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Using Abstract Harmonic Analysis and the Lie Group Theory for the Study of Parameterized Quantum Circuits

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Abstract:
Quantum computers are believed to be able to significantly outperform classical ones in terms of running time required to solve various problems. Near-term quantum computers, that can already be available in the nearest future, will have fairly limited resources, thus implying additional limitations and challenges. Near-term quantum algorithms are primarily based on parameterized quantum circuits. A parameterized quantum circuit is a quantum circuit, which is run repeatedly, while changing the numerical parameters some of the quantum operations in response to previous measurement results. Parameterized quantum circuits, however, need to be optimized, which can be simplified by endowing them with some mathematical structure, e.g., the ability to take derivatives or compute Fourier transforms. Here we study the possibility of using non-commutative Fourier transforms as a tool to find useful mathematical structure in parameterized quantum circuits.To our knowledge this thesis is the first work, where non-commutative Fourier transforms have been applied to parameterized quantum circuits. Our results include computations and theorems about non-commutative Fourier spectrum on parameterized quantum circuits. The results of this thesis provide a foundation, that opens the door for further study into derivatives and gradients of expectation functions on parameterized quantum circuits via the means of abstract harmonic analysis.

Keywords:
Quantum Computing, Near-Term Quantum Computing, Parameterized Quantum Circuits, Fourier Analysis, Non-Commutative Fourier Transforms.

CERCS:
P170 Computer science, numerical analysis, systems, control

Abstraktse Harmoonilise Analüüsi ja Lie Rühma Teooria Kasutamine Parameetriseeritud Kvantahelate Uurimiseks

Lühikokkuvõte:
Kvantarvuteid peetakse oluliselt võimekamaks oma võimsuse ning ülesande lahendamise kiiruse poolest võrreldes klassikaliste arvutitega. Kvantarvutid, mida on lähitulevikus juba võimalik kasutada, saavad olema piiratud ressurssidega, mille tõttu tekivad uued väljakutsed ning probleemid. Lähitulevikus kasutatavaid kvantalgoritme ehitatakse parameetriseeritud kvantahelate abil. Parameetriseeritud kvantahelad on kindlat tüüpi kvantahelad, mida kasutatakse järjestikku mitmeid kordi, muutes seejuures kvantoperatsioone vastavalt eelmise operatsiooni mõõtetulemustele. Parameetriseeritud kvantahelad tuleb optimeerida, mida saab teha lihtsasti, kui lisada neile kindel matemaatiline struktuur, ehk anda ahelatele võime võtta tuletisi ning arvutada Fourier’ teisendusi. Selles töös me uurime võimalust kasutada mittekommutatiivseid Fourier’ teisendusi tööriistadena selleks, et leida matemaatilisi struktuure parameetriseeritud kvantahelates. See lõputöö on esimene töö, kus parameetriseeritud kvantahelatele on lisatud mittekommutatiivsed Fourier’ teisendused. Töö tulemused sisaldavad arvutustulemusi ning teoreeme mittekommutatiivse Fourier’ spektrumi kasutamisest parmeetriseeritud kvantahelates. Selle töö tulemused aitavad luua vundamendi, mille abil saab edasi uurida tuletiste ja gradientide kasutust kvantarvutustes parameetriseeritud kvantahelates kasutades abstraktset harmoonilist analüüsi meetodilt.

Võtmesõnad: Kvantarvutid, Lähituleviku Kvantarvutid, Parmeetirseeritud Kvantahelad, Fourier’ Analüüs, Mittekommutatiivsed Fourier Teisendused.

CERCS:
P170 Arvutiteadus, arvutusmeetodid, süsteemid, juhtimine (automaatjuhtimisteooria)

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Contents

1 Introduction

Parameterized quantum circuits are the special type quantum circuits which are comprised of a specific class of quantum gates. They are of significant interest in the fields of Quantum Machine Learning and Quantum Neural Networks in near-term quantum computing.

Parameterized quantum circuits even when implemented on noisy intermediate-scale quantum (NISQ) devices may be found useful in applications either standalone or as a part of hybrid system, meaning utilizing both quantum and classical hardware (see for example [BLSF19] and [Pre18]).

Quantum operations on these quantum circuits depend on parameters, which can be iteratively modified to compute the desired function. The whole process of adjusting these parameters is similar to training models in the classical Machine Learning sense. In order to compute the desired output efficiently and precise enough it is, again just as in the classical sense, vital to be able to analyze the expectation value function of such a circuit. One way to do so, is to parameterize a unitary gate, the expectation function of which we are looking for, with some real-valued parameters and treat it as a multi-variable real function (see [SBG$^+$19], [VT18] and [Cro19] for more details). Another important aspect is that these functions must be analyzed on a quantum device, meaning there must be a way to compute their derivatives after a finite amount of circuit runs. This can be done with Fourier analysis techniques if we know the Fourier transform of the function or from (weighted) differences of function values at a finite number of sample points.

In this thesis we offer a different approach to analyzing expectation functions on parameterized quantum circuits. Instead of looking at them as multi-variable real functions, we treat them as functions on a specific type of matrices, more precisely special unitary group. We cannot rely on classical mathematical analysis and Fourier analysis there, instead we use more general theories: abstract harmonic analysis, Lie group theory and non-commutative Fourier analysis. We use this theories to build similar method for computing derivatives for expectation value functions and analyzing them in general. We hope that our approach that utilizes more advanced mathematical tools will prove itself superior to the other methods that have been developed at least in some use cases.

- Section 1 gives a brief introduction to parameterized quantum circuits and some elementary quantum computing facts.
- Section 2 provides with the essential mathematical background for non-commutative analysis on parameterized quantum circuits
- Section 3 states the main results of this thesis

2 Parameterized Quantum Circuits

In this section we briefly cover some facts from elementary quantum computing and give an overview on parameterized quantum circuits. The goal of this section is to familiarize the reader with basic properties of parameterized quantum circuits and their expectation value functions.

2.1 Basic Concepts

Definition 2.1.1 (Matrix exponential)**.** Let V be a vector space over a field $\mathbb{K}$, where $\mathbb{K}$ is either $\mathbb{C}$ or $\mathbb{R}$. Given $A \in \mathrm{End}_{\mathbb{K}}(V)$ we can define e^A in the following way:

$$e^A = \sum_{m=0}^{\infty} \frac{1}{m!} A^m$$

The following properties of matrix exponential can easily be verified:

- $e^{\mathbf{0}} = I$
- $e^{A^\dagger} = (e^A)^\dagger$, where $\dagger$ denotes conjugate transpose in case of $\mathbb{K} = \mathbb{C}$, or simply transpose when $\mathbb{K} = \mathbb{R}$.
- $\det(e^A) = e^{\mathrm{tr}(A)}$

However the property $e^{A+B} = e^A e^B$ does not hold in the general case, but only when A and B commute. For arbitrary matrices exponent of sum is described via *Lie product formula*

$$e^{A+B} = \lim_{n\to\infty} (e^{A/n} e^{B/n})^n$$

Lemma 2.1.1. *Let $\theta \in \mathbb{R}$ and $A \in M_n(\mathbb{K})$, such that $A^2 = I$ then*

$$e^{-i\theta A/2} = \cos(\theta/2) I - i \sin(\theta/2) A$$

Proof. By definition we have the following:

$$e^{-i\theta A/2} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{-i\theta A}{2} \right)^k$$

Since this power series converges absolutely we can rewrite it as the following sum of two series:

$$\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{-i\theta A}{2} \right)^k = \sum_{k=0}^{\infty} \frac{1}{(2k)!} \left(\frac{-i\theta A}{2} \right)^{2k} + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} \left(\frac{-i\theta A}{2} \right)^{2k+1}$$

Now observe that since $A^2 = I$, then $A^{2k} = I$ and $A^{2k+1} = A$. Thus we have the following:

$$\left(\sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!}\left(\frac{\theta}{2}\right)^{2k}\right) I + (-i)\left(\sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!}\left(\frac{\theta}{2}\right)^{2k+1}\right) A$$

But these two sums in big parentheses are Taylor series for $\cos(\theta/2)$ and $\sin(\theta/2)$, hence we get the desired result. □

Remark. Under the same assumptions as in lemma above, we can conclude that

$$e^{i\theta A/2} = \cos(\theta/2) I + i \sin(\theta/2) A$$

Recall, that Pauli matrices, which are represented by

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \; X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

all satisfy the property $A^2 = I$. Thus, we can define parameterized rotation gates around x, y and z axis of Bloch sphere in the following way:

$$R_x(\theta) = e^{-iX\theta/2} = \cos(\theta/2) I - i \sin(\theta/2) X$$

$$R_y(\theta) = e^{-iY\theta/2} = \cos(\theta/2) I - i \sin(\theta/2) Y$$

$$R_z(\theta) = e^{-iZ\theta/2} = \cos(\theta/2) I - i \sin(\theta/2) Z$$

Proposition 2.1.2. *Let U be a unitary single qubit gate, then there exist $\alpha, \beta, \gamma, \delta \in \mathbb{R}$, such that U can be represented in the following way:*

$$U = e^{i\alpha} R_z(\beta) R_y(\gamma) R_z(\delta)$$

Remark. As a matter of fact, instead of y and z we can take any pair of non-collinear axis.

