y^2\bar{X} - \bar{X}Y^2 - Y\bar{X}^2 \right]}{12} + O(t^4)
\]

\[
+ t^4 \cdot \text{Tr} \left[ \frac{\bar{XY}\bar{X}^3 + Y\bar{XY}\bar{X}^3 + \bar{XY}\bar{X}^3 + \bar{XY}^3 + \bar{XY}^3 - \bar{X}Y^2\bar{X} - \bar{X}Y\bar{X}^2 - Y^2\bar{X}Y - Y\bar{X}^2Y - \bar{X}Y^2 + \bar{X}Y^2}{24} \right] + O(t^5)
\]

\[
= 1 + t \cdot \text{Tr}(\bar{X} + Y) + t^2 \cdot \frac{\text{Tr}(\bar{XY} + Y\bar{X})}{2} + t^4 \cdot \frac{\text{Tr} \left( \bar{XY}\bar{X}^3 + \bar{XY}^2 \right)}{12} + O(t^5);
\]
Proof of Corollary 8.

which proves Corollary 8. Combining (105) and (106), we have

which justifies (101), and therefore also justifies (31).

Notice that \( \text{Tr}_2(X \cdot Z) = X \cdot \text{Tr}_2(Z) \) for any operator \( Z \in \mathcal{L}^H(\mathcal{H}_1 \otimes \mathcal{H}_2) \). Thus, one can easily check that (102) and (103) agree up to \( t^3 \). (Note that the coefficients of \( t^3 \) are both 0 for (102) and (103).) For matrices \( V, W \), denote \([V, W] \triangleq VW - WV\).

Using such notation, we have

\[
\text{Tr}_1[(I + tX) \circ (I + tY)] = \text{Tr}_1[(I + tX) \circ \text{Tr}_2(I + tY)] + \frac{t^4}{12} \cdot \text{Tr}_1(X \cdot [\text{Tr}_2(Y), X] \cdot \text{Tr}_2(Y)) - \text{Tr}_1[(\bar{X} \cdot [\bar{X}, Y] \cdot Y)] \cdot t^4 + O(t^5),
\]

which justifies (101), and therefore also justifies (31).

\[
\square
\]

\section*{Proof of Corollary 8}

Applying the same method used to derive (102) and (103) in above proof, we obtain the following Taylor series expansions.

\[
\text{Tr}_2[(I + tX) \circ (I + tY)] = I + t \cdot \text{Tr}_2(\bar{X} + Y) + t^2 \cdot \text{Tr}_2(\bar{X} \bar{Y} + Y \bar{X}) + \frac{t^3}{12} \cdot \text{Tr}_2(2\bar{X} \bar{Y} \bar{X} + 2 \bar{Y} \bar{X} \bar{Y} - \bar{X} \bar{Y} \bar{X} - \bar{X} \bar{Y} \bar{X} - Y^2 \bar{X} - \bar{X} Y^2 - Y \bar{X}^2) + O(t^4),
\]

(105)

\[
(I + tX) \circ \text{Tr}_2(I + tY) = I + t \cdot (X + \text{Tr}_2(Y)) + t^2 \cdot \frac{X \text{Tr}_2(Y) + \text{Tr}_2(Y) X}{12} + \frac{t^3}{2} \cdot \frac{2X \text{Tr}_2(Y) X + 2 \text{Tr}_2(Y) X \text{Tr}_2(Y) - X^2 \text{Tr}_2(Y) - \text{Tr}_2(Y)^2 X - X \text{Tr}_2(Y)^2 - \text{Tr}_2(Y) X^2}{12} + O(t^4).
\]

(106)

Combining (105) and (106), we have

\[
\text{Tr}_2[(I + tX) \circ (I + tY) = (I + tX) \circ \text{Tr}_2(I + tY)
\]

\[
+ \frac{t^3}{12} \cdot \frac{2 \left( \text{Tr}_2(Y \bar{X} Y) - \text{Tr}_2(Y) X \text{Tr}_2(Y) \right) + \left( \text{Tr}_2(Y)^2 - \text{Tr} (Y^2) \right) X + X \left( \text{Tr}_2(Y)^2 - \text{Tr} (Y^2) \right)}{12} + O(t^4),
\]

(107)

which proves Corollary 8.

\[
\square
\]

\section*{Appendix B

\textbf{Approximation of Tr \( e^{tX} \otimes e^{tY} \)}

In this appendix, we consider the relationship between \( \text{Tr}_1[e^{tX} \otimes e^{tY}] \) and \( \text{Tr}_1[e^{tX} \otimes \text{Tr}_2(e^{tY})] \). The results we present here are similar to those of Theorem 7 and Corollary 8.

\section*{Theorem 19. Consider finite-dimensional Hilbert spaces \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \). Given \( X \in \mathcal{L}^H(\mathcal{H}_1) \), and \( Y \in \mathcal{L}^H(\mathcal{H}_1 \otimes \mathcal{H}_2) \), it holds that

\[
\text{Tr}_1[e^{tX} \otimes e^{tY}] = \text{Tr}_1[e^{tX} \otimes \text{Tr}_2(e^{tY})] + O(t^4),
\]

(108)

where the real number \( t \) is in a neighborhood of 0.

\section*{Proof. We also apply the Taylor series expansions to prove this theorem. Similar to the proof of Theorem 7, we can rewrite (108) as

\[
\text{Tr}_1[e^{tX} \otimes e^{tY}] = \text{Tr}_1[e^{tX} \otimes \text{Tr}_2(e^{tY})] + O(t^4),
\]

(109)
Again, consider the Taylor series expansion of the both sides of (109); and let \( \tilde{X} \triangleq X \otimes I \in \mathcal{L}_H (\mathcal{H}_1 \otimes \mathcal{H}_2) \). We have,

\[
\begin{align*}
\mathcal{Tr}[e^{tX} \otimes e^{tY}] &= \mathcal{Tr}[I + t \cdot (X + Y) + \frac{1}{2!} t^2 \cdot (X + Y)^2 + \frac{1}{3!} t^3 \cdot (X + Y)^3 + \cdots] \\
&= 1 + t \cdot \mathcal{Tr}(X + Y) + \frac{1}{2!} t^2 \cdot \mathcal{Tr}(X + Y)^2 + \frac{1}{3!} t^3 \cdot \mathcal{Tr}(X + Y)^3 + \frac{1}{4!} t^4 \cdot \mathcal{Tr}(X + Y)^4 + O(t^5) \\
&= \mathcal{Tr}_1[e^{tX} \otimes \mathcal{Tr}_2(e^{tY})]
\end{align*}
\]

\[
= \mathcal{Tr}_1 \left[ \exp \left( t \cdot X + \log \left( 1 + t \cdot \mathcal{Tr}_2(Y) + \frac{t^2}{2!} \cdot \mathcal{Tr}_2(Y^2) + \frac{t^3}{3!} \cdot \mathcal{Tr}_2(Y^3) + \frac{t^4}{4!} \cdot \mathcal{Tr}_2(Y^4) + \cdots \right) \right) \right]
\]