Definition 2.1.2. Let U be an n-qubit unitary gate. We call an $(n+1)$-qubit operator *cU controlled gate if*

$$cU(|0\rangle|\phi\rangle) = |0\rangle|\phi\rangle$$
$$cU(|1\rangle|\phi\rangle) = |1\rangle U|\phi\rangle$$

Proposition 2.1.3. *An operator cU can be represented in the following way:*

$$cU = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U$$

Proof. Let $|\psi\rangle = (\alpha|0\rangle + \beta|1\rangle) \otimes |\phi\rangle$. Then $cU(|\psi\rangle) = \alpha|0\rangle|\phi\rangle + \beta|1\rangle U|\phi\rangle$. Also for an operator $A = |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes U$ the corresponding block matrix is of the following form:

$$\begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix}$$

Therefore

$$\begin{aligned}
A|\psi\rangle &= \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} (\alpha|0\rangle + \beta|1\rangle) \otimes |\phi\rangle \\
&= \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} (\alpha|0\rangle|\phi\rangle + \beta|1\rangle|\phi\rangle) \\
&= \alpha \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} \begin{pmatrix} |\phi\rangle \\ 0 \end{pmatrix} + \beta \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} \begin{pmatrix} 0 \\ |\phi\rangle \end{pmatrix} \\
&= \alpha|0\rangle|\phi\rangle + \beta|1\rangle U|\phi\rangle
\end{aligned}$$

Which implies $A = cU$ and that finishes the proof. □

Proposition 2.1.4. *cU is a unitary operator.*

Proof. Using the matrix representation for cU from proposition 2.1.3 we get

$$\begin{aligned}
cUcU^\dagger &= \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & U^\dagger \end{pmatrix} \\
&= \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \\
&= \begin{pmatrix} I & 0 \\ 0 & U^\dagger \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} = cU^\dagger cU
\end{aligned}$$

□

Definition 2.1.3. *Parameterized quantum circuit* is a quantum circuit comprised of single qubit unitary parameterized gates and controlled single qubit gates.

2.2 Expectation Value Functions for Parameterized Quantum Circuits

A complete measurement in the computational basis can be viewed as a projective measurement with respect to the following decomposition of the identity

$$I = \sum_{j \in \mathbb{Z}_2^n} P_j$$

where P_js are orthogonal projectors and thus can be written as $P_j = |j\rangle\langle j|$.

Suppose we have a quantum state $|\psi\rangle$, which we write with respect to its orthonormal basis $\{|\phi_j\rangle\}$ as follows

$$|\psi\rangle = \sum_j \alpha_j |\phi_j\rangle$$

A measurement of $|\psi\rangle$ with respect to $\{|\phi_j\rangle\}$ is described via orthogonal projectors $\{|\phi_j\rangle\langle\phi_j|\}$ and will output the result j with probability

$$\begin{aligned}
\operatorname{tr}(|\psi\rangle\langle\psi||\phi_j\rangle\langle\phi_j|) &= \operatorname{tr}(\langle\phi_j|\psi\rangle\langle\psi|\phi_j\rangle) \\
&= \langle\phi_j|\psi\rangle\langle\psi|\phi_j\rangle \\
&= |\langle\psi|\phi_j\rangle|^2 \\
&= |\alpha_j|^2
\end{aligned}$$

Definition 2.2.1. An *observable* is a Hermitian operator H acting on a state space of a system. It has a spectral decomposition of the form

$$H = \sum_j \lambda_j P_j$$

where P_j is an orthogonal projector on the eigenspace of M with corresponding real eigenvector λ_j.

Measuring an observable then means performing a projective measurement with respect to decomposition

$$I = \sum_j P_j$$

where a measurement j corresponds to the eigenvalue λ_j.

Theorem 2.2.1. *For a projective measurement described by projectors P_j suppose we measure a quantum state $|\psi\rangle$. Then the expectation value when measuring H, given that the system is in state $|\psi\rangle$ is*

$$\mathbb{E}(H) = \operatorname{tr}(H|\psi\rangle\langle\psi|)$$

Proof. We refer to [KLM+07]. □

Let the unitary $V(\theta)$ be composed of chains of unitary transformations $\{V_j(\theta)\}_{j=1}^m$, more precisely

$$V(\theta) = \prod_{j=1}^m V_j(\theta_j)$$

acting on a state ϱ and suppose we measure an observable μ. Additionally assume, that each $V_j(\theta_j)$ is represented as $e^{-i\theta_j P_j/2}$, where each P_j denotes one of the Pauli matrices. Denote

$$V_{l:k} := \prod_{j=l}^{k} V_j$$

The expectation function $\mathbb{E}(\mu(\theta))$ is then given by

$$\mathbb{E}(\mu(\theta)) = \mathrm{tr}(\mu V_{m:1} \varrho V_{m:1}^{\dagger})$$

Proposition 2.2.2. *Gradient of the expectation value function* $\mathbb{E}(\mu(\theta))$ *is represented by*

$$\frac{\partial \mathbb{E}(\mu(\theta))}{\partial \theta} = -\frac{i}{2} \mathrm{tr}(\mu V_{m:j} [P_j, V_{j-1:1} \varrho V_{j-1:1}^{\dagger}] V_{m:j}^{\dagger})$$

where $[\ ,\ ]$ *denotes a commutator.*

Proof. For more details we refer to Mitarai et al. paper, see [MNKF18]. □

3 Analysis on Topological Groups

In this section we aim to develop essential mathematical techniques required to be able to compute non-commutative Fourier transforms. We shall be primarily relying on [AH14] and [Hal15]. We begin with the introduction to topological groups and integration over them as well as elements of representation theory. We define a non-commutative Fourier transform and list some of its properties. Finally we focus more on Lie groups and in particular $SU(2)$ which we will then be employing in the next section. We try to stay brief and focus primarily on the essentials, however we do state some auxiliary facts which we find to be of interest in general.

3.1 Integration over Topological Groups and Unitary Representations

Definition 3.1.1. Let G be a group together with a binary operation $\mu : G \times G \to G$, such that for any $g, h \in G$ maps a pair (g, h) onto $\mu(g, h)$. We call G a *topological group* if it is additionally equipped with a topological space structure and the mapping given by $(g, h) \mapsto \mu(g, h^{-1})$ is continuous.

From now on we shall omit the bulky notation $\mu(g, h)$ for the binary operation and will write gh instead.

Definition 3.1.2. For a topological group G and $g \in G$ we define *left translation* l_g, *right translation* r_g, *conjugation* c_g and *inversion* I_g in the following way:

$$I_g = g^{-1} \text{ and } \forall h \in G :\ l_g(h) = g^{-1}h,\ r_g(h) = hg,\ c_g(h) = ghg^{-1}$$

Clearly all these mappings are homeomorphisms with

$$l_g^{-1} = l_{g^{-1}},\ r_g^{-1} = r_{g^{-1}} \text{ and } c_g^{-1} = c_{g^{-1}}$$

Moreover c_g is an automorphism and I_g is an anti-automorphism (meaning bijection and $I(g_1, g_2) = I(g_2)I(g_1)$ for all $g_1, g_2 \in G$).

Definition 3.1.3. Consider a continuous function $f : G \to \mathbb{C}$. We call it *vanishing at infinity* if for any $\epsilon > 0$ there exists a compact set $K \subset G$ such that $|f(x)| < \epsilon$ whenever $x \in K^c$.
Denote the space of all such functions as $C_0(G)$. Moreover $C_0(G)$ is a Banach space with respect to the following norm:

$$||f||_\infty := \sup_{g \in G} |f(g)|$$

Denote by $C_c(G)$ a linear space of complex-valued functions on G with compact support.

Theorem 3.1.1. *$C_c(G)$ is dense in $C_0(G)$.*

Proof. See [AH14]. □

For each $f \in C_0(G)$ and $g \in G$ we define

$$L_g f = f \circ l_g,\ R_g f = f \circ r_g,\ C_g f = f \circ c_g,\ i(f) = f \circ I$$

One can show that all these maps are isometric isomorphisms on $C_0(G)$.

Definition 3.1.4. Consider a function $f : G \to \mathbb{C}$. We say that f is *left uniformly continuous* (resp. *right uniformly continuous*) if for any $\epsilon > 0$ there exist an open neighborhood of the identity element of G (denote it as e), such that for all $g \in U$: $||L_g f - f||_\infty < \epsilon$ (resp. $||R_g f - f||_\infty < \epsilon$).

Theorem 3.1.2. *Let $f : G \to \mathbb{C}$ be a function in $C_c(G)$, then f is both left and right uniformly continuous.*

Proof. See [AH14]. □

Definition 3.1.5. Let $\mathcal{B}(G)$ be the Borel σ-algebra of G. A non-trivial regular Borel measure m_L on G is called *left Haar measure* if for all $A \in \mathcal{B}(G)$ and $g \in G$: $m_L(gA) = m_L(A)$. In a similar way we define m_R as a *right Haar measure*. That is for all $A \in \mathcal{B}(G)$ and $g \in G$: $m_R(Ag) = m_R(A)$.

Theorem 3.1.3. *Let G be a locally compact Hausdorff topological group. Then both left and right Haar measures exist and are unique up to a positive multiplicative factor. Moreover for a compact set $C \subset G$: $m_L(C)$, $m_R(C) < \infty$.*

Proof. See [AH14] and [HR12]. □

Remark. We shall define integrals $\int_G f(x) m_L(dx)$ and $\int_G f(x) m_R(dx)$ with respect to left and right Haar measures respectively in the usual Lebesgue sense.

We can form Banach spaces $L^p(G, \mathcal{B}(G), m_L, \mathbb{C})$ and $L^p(G, \mathcal{B}(G), m_R, \mathbb{C})$ for $1 \leq p \leq \infty$. In particular $L^p(G, \mathcal{B}(G), m_L, \mathbb{C})$ consists of classes of functions that agree almost everywhere with respect to m_L and satisfy the following norm property:

$$||f||_p := \Big(\int\limits_G |f(x)|^p m_L(dx) \Big)^{\frac{1}{p}} < \infty$$

In particular for $L^\infty(G, \mathcal{B}(G), m_L, \mathbb{C})$ we have

$$||f||_\infty := \inf\{c > 0 : |f(x)| \leq c \text{ almost everywhere}\} < \infty$$

We can then define an inner product in the following way:

$$\langle f_1, f_2 \rangle = \int\limits_G f_1(x)\overline{f_2(x)} m_L(dx)$$

Note that $L^p(G, \mathcal{B}(G), m_L, \mathbb{C})$ together with defined above inner product is a Hilbert space.

Theorem 3.1.4. *Consider $f : G \mapsto \mathbb{C}$. For any $1 \leq p < \infty$ the mapping $g \mapsto L_g f$ (resp. $g \mapsto R_g f$) is a continuous map from G to $L^p(G, \mathcal{B}(G), m_L, \mathbb{C})$ (resp. from G to $L^p(G, \mathcal{B}(G), m_R, \mathbb{C})$).*

Proof. We shall introduce the proof for the case of left translation. Right translation situation is similar and verification of that fact is left to a reader.

Firstly fix p. It will suffice to show that for a given $f \in L^p(G, \mathcal{B}(G), m_L, \mathbb{C})$ for any $\epsilon > 0$ there exists a neighbourhood U of the identity element, such that U^c is compact and for any $g \in U$: $||L_g f - f||_p < \epsilon$. Since $C_c(G)$ is dense in $L^p(G, \mathcal{B}(G), m_L, \mathbb{C})$ we can find such $\phi \in C_c(G)$, that $||f - \phi||_p < \frac{\epsilon}{3}$. Using triangle inequality and $L_g f$ being an isometry, we get:

$$\begin{aligned} ||L_g f - f||_p &\leq ||L_g f - L_g \phi||_p + ||L_g \phi - \phi||_p + ||f - f\phi||_p \\ &< ||L_g \phi - \phi||_p + \frac{2\epsilon}{3} \end{aligned}$$

By theorem 3.1.2 ϕ is left uniformly continuous, thus choosing a smaller U if necessary, we get that $g \in U$ implies

$$||L_g \phi - \phi||_\infty < \frac{\epsilon}{3 m_L(U \operatorname{supp}(\phi))^{\frac{1}{p}}}$$

Therefore $||f - \phi||_p < \frac{\epsilon}{3}$ which proves the claim. □

Definition 3.1.6. Consider a left Haar measure m_L on topological group G. For a fixed $p \in G$ and for each $A \in \mathcal{B}(G)$ define

$$m_L^p(A) := m_L(Ap)$$

Then m_L^p is another Haar measure, therefore by theorem 3.1.3 there exists a positive constant $\Delta(p)$, such that

$$m_L^p(A) = \Delta(p) m_L(A)$$

for all $A \in \mathcal{B}(G)$. We call a mapping $p \mapsto \Delta(p)$ from G to a multiplicative group $(0, \infty)$ the *modular function* of G.

Theorem 3.1.5. *The modular function is a continuous homomorphism from G to* $(0, \infty)$.

Proof. Pick a non-trivial $f \in C_c(G)$, such that $f \geq 0$, then for all $p_1, p_2 \in G$

$$\int_G f(xp_2^{-1}p_1^{-1})m_L(dx) = \Delta(p_1p_2)\int_G f(x)m_L(dx)$$

On the other hand

$$\begin{aligned}\int_G f(xp_2^{-1}p_1^{-1})m_L(dx) &= \Delta(p_2)\int_G f(xp_1^{-1})m_L(dx) \\ &= \Delta(p_2)\Delta(p_1)\int_G f(x)m_L(dx) \\ &= \Delta(p_1)\Delta(p_2)\int_G f(x)m_L(dx)\end{aligned}$$

Which establishes the homomorphism.
To show continuity, pick f as above with an additional property $\int_G f(x)m_L(dx) = 1$. Then for all $g \in G$:

$$\Delta(p) = \int_G f(xp^{-1})m_L(dx)$$

And we get that $|\Delta(p_1) - \Delta(p_2)| \leq ||L_{p_1}f - L_{p_2}f||_1$, thus by theorem 3.1.4 the continuity holds. □

Definition 3.1.7. If $\Delta(p) = 1$ for all $p \in G$, then G is called *unimodular*.

Theorem 3.1.6. *Every compact topological group G is unimodular.*

Proof. By continuity of Δ compactness of G implies compactness of $\mathrm{Im}(G)$, since Δ on the other hand is a homomorphism, then $\mathrm{Im}(G)$ is a subgroup of $(0, \infty)$. However the only compact subgroup of $(0, \infty)$ is $\{1\}$. □

From now on all our topological groups are considered to be compact, Hausdorff and additionally equipped with normalized Haar measure, meaning that for all $f \in C_c(G)$:

$$\int_G f(x)m_L(dx) = 1$$

Definition 3.1.8. Let G be a topological group. A *linear representation* of G is a homomorphism π from G to the group of bounded invertible operators on some topological vector space V_π, such that for any fixed $\psi \in V_\pi$, the mapping $g \mapsto \pi(g)\psi$ is a continuous mapping from G to V_π.

Definition 3.1.9. A representation π is called a *unitary representation* if V_π is a complex separable Hilbert space and $\pi(g)$ is a unitary operator on V_π for all $g \in G$.

From now on we shall automatically assume all our representations to be unitary, unless stated otherwise.

Definition 3.1.10. Let $\{\pi_i\}_{i=1}^m$ be a collection of representations of G acting on Hilbert spaces $\{V_i\}_{i=1}^m$. Then for a fixed collection of $\psi_i \in V_i$ and for any $g \in G$ the *direct sum* of representations $\{\pi_i\}_{i=1}^m$ is defined as

$$\Big(\bigoplus_{i=1}^m \pi_i\Big)(g)\psi := \bigoplus_{i=1}^m \Big(\pi_i(g)\psi_i\Big)$$

Where $\psi = \bigoplus_{i=1}^m \psi_i \in \bigoplus_{i=1}^m V_i$.
Similarly *tensor product* of $\{\pi_i\}_{i=1}^m$ is

$$\Big(\bigotimes_{i=1}^m \pi_i\Big)(g)\psi := \bigotimes_{i=1}^m \Big(\pi_i(g)\psi_i\Big)$$

And $\psi = \bigotimes_{i=1}^m \psi_i \in \bigotimes_{i=1}^m V_i$.

Definition 3.1.11. If π is a representation of G acting on a space V then we can define a *conjugate representation* $\bar{\pi}$ that acts on the dual space V^*. There exists a natural isomorphism $J : V \to V^*$, such that $\langle J\phi, J\psi\rangle = \langle \psi, \phi\rangle$ for $\phi, \psi \in V$. Then we define $\bar{\pi}(g)$ as follows:

$$\bar{\pi}(g) = J\pi(g)J^{-1}$$

Moreover

$$\langle \bar{\pi}(g)\bar{\phi}, \bar{\psi}\rangle = \langle \psi, \pi(g)\phi\rangle$$

for all $g \in G$ and $\phi, \psi \in V$.

Definition 3.1.12. Let π be representation of G on V and $W \subset V$ a closed linear subspace. We call W an *invariant subspace* if $\pi(g)W \subset W$ for all $g \in G$. Moreover $\pi|_W$ defines another representation of G, which we call a *subrepresentation*.

Definition 3.1.13. Let π be representation of G on V. If W being an invariant subspace implies that either $W = V$ or $W = \{0\}$ then π is called *irreducible representation*.

Definition 3.1.14. Let $\pi_1 : G \to V_1$ and $\pi_2 : G \to V_2$ be representations. A bounded linear operator $T : V_1 \to V_2$ is called an *intertwining map* if for all $g \in G$ the following diagram commutes:

$$\begin{array}{ccc} V_1 & \xrightarrow{T} & V_2 \\ \downarrow{\scriptstyle \pi_1(g)} & & \downarrow{\scriptstyle \pi_2(g)} \\ V_1 & \xrightarrow{T} & V_2 \end{array}$$

Moreover two representations are called *equivalent* (denote by $\pi_1 \sim \pi_2$) if there exists a unitary intertwining map between them.

It is easy to see, that $\sim$ as defined above is an equivalence relation.

Definition 3.1.15. Let $\widehat{G}$ be a set of all equivalence classes of irreducible representations of G, then we call $\widehat{G}$ the *unitary dual* of G.