\[
= \mathcal{Tr}_1 \left\{ \exp \left[ t \cdot X + t \cdot \mathcal{Tr}_2(Y) + \frac{t^2}{2} \cdot \mathcal{Tr}_2(Y^2) + \frac{t^3}{3!} \cdot \mathcal{Tr}_2(Y^3) + \frac{t^4}{4!} \cdot \mathcal{Tr}_2(Y^4) \right] \\
- \frac{1}{2} \left( t \cdot \mathcal{Tr}_2(Y) + \frac{t^2}{2} \cdot \mathcal{Tr}_2(Y^2) + \frac{t^3}{3!} \cdot \mathcal{Tr}_2(Y^3) + \frac{t^4}{4!} \cdot \mathcal{Tr}_2(Y^4) \right)^2 \\
+ \frac{1}{3} \left( t \cdot \mathcal{Tr}_2(Y) + \frac{t^2}{2} \cdot \mathcal{Tr}_2(Y^2) + \frac{t^3}{3!} \cdot \mathcal{Tr}_2(Y^3) + \frac{t^4}{4!} \cdot \mathcal{Tr}_2(Y^4) \right)^3 \\
- \frac{1}{4} \left( t \cdot \mathcal{Tr}_2(Y) + \frac{t^2}{2} \cdot \mathcal{Tr}_2(Y^2) + \frac{t^3}{3!} \cdot \mathcal{Tr}_2(Y^3) + \frac{t^4}{4!} \cdot \mathcal{Tr}_2(Y^4) \right)^4 + \cdots \}
\]

\[
= \mathcal{Tr}_1 \left\{ \exp \left[ t \cdot (X + \mathcal{Tr}_2(Y)) + \frac{t^2}{2} \cdot \left( \mathcal{Tr}_2(Y^2) - \mathcal{Tr}_2^2(Y) \right) \right] \\
+ \frac{t^3}{12} \left( 2 \cdot \mathcal{Tr}_2(Y^3) - 3 \cdot \mathcal{Tr}_2(Y) \cdot \mathcal{Tr}_2(Y^2) - 3 \cdot \mathcal{Tr}_2^2(Y^2) \cdot \mathcal{Tr}_2(Y) + 4 \cdot \mathcal{Tr}_2^3(Y) \right) \\
+ \frac{t^4}{24} \cdot \mathcal{Tr}_1 \left[ \mathcal{Tr}_2(Y^4) - 3 \cdot \mathcal{Tr}_2(Y^2)^2 - 2 \cdot \mathcal{Tr}_2(Y) \cdot \mathcal{Tr}_2(Y^3) - 2 \cdot \mathcal{Tr}_2^2(Y^2) \cdot \mathcal{Tr}_2(Y) \\
+ 4 \cdot \mathcal{Tr}_2^2(Y) \cdot \mathcal{Tr}_2(Y^2) + 4 \cdot \mathcal{Tr}_2(Y) \cdot \mathcal{Tr}_2(Y^2) \cdot \mathcal{Tr}_2(Y) + 4 \cdot \mathcal{Tr}_2(Y^2) \cdot \mathcal{Tr}_2^2(Y) - 6 \cdot \mathcal{Tr}_2^3(Y) \right] \\
+ \cdots \} \right\}
\]

\[
= 1 + t \cdot \mathcal{Tr}_1 (X + \mathcal{Tr}_2(Y)) + \frac{t^2}{2} \cdot \mathcal{Tr}_1 (X^2 + X \mathcal{Tr}_2(Y) + \mathcal{Tr}_2(Y) X + \mathcal{Tr}_2(Y^2)) \\
+ \frac{t^3}{6} \cdot \mathcal{Tr}_1 (X^3 + 3 \cdot X \mathcal{Tr}_2(Y) + 3 \cdot X \cdot \mathcal{Tr}_2(Y^2) + 3 \cdot \mathcal{Tr}_2(Y) \cdot \mathcal{Tr}_2(Y^2) \cdot \mathcal{Tr}_2(Y) + \mathcal{Tr}_2(Y^3)) + O(t^4)
\]

Notice that (110) and (111) agree up to \( t^3 \). Thus, (109) is justified and so is (108).

We can also prove the following corollary in a similar way.

**Corollary 20.** Given the same setup as in Theorem 19, we have

\[
\mathcal{Tr}_2[e^{tX} \otimes e^{tY}] = e^{tX} \otimes \mathcal{Tr}_2(e^{tY}) + O(t^3).
\]

**Proof.** Based on the proof of Theorem 19, we have

\[
\begin{align*}
\mathcal{Tr}_2[e^{tX} \otimes e^{tY}] &= 1 + t \cdot \mathcal{Tr}_2(\tilde{X} + Y) + \frac{1}{2!} t^2 \cdot \mathcal{Tr}_2(\tilde{X} + Y)^2 + \frac{1}{3!} t^3 \cdot \mathcal{Tr}_2(\tilde{X} + Y)^3 + O(t^4), \\
e^{tX} \otimes \mathcal{Tr}_2(e^{tY}) &= I + t \cdot (X + \mathcal{Tr}_2(Y)) + \frac{t^2}{2} \cdot (X^2 + X \mathcal{Tr}_2(Y) + \mathcal{Tr}_2(Y) X + \mathcal{Tr}_2(Y^2)) + O(t^3),
\end{align*}
\]

which justified the corollary since the above two expressions agree up to \( t^2 \).

**Appendix C**

**Quantum Exponential Family**

**Definition 21** (Quantum Exponential Family [14]). Similar to classical exponential families, a **quantum exponential family** (of degree \( d \)) is a parametric family of quantum operators in form of

\[
\rho_\theta \triangleq \exp \left[ \sum_{k=1}^{d} \theta_k \cdot T_k - \Psi(\theta) \right]
\]
for natural parameter $\theta$ in some open subset $\Theta \subset \mathbb{R}^d$, where $T_k \in \mathcal{L}^{\text{II}}(\mathcal{H}_{\partial k}) = \mathcal{L}^{\text{II}}(\bigotimes_{i \in \partial k} \mathcal{H}_i)$ are some given Hermitian operators ($\partial k \subseteq \{1, \ldots, N\}$), and conventions as in (16) are applied in the summation in (115). Moreover,

$$
\Psi(\theta) \triangleq \log \left( \text{Tr} \left\{ \exp \left[ \sum_{k=1}^{d} \theta_k \cdot T_k \right] \right\} \right). 
$$

As a result, $\rho_\theta$ is a density operator on the global Hilbert space $\mathcal{H}_{\partial \partial k}$.

Note that if $\{T_k\}_{k=1}^{d}$ is linearly independent then the mapping $\theta \mapsto \rho_\theta$ is injective. In this report, we always assume $\{T_k\}_{k=1}^{d}$ to be linearly independent. In this case, the (strict) convexity of the function $\Psi$ follows naturally from the (strict) convexity of the exponential function.\(^3\)

**Example 22.** As an example, consider the following quantum exponential family

$$
\sigma_\theta = \exp \left( \sum_{a \in \mathcal{F}} \sum_{k} \theta_k^{(a)} \cdot T_k^{(a)} - \Psi(\theta) \right),
$$

where $\theta \in \mathbb{R}^d$, $\{T_k^{(a)}\}_{k}$ form a basis of $\mathcal{L}^{\text{II}}(\mathcal{H}_{\partial a})$. Comparing (117) with (17), it is straightforward to see that the parametrization of $\sigma_\theta$ corresponds to all the density operators that can be decomposed as

$$
\sigma \propto \bigotimes_{a \in \mathcal{F}} \sigma_a = \exp \left( \sum_{a \in \mathcal{F}} \log(\sigma_a) \right).
$$

**Definition 23.** The dual parameter $\eta = (\eta_i)_{i=1}^{d}$ (w.r.t. $\theta$) of a quantum exponential family is defined as

$$
\eta_i = \frac{\partial}{\partial \theta_i} \eta(\theta) = \frac{\partial}{\partial \theta_i} \log \left( \text{Tr} \left\{ \exp \left[ \sum_{k=1}^{d} \theta_k \cdot T_k \right] \right\} \right)
= \text{Tr} \left\{ \exp \left[ \sum_{k=1}^{d} \theta_k T_k \right] \right\}^{-1} \frac{\partial}{\partial \theta_i} \text{Tr} \left\{ \exp \left[ \sum_{k=1}^{d} \theta_k T_k \right] \right\}
= \text{Tr} \left\{ \exp \left[ \sum_{k=1}^{d} \theta_k T_k \right] \right\}^{-1} \text{Tr} \left\{ \exp \left[ \sum_{k=1}^{d} \theta_k T_k \right] \cdot T_l \right\}
= \text{Tr} \left( \rho_\theta \cdot T_l \right) = \langle \rho_\theta, T_l \rangle \ \forall l = 1, 2, \ldots, d,
$$

where (119) was obtained by applying the first-order perturbation theory [21].