Theorem 3.1.7 (Schur's lemma)**.** *Let π_1, π_2 be finite-dimensional (meaning $d_{\pi_i} := \dim(V_i) < \infty$ for $i \in \{1, 2\}$) irreducible representations of G acting on complex Hilbert spaces V_1 and V_2 respectively.*

1. *Let $T : V_1 \to V_2$ be an intertwining map, then either T is an isomorphism or $T = 0$.*

2. *Let $T \in \mathrm{End}(V_1)$ be such that $T\pi_1(g) = \pi_1(g)T$, then there exists $\lambda \in \mathbb{C}$, such that $T = \lambda I_{d_{\pi_1}}$.*

Proof. 1. Assume $\mathrm{Ker}(T) = 0$ and $T \neq 0$, hence T is injective. $\mathrm{Im}(T)$ is a closed linear subspace in V_2. Pick $\psi \in \mathrm{Im}(T)$, then there exists $\phi \in V_1$, such that $T\phi = \psi$. Therefore $\pi_2(g)\psi = \pi_2(g)T\phi = T\pi_1(g)\phi$ and by irreducibility of π_2 it follows that $\mathrm{Im}(T) = V_1$. Hence T is an isomorphism.
Now take $\mathrm{Ker}(T) \neq 0$. Since $\mathrm{Ker}(T)$ is invariant for $\phi \in \mathrm{Ker}(T)$ and for all $g \in G$ we have $T\pi_1(g)\psi = \pi_2(g)T\psi = 0$. Due to irreducibility of π_1 we get $\mathrm{Ker}(T) = V_1$ and hence $T = 0$.

2. T has at least one eigenvalue from the assumption $(T - \lambda I_{d_{\pi_1}})\pi_1(g) = \pi_1(g)(T - \lambda I_{d_{\pi_1}})$. At the same time $(T - \lambda I_{d_{\pi_1}})$ cannot be an isomorphism since the corresponding eigenvector ϕ belongs to $\mathrm{Ker}(T - \lambda I_{d_{\pi_1}})$, hence by (1) we have $(T - \lambda I_{d_{\pi_1}}) = 0$.

□

Theorem 3.1.8. *Let G and H be compact topological groups and $\{\pi_j\}_{j \in J}$ and $\{\sigma_i\}_{i \in I}$ their respective complete collections of irreducible representations, then the complete collection of irreducible representations for $G \times H$ is*

$$\{\pi_j \otimes \sigma_i\}_{j \in J, i \in I}$$

Proof. See [Tel05] □

Theorem 3.1.9. *Every irreducible representation of a compact Hausdorff group is finite dimensional.*

Proof. See [AH14] □

Theorem 3.1.10. *Let π be an irreducible representation acting on V. Then for all $\phi_i, \psi_i \in V$, $i \in \{1, 2\}$:*

$$\int_G \langle \pi(g)\phi_1, \psi_1 \rangle \langle \psi_2, \pi(g)\phi_2 \rangle dg = \frac{1}{d_\pi} \langle \phi_1, \phi_2 \rangle \langle \psi_2, \psi_1 \rangle \tag{1}$$

Proof. See [AH14]. □

Let π be an irreducible representation. Denote by $\mathcal{M}_\pi$ a linear span of all maps of the form $g \mapsto \langle \pi(g)\phi, \psi \rangle$.

Proposition 3.1.11. $\pi_1 \sim \pi_2$ *implies* $\mathcal{M}_{\pi_1} = \mathcal{M}_{\pi_1}$. *If* π_1 *and* π_2 *are distinct elements of* $\widehat{G}$ *then* $\mathcal{M}_{\pi_1}$ *is orthogonal to* $\mathcal{M}_{\pi_2}$.

Proof. See [AH14]. □

Let $\mathcal{E}(G)$ be the smallest linear subspace of $L^2(G)$ which contains all $\mathcal{M}_\pi$s, meaning $\mathcal{E}(G)$ is a linear span of maps

$$\{g \to \langle \pi(g)\psi, \phi \rangle | \psi, \phi \in V, \pi \in \widehat{G}\}$$

Theorem 3.1.12 (Peter-Weyl I)**.** $\mathcal{E}(G)$ *is dense in* $L^2(G)$.

Proof. See [AH14]. □

Fix a basis $\{e_j^{(\pi)}, 1 \leq j \leq d_\pi\}$ in each V and define, relative to these bases, coordinate functions $\pi_{ij}(g) = \pi(g)_{ij}$ for each $g \in G$, where $\pi(g)_{ij}$ is the (i, j)-th matrix entry of $\pi(g)$, meaning

$$\pi(g)_{ij} = \langle \pi(g)e_i^{(\pi)}, e_j^{(\pi)} \rangle$$

Theorem 3.1.13 (Peter-Weyl II)**.** *The set* $\{\sqrt{d_\pi}\pi_{ij}, \pi \in \widehat{G}\}$ *is an orthonormal basis in* $L^2(G)$.

Proof. See [AH14]. □

3.2 Non-Commutative Fourier Transforms

Definition 3.2.1. For a matrix algebra $M_n(\mathbb{C})$ and for all $M, N \in M_n(\mathbb{C})$ a *Hilbert-Schmidt norm* is defined by

$$||M||_{HS} = (\mathrm{tr}(MM^*))^{\frac{1}{2}}$$

and the associated inner product is

$$\langle M, N\rangle_{HS} = (\mathrm{tr}(MN^*))^{\frac{1}{2}}$$

Definition 3.2.2. Let G be a compact, second countable Hausdorff group. Define a set

$$\mathcal{M}(\widehat{G}) = \bigcup_{\pi \in \widehat{G}} M_{d_\pi}(\mathbb{C})$$

A mapping $F : \widehat{G} \to \mathcal{M}(\widehat{G})$ is called *compatible* if $F(\pi) \in M_{d_\pi}(\mathbb{C})$.

The set of all compatible maps forms a linear complex space (which we denote as $\mathcal{L}(\widehat{G})$) under the pointwise operations for all $\lambda \in \mathbb{C}$, $F, G \in \mathcal{L}(\widehat{G})$, $\pi \in \widehat{G}$:

$$(\lambda F + G)(\pi) = \lambda F(\pi) + G(\pi)$$

Let $\mathcal{H}_2(\widehat{G})$ be a linear subspace of all $F \in \mathcal{L}(\widehat{G})$ for which

$$|||F|||_2^2 := \sum_{\pi \in \widehat{G}} d_\pi ||F(\pi)||_{HS}^2 < \infty$$

Then $\mathcal{H}_2(\widehat{G})$ is a complex Hilbert space together with an inner product

$$\langle F, G\rangle := \sum_{\pi \in \widehat{G}} d_\pi \langle F(\pi), G(\pi)\rangle_{HS}$$

and an associated norm $|||.|||_2$.

Definition 3.2.3. Let $f \in L^1(G)$, for each $\pi \in \widehat{G}$ we introduce the *non-commutative Fourier transform*:

$$\hat{f}(\pi) = \int_G \pi(g^{-1}) f(g) dg$$

Moreover for each $0 \leq i, j, \leq d_\pi$ we have

$$\hat{f}(\pi)_{ij} = \int_G \pi_{ij}(g^{-1}) f(g) dg$$

Theorem 3.2.1. *For each $f \in L^2(G)$ we have*

$$f = \sum_{\pi \in \widehat{G}} d_\pi \mathrm{tr}(\hat{f}(\pi)\pi)$$

which we call a Fourier expansion of f, where convergence is considered in L^2 sense.

Proof. Using Peter-Weyl theorem we get

$$\begin{aligned}
f &= \sum_{\pi \in \widehat{G}} d_\pi \sum_{i,j=1}^{d_\pi} \langle f, \pi_{ij} \rangle \pi_{ij} \\
&= \sum_{\pi \in \widehat{G}} d_\pi \sum_{i,j=1}^{d_\pi} \left(\int\limits_G f(g)\overline{\pi_{ij}(g)} dg \right) \pi_{ij} \\
&= \sum_{\pi \in \widehat{G}} d_\pi \sum_{i,j=1}^{d_\pi} \left(\int\limits_G f(g)\pi_{ji}(g^{-1}) dg \right) \pi_{ij} \\
&= \sum_{\pi \in \widehat{G}} d_\pi \sum_{i,j=1}^{d_\pi} \hat{f}(\pi_{ij})\pi_{ji} \\
&= \sum_{\pi \in \widehat{G}} d_\pi \mathrm{tr}(\hat{f}(\pi)\pi)
\end{aligned}$$

□

Lemma 3.2.2 (Parseval-Plancherel identity)**.** *Denote by $\mathcal{F} : L^1(G) \to \mathcal{L}(\widehat{G})$ the Fourier transformation mapping given by $\mathcal{F}(f) = \hat{f}$ and consider its restriction to $L^2(G)$. The operator $\mathcal{F}$ is an isometry from $L^2(G)$ to $\mathcal{H}_2(G)$, such that for all $f_1, f_2 \in L^2(G)$*

$$\int\limits_G f_1(g)\overline{f}_2(g) dg = \sum_{\pi \in \widehat{G}} d_\pi ||\hat{f}_1(\pi)||_{HS}^2$$

and

$$\int\limits_G |f_1(g)|^2 dg = \sum_{\pi \in \widehat{G}} d_\pi \langle \hat{f}_1(\pi), \hat{f}_2(\pi) \rangle_{HS}$$

Proof. See [AH14]. □

Definition 3.2.4. Let f be a complex valued function on a group G. We call f a *central function* if for all $g, h \in G$

$$f(g) = f(hgh^{-1})$$

or equivalently $f(gh) = f(hg)$.