Due to the strict convexity of $\Psi$, the mapping $\eta(\theta) : \theta \mapsto (\langle \rho_\theta, T_k \rangle)$ is always injective. On the other hand by considering the conjugate function of $\Psi$ given as (which is also strictly convex)

$$
\Phi(\eta) \triangleq \sup_{\theta} \left\{ \sum_{k=1}^{d} \theta_k \eta_k - \Psi(\theta) \right\},
$$

the inverse mapping can be written as

$$
\theta(\eta) : \eta \mapsto \left( \frac{\partial}{\partial \eta_k} \Phi(\eta) \right)_k.
$$

In other words, the correspondence between the natural parameters and the dual parameters is bijective or one-to-one.

**Example 24.** We continue Example 22. In this case, the dual variables can be written as

$$
\eta_k^{(a)} = \text{Tr} \left( \sigma_\theta \cdot T_k^{(a)} \right) = \text{Tr} \left( \sigma_\theta \right) \left( \text{Tr} \left\{ \exp \left[ \sum_{k=1}^{d} \theta_k \cdot T_k \right] \right\} \right)
= \text{Tr} \left( \sigma_a \cdot T_k^{(a)} \right),
$$

where $\sigma_a = \text{Tr}_{\mathcal{V} \setminus \partial a}(\sigma_\theta)$. Since $\{T_k^{(a)}\}_{k}$ is a basis of $\mathcal{L}^{\text{II}}(\mathcal{H}_{\partial a})$, (123) establishes an injection from $\sigma_a$ to $\eta^{(a)}$. In other words, marginal densities fix the global density if such a global density exists.\(^\blacksquare\)

\(^3\)This can be easily derived if one is familiar with the results on trace functions as in [24]
APPENDIX D

JUSTIFICATION OF THE DIFFERENTIABILITY OF $f(\eta) \equiv -\mathrm{Tr}(\sigma \cdot \log(\rho(\eta)))$

Firstly, we verify the bijective mapping $\eta : \theta \mapsto (\{\rho_\theta, T_i\})$, to be differentiable. Notice that,

$$\frac{\partial \eta_j}{\partial \theta_j} = \frac{\partial \mathrm{Tr}(\rho_\theta \cdot T_i)}{\partial \theta_j} = \frac{d}{dt} \mathrm{Tr} \left( \exp \left[ \sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i - \Psi(\theta + t \cdot e_i) \right] \cdot T_i \right) \bigg|_{t=0}$$

(124)

$$= \frac{d}{dt} \mathrm{Tr} \left( \exp \left( \sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i \right) \cdot T_i \right) \bigg|_{t=0} = \exp(\sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i) \cdot T_i$$

(125)

Since function $\exp \circ \Psi$ is obviously differentiable, it suffice to justify the differentiability of $t \mapsto \mathrm{Tr}(\sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i) \cdot T_i$ at $t = 0$. However, by the Taylor series expansion, we can write

$$\mathrm{Tr} \left( \exp(\sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i) \right) - \mathrm{Tr} \left( \exp(\sum_{k=1}^{d} \theta_k \cdot T_k) \cdot T_i \right) = \mathrm{Tr} \left\{ \sum_{n=0}^{\infty} \frac{t^n}{n!} \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i \right)^n \right\} - \mathrm{Tr} \left\{ \sum_{n=0}^{\infty} \frac{t^n}{n!} \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right)^n \right\}$$