Denote by $L_c^2(G)$ a closed subspace of $L^2(G)$ comprised of square-integrable functions that are central almost everywhere, meaning for all $h \in G$ and almost all $g \in G$ it holds that $f(g) = f(hgh^{-1})$.

Lemma 3.2.3. *$f \in L^2(G)$ implies $f \in L_c^2(G)$ iff for all $\pi \in \widehat{G}$, $\hat{f}(\pi) = I_\pi c_\pi$ for some $c_\pi \in \mathbb{C}$.*

Proof. See [AH14]. □

Definition 3.2.5. Let π be a finite-dimensional representation of compact group G. We define a *character* of representation χ_π by

$$\chi_\pi(g) = \mathrm{tr}(\pi(\mathrm{g}))$$

for all $g \in G$.

Clearly characters are continuous and central functions.

Proposition 3.2.4. *Let π_1, π_2 be finite-dimensional representations of a compact group G. Then*

- $\chi_{\pi_1 \oplus \pi_2} = \chi_{\pi_1} + \chi_{\pi_2}$
- $\chi_{\pi_1 \otimes \pi_2} = \chi_{\pi_1} \chi_{\pi_2}$
- $\chi_{\overline{\pi}_1} = \overline{\chi_{\pi_1}}$

Proof. See [AH14]. □

Theorem 3.2.5. *The set $\{\chi_\pi, \pi \in \widehat{G}\}$ is an orthonormal basis in $L_c^2(G)$*

Proof. See [AH14]. □

Definition 3.2.6. For a central function $f \in L^1(G)$ we can define its *central Fourier transform* to be

$$\hat{f}(\chi_\pi) \int_G f(g) \chi_\pi(g^{-1}) dg$$

for all $\pi \in \widehat{G}$.

Notice that Fourier expansion then takes the form

$$\sum_{\pi \in \widehat{G}} \hat{f}(\chi_\pi) \chi_\pi$$

It is worth mentioning that being central is a very strong property in a sense that it significantly simplifies Fourier analysis of such function. A curious reader may refer, for example, to [Fol16] and [RT09] for more details. Unfortunately functions that we are going to study in section 3 do not possess the centrality property.

3.3 Representations of $SU(2)$

Proposition 3.3.1. *Let G be a matrix Lie group with associated Lie algebra $\mathfrak{g}$ and let π be a finite-dimensional representation of G. There exists a unique representation Π of $\mathfrak{g}$ acting on the same space, such that for all $X \in \mathfrak{g}$*

$$\pi(e^X) = e^{\Pi(X)}$$

and Π can be computed as

$$\Pi(X) = \frac{d}{dt}\pi(e^{tX})\Big|_{t=0}$$

Proof. We refer to [Hal15]. □

Lemma 3.3.2. *Denote by $\mathcal{P}$ a space of polynomials of two variables with complex coefficients and by $\mathcal{P}_m \subset \mathcal{P}$ a space of degree-m homogeneous polynomials. For each $g \in SU(2)$ define the following linear transformation*

$$\pi_m(g) \mapsto \mathcal{P}_m$$

such that

$$(\pi_m(g)f)(z_1, z_2) = f(g^{-1}(z_1, z_2))$$

and where for $a_j \in \mathbb{C}$

$$f(z_1, z_2) = \sum_{j=0}^{m} a_j z_1^j z_2^{m-j}$$

then π_m is a representation of $SU(2)$.

Proof. Notice that $\pi_m f$ is again a homogeneous polynomial of degree m hence $\pi \in \mathrm{Aut}_{\mathbb{C}}(\mathcal{P}_m)$. Now observe

$$\begin{aligned}\pi_m(g_1)(\pi_m(g_2)f)(z_1, z_2) &= (\pi_m(g_2)f)(g_1^{-1}(z_1, z_2)) \\ &= f(g_2^{-1}g_1^{-1}(z_1, z_2)) \\ &= (\pi_m(g_1g_2)f)(z_1, z_2)\end{aligned}$$

And that finishes the proof. □

Theorem 3.3.3. *π_m is irreducible for all $m \geq 0$.*

Proof. See [Hal15]. □

We define an inner product on $\mathcal{P}$ by regarding it as a subset of $L^2(\sigma)$, where σ is a normalized surface measure on a sphere S^3, as follows: for $f, h \in \mathcal{P}$

$$\langle f, h\rangle = \int_{S^3} f\overline{h}d\sigma$$

$\mathcal{P}$ is not complete with respect to this inner product, but each $\mathcal{P}_m$ is.

Proposition 3.3.4. *The spaces $\mathcal{P}_m$ are mutually orthogonal in $L^2(\sigma)$, moreover a set*

$$\left\{ \sqrt{\frac{(m+1)!}{j!(m-j)!}} z_1^j z_2^{m-j} \ : \ 0 \leq j \leq m \right\}$$

is an orthonormal basis for $\mathcal{P}_m$.

Proof. See [Fol16]. □

Definition 3.3.1. Let V be a finite-dimensional vector space over $\mathbb{R}$. For $v_1, v_2 \in V$ the space of formal linear combinations of the form

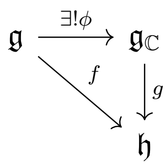
$$v_1 + iv_2$$

is called *complexification* of real space V and is denoted by $V_{\mathbb{C}}$.

Proposition 3.3.5. *Let $\mathfrak{g}$ be a finite-dimensional real Lie algebra and $\mathfrak{g}_{\mathbb{C}}$ its complexification as a vector space. There exists a unique extension of the bracket operation on $\mathfrak{g}$ to $\mathfrak{g}_{\mathbb{C}}$ that makes $\mathfrak{g}_{\mathbb{C}}$ into a complex Lie algebra. $\mathfrak{g}_{\mathbb{C}}$ is then called the complexification of the real Lie algebra.*

Proof. See [Hal15]. □

Proposition 3.3.6 (Universal property of complexification of a real Lie algebra)**.** *Let $\mathfrak{g}$ be a real Lie algebra, $\mathfrak{g}_{\mathbb{C}}$ – its complexification and $\mathfrak{h}$ some arbitrary complex Lie algebra. For every real Lie algebra homomorphism $f : \mathfrak{g} \to \mathfrak{h}$ and a complex Lie algebra homomorphism $g : \mathfrak{g}_{\mathbb{C}} \to \mathfrak{h}$ there exists a unique extension $\phi : \mathfrak{g} \to \mathfrak{g}_{\mathbb{C}}$ making the following diagram commutative:*



Proof. For all $X, Y \in \mathfrak{g}$ the unique extension is given by $\phi(X + iY) = \phi(X) + i\phi(Y)$. One can show that this is indeed a Lie algebra homomorphism. See [Hal15] for more details. □

The associated representation of Lie algebra $\mathfrak{sl}(2, \mathbb{C})$ (complexification of the real Lie algebra $\mathfrak{su}(2)$) can then be computed as follows:

$$(\Pi_m(X)f)(z_1, z_2) = \frac{d}{dt} f(e^{-tX})(z_1, z_2)\Big|_{t=0}$$

Now let $z(t) = (z_1(t), z_2(t))$ be a curve on $\mathbb{C}^2$, such that $z(t) = e^{tX}z$, then

$$(\Pi_m(X)f)(z_1, z_2) = \frac{\partial f}{\partial z_1}\frac{dz_1}{dt}\Big|_{t=0} + \frac{\partial f}{\partial z_2}\frac{dz_2}{dt}\Big|_{t=0}$$

and since

$$\frac{dz}{dt}\Big|_{t=0} = -Xz$$

we get

$$(\Pi_m(X)f)(z_1, z_2) = -\frac{\partial f}{\partial z_1}(X_{11}z_1 + X_{12}z_2) - \frac{\partial f}{\partial z_2}(X_{21}z_1 + X_{22}z_2)$$

Theorem 3.3.7. *Π_m is an irreducible representation for all $m \geq 0$.*

Proof. See [Hal15]. □

Theorem 3.3.8 (Clebsch-Gordan formula)**.** *Let π_m and π_n be irreducible representations of $SU(2)$, then for a tensor product of π_m and π_n we have*

$$\pi_m \otimes \pi_n = \bigoplus_{j=0}^{\min\{n,m\}} \pi_{n+m-2j}$$

Proof. We refer to [Tho04]. □

Definition 3.3.2. Let G be a matrix Lie group and $\mathfrak{g}$ its associated Lie algebra. Let $f : G \to \mathbb{C}$ be an analytic function. Then for $X \in \mathfrak{g}$ we define *left Lie derivative* at point $g \in G$ to be

$$\partial_X^l(g) = \frac{d}{dt}f(e^{tX}g)\Big|_{t=0}$$

Similarly right derivative is

$$\partial_X^r(g) = \frac{d}{dt}f(ge^{tX})\Big|_{t=0}$$

Remark. This definitions agree with

$$\partial_X^l(g) = \lim_{t\to\infty}\frac{f(e^{tX}g) - f(g)}{t}$$

and

$$\partial_X^r(g) = \lim_{t\to\infty}\frac{f(ge^{tX}) - f(g)}{t}$$

See [Chi11] for more properties of Lie derivatives.

4 Results

This section introduces the primary results of this thesis. We compute the non-commutative Fourier transform of the expectation value function for parameterized quantum circuits. We show that it has some good properties that allow us to easily find derivatives of this function. We also develop an approach for computing these derivatives.

4.1 Preparatory Theorems

Before we begin with some actual computations we have to justify why we can reduce the study of a single unit qubit unitary's expectation value function to analysis of functions on $SU(2)$. Parameterized quantum circuit in principle can have any number of qubits, which would suggest we have to be looking at $SU(2^n)$, where n is the number of qubits. The next theorem clarifies this situation.

Theorem 4.1.1. *Let $M,\ P,\ \{V_j\}_{j=1}^n \in U(2^m)$ be some fixed unitary matrices. There exist $\mu, \varrho \in M_2(\mathbb{C})$ and $a_j \in \mathbb{C}$ such that for all $g \in SU(2)$ and G of the form*

$$G := \underbrace{\mathbf{1}_2 \otimes \cdots \otimes \mathbf{1}_2}_{k} \otimes g \otimes \underbrace{\mathbf{1}_2 \otimes \ldots \otimes \mathbf{1}_2}_{n-k-1}$$

The following equation holds:

$$\operatorname{tr}(MV_m \ldots V_i G V_{i-1} \ldots V_1 P V_1^{-1} \ldots V_{i-1}^{-1} G^{-1} V_i^{-1} \ldots V_m^{-1}) = \sum_{j \in J} a_j \operatorname{tr}(\mu_j g \varrho_j g^{-1})$$

Proof. First of all observe, that since trace is invariant under cyclic permutations we can write

$$\begin{aligned} &\operatorname{tr}(MV_m \ldots V_i G V_{i-1} \ldots V_1 P V_1^{-1} \ldots V_{i-1}^{-1} G^{-1} V_i^{-1} \ldots V_m^{-1}) \\ &= \operatorname{tr}(V_i^{-1} \ldots V_m^{-1} M V_m \ldots V_i G V_{i-1} \ldots V_1 P V_1^{-1} \ldots V_{i-1}^{-1} G^{-1}) \end{aligned}$$

Now denote $V_i^{-1} \ldots V_m^{-1} M V_m \ldots V_i$ and $V_{i-1} \ldots V_1 P V_1^{-1} \ldots V_{i-1}^{-1}$ as $\mathbf{M}$ and $\mathbf{P}$ respectively, which leads to the expression of the form

$$\operatorname{tr}(\mathbf{M} G \mathbf{P} G^{-1})$$

Without loss of generality we can assume that G acts on a first qubit, meaning we can represent G as $g \otimes I$, where $I = \mathbf{1}_2^{\otimes n-1}$. $\mathbf{M}$ and $\mathbf{P}$ we can rewrite as

$$\mathbf{M} = \sum_{k \in K} \mu_k^{(1)} \otimes \mu_k^{(rest)}$$

$$\mathbf{P} = \sum_{l \in L} \varrho_l^{(1)} \otimes \varrho_l^{(rest)}$$

where $\mu_k^{(1)}$ and $\varrho_l^{(1)}$ act on a first qubit and $\mu_k^{(rest)}$ and $\varrho_l^{(rest)}$ on the rest of them. We now have

$$\begin{aligned}
\operatorname{tr}(\mathbf{M}G\mathbf{P}G^{-1}) &= \operatorname{tr}\left(\left[\sum_{k\in K}\mu_k^{(1)}\otimes\mu_k^{(rest)}\right](g\otimes I)\left[\sum_{l\in L}\varrho_l^{(1)}\otimes\varrho_l^{(rest)}\right](g^{-1}\otimes I)\right)\\
&= \sum_{k\in K}\sum_{l\in L}\operatorname{tr}\left(\left[\mu_k^{(1)}\otimes\mu_k^{(rest)}\right](g\otimes I)\left[\varrho_l^{(1)}\otimes\varrho_l^{(rest)}\right](g^{-1}\otimes I)\right)\\
&= \sum_{k\in K}\sum_{l\in L}\operatorname{tr}\left(\left[\mu_k^{(1)}g\varrho_l^{(1)}g^{-1}\right]\otimes\left[\mu_k^{(rest)}\varrho_l^{(rest)}\right]\right)\\
&= \sum_{k\in K}\sum_{l\in L}\operatorname{tr}\left[\mu_k^{(1)}g\varrho_l^{(1)}g^{-1}\right]\operatorname{tr}\left[\mu_k^{(rest)}\varrho_l^{(rest)}\right]\\
&\sum_{k\in K}\sum_{l\in L}\sum_{t,v\in N}\mu_{k(t,v)}^{(rest)}\varrho_{l(v,t)}^{(rest)}\operatorname{tr}\left[\mu_k^{(1)}g\varrho_l^{(1)}g^{-1}\right]
\end{aligned}$$

By re-indexing the quadruple sum via any set theoretical bijection $b : K \times L \times N \to J$, thus reducing it to a single sum, denoting $\mu_{k(t,v)}^{(rest)}\varrho_{l(v,t)}^{(rest)}$ as a_j for $j \in J$ and omitting upper indexes for $\mu_k^{(1)}$ and $\varrho_l^{(1)}$ we obtain the desired expression. □

One other important aspect is that up until this point we have mostly been dealing with equivalence classes of representations in the context of non-commutative Fourier transforms. While this totally makes sense for developing general theory and helps us to omit unnecessary bulky constructions with multiple indexes, once we start performing actual computations we will have no other option but to pick some concrete representatives of these equivalence classes.

Proposition 4.1.2. *Let G be a compact Hausdorff group, $\pi : G \to V_1$ and $\pi' : G \to V_2$ two equivalent irreducible representations and $T : V_1 \to V_2$ an intertwining map, then for $f \in L^1(G)$ and all $g \in G$*

$$T\hat{f}(\pi) = \hat{f}(\pi')T$$

Proof. By definition equivalence of representations implies that there exists an intertwining map $T : V_1 \to V_2$ such that for all $g \in G$ it holds that

$$T\pi(g) = \pi'(g)T$$

By Schur's lemma T is either an isomorphism or $T = 0$.

- If T is a zero map we are done.

- If T is an isomorphism then $T\pi(g) = \pi^{'}(g)T$ implies $\pi(g) = T^{-1}\pi^{'}(g)T$. Now observe

$$\begin{aligned}\hat{f}(\pi) &= \int\limits_G \pi(g^{-1})f(g)dg \\ &= \int\limits_G T^{-1}\pi^{'}(g^{-1})Tf(g)dg \\ &= T^{-1}\left(\int\limits_G \pi^{'}(g^{-1})f(g)dg\right)T \\ &= T^{-1}\hat{f}(\pi^{'})T\end{aligned}$$

Applying T to the left of both sides of the equation gives the desired result.

□

4.2 Non-Commutative Fourier Transforms of Functions on Parameterized Quantum Circuits

The goal of this subsection is to find the non-commutative Fourier transform for the expectation value function of a parameterized quantum circuit. The definition 3.2.3 of the non-commutative Fourier transform and its properties, we have listed up until this point, give us little hints on how to perform such computations so far.
One way to approach this problem would be to find a proper parameterization for an element $g \in SU(2)$ that would help us reduce an integral with respect to Haar measure on $SU(2)$ to something we could actually compute. Such approach can be found for instance in [Far08].
We shall however take an alternative route. Take $g \in SU(2)$ of the form

$$g = \begin{pmatrix} u_1 & -\bar{u}_2 \\ u_2 & \bar{u}_1 \end{pmatrix}$$

It is clear that $f(g) = \mathrm{tr}(\mu g \varrho g^{-1})$ where μ, $\varrho \in M_2(\mathbb{C})$ can be viewed as a degree 2 polynomial of four variables u_1, u_2, $\bar{u}_1$ and $\bar{u}_2$. Additionally, as we shall see later on, all the matrix entries of $\pi_2(g^{-1})$ with respect to an orthonormal basis (as in proposition 3.3.4) in $\mathcal{P}_2$ are as well degree 2 polynomials of the same four variables. Finally we consider Fourier expansion

$$f(g) = \sum_{m=0}^{\infty} d_{\pi_m}\mathrm{tr}(\hat{f}(\pi_m)\pi_m) = \sum_{m=0}^{\infty} d_{\pi_m} \sum_{i,j=1}^{d_{\pi_m}} \hat{f}^{ji}(\pi_m)\pi_m^{ij}$$

that points us to the fact, that all $\hat{f}(\pi_m) = 0$ for $m > 2$, meaning we only have to track down $\hat{f}(\pi_0)$, $\hat{f}(\pi_1)$ and $\hat{f}(\pi_2)$.
Before we do so however, let us first consider a couple of toy examples employing this technique.