(126)

$$= \mathrm{Tr} \left\{ \sum_{n=1}^{\infty} \frac{t^n}{n!} \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right)^{n-1} \cdot T_i (\sum_{k=1}^{d} \theta_k \cdot T_k) + O(t^2) \right\}$$

(127)

$$= \mathrm{Tr} \left\{ \sum_{n=1}^{\infty} \frac{t^n}{n!} \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right)^{n-1} \cdot T_i (\sum_{k=1}^{d} \theta_k \cdot T_k) \right\} + O(t^2).$$

(128)

Notice that

$$\sum_{n=1}^{\infty} \frac{t^n}{n!} \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right)^{n-1} \cdot T_i (\sum_{k=1}^{d} \theta_k \cdot T_k)$$

(129)

$$\leq \dim \cdot \mathrm{Tr} (\sum_{k=1}^{d} \theta_k \cdot T_k)_{n-1} \cdot \|\mathrm{Tr}(T)\|^2$$

(130)

where, for any matrix $A$, $\|A\|$ stands for the spectral radius of $A$, and $\dim$ is the dimension of the global Hilbert space of the problem. Here, we apply the following inequality in deriving (131):

$$\|\mathrm{Tr}(A_1 \cdot A_2 \cdots \cdot A_m)\| \leq \dim \cdot \|A_1\| \cdot \|A_2\| \cdots \cdot \|A_m\| \quad \forall A_1, A_2, \cdots, A_m \in \mathcal{L}(\mathcal{H}), \forall m \in \mathbb{Z}_+.$$  

(131)

Equation (132) implies that the series

$$\sum_{n=1}^{\infty} \frac{t^n}{n!} \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right)^{n-1} \cdot T_i (\sum_{k=1}^{d} \theta_k \cdot T_k)$$

(132)

$$\sum_{n=1}^{\infty} \frac{t^n}{n!} \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right)^{n-1} \cdot T_i (\sum_{k=1}^{d} \theta_k \cdot T_k)$$

(133)
is absolute convergent, and thus is convergent. Therefore, we know that the following limit exists:

\[
\lim_{t \to 0} \frac{\text{Tr} \left( \exp \left( \sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i \right) \cdot T_i \right) - \text{Tr} \left( \exp \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right) \cdot T_i \right)}{t},
\]

which justifies the differentiability of \( t \mapsto \text{Tr} \left( \exp \left( \sum_{k=1}^{d} \theta_k \cdot T_k + t \cdot T_i \right) \cdot T_i \right) \) at \( t = 0 \), and also justifies the differentiability of \( \eta : \theta \mapsto \left( \langle \rho_{\theta}, T_i \rangle \right)_i \).

Secondly, we consider the function \( \hat{f}(\theta) \triangleq -\text{Tr} \left( \sigma \cdot \log \left( \rho(\theta) \right) \right) \), where \( \rho(\theta) \) is the density operator defined by (115). By rewriting \( \hat{f} \) as (note that \( \text{Tr} \left( \sigma \right) = 1 \))

\[
\hat{f}(\theta + h \cdot e_j) = \text{Tr} \left( \sigma \cdot \left[ \sum_{k=1}^{d} \theta_k \cdot T_k + h \cdot T_i - \Psi(\theta + h \cdot e_i) \cdot I \right] \right)
\]

\[
= \text{Tr} \left( \sigma \cdot \left( \sum_{k=1}^{d} \theta_k \cdot T_k \right) \right) + h \cdot \text{Tr} \left( \sigma \cdot T_i \right) - \Psi(\theta + h \cdot e_i),
\]

it is then straightforward to verify the differentiability of \( \hat{f} \).

Now, consider that \( f(\eta) = \hat{f}(\theta(\eta)) \). Since the mapping \( \theta \mapsto \eta \) is differentiable, then so the inverse mapping \( \eta \mapsto \theta \). Therefore, the differentiability of \( f \) follows right away from the differentiability of \( \hat{f} \).