Proposition 4.2.1. *Consider a function $f : SU(2) \to \mathbb{C}$, such that $f(g) = c$ where $c \in \mathbb{C}$, then*

$$\hat{f}(\pi_m) = \begin{cases} c, & \textit{for } m = 0 \\ 0, & \textit{otherwise} \end{cases}$$

Proof. First of all it is easy to see, that $\pi_0(g^{-1}) = 1$ and that $\hat{f}(\pi_m) = 0$ for $m > 0$. Now we have

$$\begin{aligned} f(g) &= \sum_{m=0}^{\infty} d_{\pi_m} \operatorname{tr}(\hat{f}(\pi_m)\pi_m) \\ &= d_{\pi_0} \operatorname{tr}(\hat{f}(\pi_0)\pi_0) \\ &= \hat{f}(\pi_0)\pi_0 \\ &= \hat{f}(\pi_0) \end{aligned}$$

And that finishes the proof. □

Proposition 4.2.2. *Given a function $f : SU(2) \to \mathbb{C}$, such that $f(g) = \operatorname{tr}(\mu g)$, where $\mu \in M_2(\mathbb{C})$, which we denote as*

$$\mu = \begin{pmatrix} \mu_{11} & \mu_{12} \\ \mu_{21} & \mu_{22} \end{pmatrix}$$

we have

$$\hat{f}(\pi_1) = \frac{1}{2} \begin{pmatrix} \mu_{22} & -\mu_{12} \\ -\mu_{21} & \mu_{11} \end{pmatrix}$$

Moreover $\hat{f}(\pi_m) \neq 0$ only if $m = 1$.

Proof. We begin with computing $\pi_1(g^{-1})$: take

$$g = \begin{pmatrix} u_1 & -\bar{u}_2 \\ u_2 & \bar{u}_1 \end{pmatrix}$$

then

$$g^{-1} = \begin{pmatrix} \bar{u}_1 & \bar{u}_2 \\ -u_2 & u_1 \end{pmatrix}$$

By definition for all $p \in \mathcal{P}_m$:

$$[\pi(g)p](z_1, z_2) = p(g^{-1}(z_1, z_2))$$

with $\{z_1, z_2\}$ as a basis for f in case of π_1. Notice that by proposition 3.3.4 this basis is already orthonormal in $\mathcal{P}_1$. We get

$$g^{-1}(z_1, z_2) = \begin{pmatrix} \bar{u}_1 z_1 + \bar{u}_2 z_2 \\ -u_2 z_1 + u_1 z_2 \end{pmatrix}$$

and therefore

$$\pi_1(g^{-1}) = \begin{pmatrix} \bar{u}_1 & \bar{u}_2 \\ -u_2 & u_1 \end{pmatrix} = g^{-1}$$

Now observe, that $\mathrm{tr}(\mu g) = \mu_{11}u_1 + \mu_{12}u_2 - \mu_{21}\bar{u}_2 + \mu_{22}\bar{u}_1$. We can now decompose f using Fourier expansion in the following way:

$$f(g) = \sum_{m=0}^{\infty} d_{\pi_m} \mathrm{tr}(\hat{f}(\pi_m)\pi_m) = \sum_{m=0}^{\infty} d_{\pi_m} \sum_{i,j=1}^{d_{\pi_m}} \hat{f}^{ji}(\pi_m)\pi_m^{ij}$$

Taking into account, that $d_{\pi_1} = 2$ we can compute the matrix entries for $\hat{f}(\pi_1)$ in the following way:

- $\pi_2^{11} = \bar{u}_1$ implies $\hat{f}^{11}(\pi_1) = \frac{1}{2}\mu_{22}$
- $\pi_2^{22} = u_1$ implies $\hat{f}^{22}(\pi_1) = \frac{1}{2}\mu_{11}$
- $\pi_2^{12} = \bar{u}_2$ implies $\hat{f}^{21}(\pi_1) = -\frac{1}{2}\mu_{21}$
- $\pi_2^{21} = -u_2$ implies $\hat{f}^{12}(\pi_1) = -\frac{1}{2}\mu_{12}$

Hence we obtain the following matrix:

$$\hat{f}(\pi_1) = \frac{1}{2}\begin{pmatrix} \mu_{22} & -\mu_{12} \\ -\mu_{21} & \mu_{11} \end{pmatrix}$$

but since $2\mathrm{tr}(\hat{f}(\pi_1)\pi_1) = f$, it means that

$$\hat{f}(\pi_m) = \begin{cases} \frac{1}{2}\begin{pmatrix} \mu_{22} & -\mu_{12} \\ -\mu_{21} & \mu_{11} \end{pmatrix}, & \text{for } m = 1 \\ 0, & \text{otherwise} \end{cases}$$

And we get the desired result. □

Now we are going to find non-commutative Fourier transform for $f(g) = \mathrm{tr}(\mu g \varrho g^{-1})$, but we shall do it in two steps. We begin with computing π_2.

Lemma 4.2.3. *Consider $g \in SU(2)$ as in theorem 4.2.2, then*

$$\pi_2(g) = \begin{pmatrix} \bar{u}_1^2 & -\frac{1}{\sqrt{2}}\bar{u}_1 u_2 & u_2^2 \\ \sqrt{2}\,\bar{u}_1\bar{u}_2 & u_1\bar{u}_1 - u_2\bar{u}_2 & -\sqrt{2}\,u_1 u_2 \\ \bar{u}_2^2 & \frac{1}{\sqrt{2}}u_1\bar{u}_2 & u_1^2 \end{pmatrix}$$

with respect to an orthonormal basis $\{\sqrt{3/2}z_1^2, \sqrt{3}z_1z_2, \sqrt{3/2}z_2^2\}$ in $\mathcal{P}_2$.

Proof. Notice that orthonormality comes from proposition 3.3.4.
However we first use $[\pi(g)p](z_1, z_2) = f(g^{-1}(z_1, z_2))$ with the basis $\{z_1^2, z_1z_2, z_2^2\}$ for $p \in \mathcal{P}_2$. Similarly we have

$$g^{-1} = \begin{pmatrix} \bar{u}_1 & \bar{u}_2 \\ -u_2 & u_1 \end{pmatrix} \text{ and } g^{-1}(z_1, z_2) = \begin{pmatrix} \bar{u}_1 z_1 + \bar{u}_2 z_2 \\ -u_2 z_1 + u_1 z_2 \end{pmatrix}$$

Now we write $g^{-1}(z_1, z_2)$ as a linear combination of basis elements for p. We get the following:

z_1^2: $\bar{u}_1^2 z_1^2 + 2\bar{u}_1\bar{u}_2 z_1 z_2 + \bar{u}_2^2 z_2^2$

z_1z_2: $-\bar{u}_1 u_2 z_1^2 + (u_1\bar{u}_1 - u_2\bar{u}_2)z_1z_2 + u_1\bar{u}_2 z_2^2$

z_2^2: $u_2^2 z_1^2 - 2u_1u_2 z_1 z_2 + u_1^2 z_2^2$

Thus we can find the following matrix for $\pi_2(g)$:

$$\begin{pmatrix} \bar{u}_1^2 & -\bar{u}_1 u_2 & u_2^2 \\ 2\bar{u}_1\bar{u}_2 & u_1\bar{u}_1 - u_2\bar{u}_2 & -2u_1 u_2 \\ \bar{u}_2^2 & u_1\bar{u}_2 & u_1^2 \end{pmatrix}$$

Now we adjust the matrix coefficients in accordance with the basis $\{\sqrt{3/2}z_1^2, \sqrt{3}z_1z_2, \sqrt{3/2}z_2^2\}$ and get the following result:

$$\pi_2(g) = \begin{pmatrix} \bar{u}_1^2 & -\frac{1}{\sqrt{2}}\bar{u}_1 u_2 & u_2^2 \\ \sqrt{2}\,\bar{u}_1\bar{u}_2 & u_1\bar{u}_1 - u_2\bar{u}_2 & -\sqrt{2}\,u_1 u_2 \\ \bar{u}_2^2 & \frac{1}{\sqrt{2}}u_1\bar{u}_2 & u_1^2 \end{pmatrix}$$

□

Theorem 4.2.4. *For any $g \in SU(2)$ and μ, $\varrho \in M_2(\mathbb{C})$ there exists $c \in \mathbb{C}$ and $C \in M_3(\mathbb{C})$, such that $f(g) = \operatorname{tr}(\mu g \varrho g^{-1})$ can be represented as $c + \operatorname{tr}(C\pi_3(g))$, where $c = \hat{f}(\pi_0)$ and $C = 3\hat{f}(\pi_2)$. In particular this means that non-commutative Fourier spectrum of f is supported on π_0 and π_2.*

Proof. Take

$$\mu = \begin{pmatrix} \mu_{11} & \mu_{12} \\ \mu_{21} & \mu_{22} \end{pmatrix}$$

and

$$\varrho = \begin{pmatrix} \varrho_{11} & \varrho_{12} \\ \varrho_{21} & \varrho_{22} \end{pmatrix}$$

Then we have the following expression for f:

$$\begin{aligned} \operatorname{tr}(\mu g \varrho g^{-1}) = (&\mu_{11}\varrho_{11} + \mu_{22}\varrho_{22})u_1\bar{u}_1 \\ &+ (-\mu_{11}\varrho_{12} + \mu_{22}\varrho_{12})u_1u_2 \\ &+ (\mu_{12}\varrho_{11} - \mu_{12}\varrho_{22})\bar{u}_1u_2 \\ &+ (-\mu_{11}\varrho_{21} + \mu_{22}\varrho_{21})\bar{u}_1\bar{u}_2 \\ &+ (\mu_{11}\varrho_{22} + \mu_{22}\varrho_{11})u_2\bar{u}_2 \\ &+ (\mu_{21}\varrho_{11} - \mu_{21}\varrho_{22})u_1\bar{u}_2 \\ &- \mu_{12}\varrho_{12}u_2^2 + \mu_{12}\varrho_{21}\bar{u}_1^2 \\ &+ \mu_{21}\varrho_{12}u_1^2 - \mu_{21}\varrho_{21}\bar{u}_2^2 \end{aligned}$$

Again we use the Fourier expansion to compute c and C. Notice however, that for any $g \in SU(2)$ the following relation holds:

$$u_1\bar{u}_1 + u_2\bar{u}_2 = 1$$

Meaning that $\pi_2^{22} = u_1\bar{u}_1 - u_2\bar{u}_2 = 2u_1\bar{u}_1 - 1$. Let C be $d_{\pi_2}\hat{f}(\pi_2)$. Similarly to theorem 4.2.2 we compute C:

- $\pi_2^{11} = \bar{u}_1^2$ implies $C_{11} = \mu_{21}\varrho_{21}$
- $\pi_2^{12} = -\frac{1}{\sqrt{2}}\bar{u}_1u_2$ implies $C_{21} = -\sqrt{2}(\mu_{12}\varrho_{11} - \mu_{12}\varrho_{22})$
- $\pi_2^{13} = u_2^2$ implies $C_{31} = -\mu_{12}\varrho_{12}$
- $\pi_2^{21} = \sqrt{2}\,\bar{u}_1\bar{u}_2$ implies $C_{12} = \frac{1}{\sqrt{2}}(-\mu_{11}\varrho_{21} + \mu_{22}\varrho_{21})$
- $\pi_2^{22} = 2u_1\bar{u}_1 - 1$ implies $C_{22} = \frac{1}{2}(\mu_{11}\varrho_{22} + \mu_{22}\varrho_{11} - \mu_{11}\varrho_{11} - \mu_{22}\varrho_{22})$ and $c := \hat{f}(\pi_0) = -(\mu_{11}\varrho_{11} + \mu_{22}\varrho_{22})$
- $\pi_2^{23} = -\sqrt{2}\,u_1u_2$ implies $C_{32} = -\frac{1}{\sqrt{2}}(-\mu_{11}\varrho_{12} + \mu_{22}\varrho_{12})$
- $\pi_2^{31} = \bar{u}_2^2$ implies $C_{13} = -\mu_{21}\varrho_{21}$
- $\pi_2^{32} = \frac{1}{\sqrt{2}}u_1\bar{u}_2$ implies $C_{23} = \sqrt{2}(\mu_{21}\varrho_{11} - \mu_{21}\varrho_{22})$

- $\pi_2^{33} = u_1^2$ implies $C_{33} = \mu_{21}\varrho_{12}$

Overall we obtain:

$$\hat{f}(\pi_0) = c = -(\mu_{11}\varrho_{11} + \mu_{22}\varrho_{22})$$

and $\hat{f}(\pi_2) = \frac{1}{3}C$, where C is represented by the following matrix:

$$\begin{pmatrix} \mu_{12}\varrho_{21} & \frac{1}{\sqrt{2}}(-\mu_{11}\varrho_{21} + \mu_{22}\varrho_{21}) & -\mu_{12}\varrho_{12} \\ -\sqrt{2}(\mu_{12}\varrho_{11} - \mu_{12}\varrho_{22}) & \frac{\mu_{11}\varrho_{22}+\mu_{22}\varrho_{11}-\mu_{11}\varrho_{11}-\mu_{22}\varrho_{22}}{2} & \sqrt{2}(\mu_{21}\varrho_{11} - \mu_{21}\varrho_{22}) \\ -\mu_{21}\varrho_{21} & \frac{1}{\sqrt{2}}(\mu_{11}\varrho_{12} - \mu_{22}\varrho_{12}) & \mu_{21}\varrho_{12} \end{pmatrix}$$

Therefore the non-commutative Fourier transform of function $f(g) = \mathrm{tr}(\mu g \varrho g^{-1})$ is as follows:

$$\hat{f}(\pi_m) = \begin{cases} \frac{1}{3}C, & \text{for } m = 2 \\ -(\mu_{11}\varrho_{11} + \mu_{22}\varrho_{22}), & \text{for } m = 0 \\ 0, & \text{otherwise} \end{cases}$$

□

4.3 Products of $SU(2)$ and Tensor Representations

Our next goal is to consider non-commutative Fourier transforms of multi-variable functions. In the commutative situation we have an elegant way to so. Let $\mathbb{T}_1$ be a one-torus, meaning $\mathbb{T}_1 \cong \mathbb{R}/\mathbb{Z}$, and let $x = (x_1, x_2)$ and $\xi = (\xi_1, \xi_2)$, we then have

$$\hat{f}(\xi) = \int\limits_{\mathbb{T}_1^2} e^{-2\pi i \xi \bullet x} f(x)dx = \int\limits_{\mathbb{T}_1} e^{-2\pi i \xi_1 x_1} \int\limits_{\mathbb{T}_1} e^{-2\pi i \xi_2 x_2} f(x_1, x_2)dx_2 dx_1$$

where

$$\int\limits_{\mathbb{T}_1} e^{-2\pi i \xi_2 x_2} f(x_1, x_2)dx_2 = \widehat{f(x_1, \square)}(\xi_2)$$

Now consider a group $SU(2)^2 := SU(2) \times SU(2)$. The following lemma introduces a similar result for the non-commutative case:

Lemma 4.3.1. *Let π and σ be irreducible representations of $SU(2)$, then for all $f(g, h) \in L^1(SU(2)^2)$*

$$\hat{f}(\pi \otimes \sigma) = 0$$

if $\sigma \notin \mathrm{supp}(\widehat{f(g, \square)})$ or $\pi \notin \mathrm{supp}(\widehat{f(\square, h)})$.

Proof. According to definition 3.1.10 for $g, h \in SU(2)$ we have

$$\hat{f}(\pi \otimes \sigma) = \int\limits_{SU(2)} \int\limits_{SU(2)} \pi \otimes \sigma(g^{-1}, h^{-1}) f(g,h) dg dh$$
$$= \int\limits_{SU(2)} \int\limits_{SU(2)} \pi(g^{-1}) \otimes \sigma(h^{-1}) f(g,h) dg dh$$

We are now going to look at the matrix elements, we have

$$\hat{f}(\pi \otimes \sigma)_{(k_1,k_2),(l_1,l_2)} = \int\limits_{SU(2)} \int\limits_{SU(2)} \pi_{k_1,l_1}(g^{-1}) \cdot \sigma_{k_2,l_2}(h^{-1}) f(g,h) dg dh$$
$$= \int\limits_{SU(2)} \pi_{k_1,l_1}(g^{-1}) \int\limits_{SU(2)} \sigma_{k_2,l_2}(h^{-1}) f(g,h) dg dh$$

Thus for all $\sigma \notin \operatorname{supp}(\widehat{f(g,\Box)})$ we obtain

$$\int_{SU(2)} \sigma_{k_2,l_2}(h^{-1}) f(g,h) dh = 0$$

and hence $\hat{f}(\pi \otimes \sigma) = 0$.
In a similar way we can show, that

$$\hat{f}(\pi \otimes \sigma)_{(k_1,k_2),(l_1,l_2)} = \int\limits_{SU(2)} \int\limits_{SU(2)} \pi_{k_1,l_1}(g^{-1}) \cdot \sigma_{k_2,l_2}(h^{-1}) f(g,h) dg dh$$
$$= \int\limits_{SU(2)} \int\limits_{SU(2)} \sigma_{k_2,l_2}(h^{-1}) \cdot \pi_{k_1,l_1}(g^{-1}) f(g,h) dg dh$$
$$= \int\limits_{SU(2)} \sigma_{k_2,l_2}(h^{-1}) \int\limits_{SU(2)} \pi_{k_1,l_1}(g^{-1}) f(g,h) dg dh$$

Which implies, that $\hat{f}(\pi \otimes \sigma) = 0$ for all $\pi \notin \operatorname{supp}(\widehat{f(\Box,h)})$, and this finishes the proof. $\Box$

Consider a function f of the following form:

$$f : SU(2)^2 \to \mathbb{C}$$
$$(g,h) \mapsto \operatorname{tr}(\mu g v h \varrho h^{-1} v^{-1} g^{-1})$$

where $\mu, \varrho \in M_2(\mathbb{C})$ and v is unitary. As we have showed above, to compute this function's non-commutative Fourier transform we can first fix one of its variables.

Let us fix h. Note, that we can then write $vh\varrho h^{-1}v^{-1}$ as ρ, and we obtain the following expression for $\hat{f}(\pi \otimes \square)$:

$$\hat{f}(\pi \otimes \square)_{k_1,l_1} = \int\limits_{SU(2)} \pi_{k_1,l_1}(g^{-1})\mathrm{tr}(\mu g \rho g^{-1})dg$$

Now we fix g. Since trace is invariant under cyclic permutations we can rewrite f as

$$f(g,h) = \mathrm{tr}(v^{-1}g^{-1}\mu g v h \varrho h^{-1})$$

Denote $v^{-1}g^{-1}\mu g v$ as ν, we now have

$$\hat{f}(\square \otimes \sigma)_{k_2,l_2} = \int\limits_{SU(2)} \sigma_{k_2,l_2}(h^{-1})\mathrm{tr}(\nu h \varrho h^{-1})dh$$

As a matter of fact this implies, that we can reduce our problem to the one stated in theorem 4.2.4.

Theorem 4.3.2. *Fourier spectrum $\hat{f}(\pi \otimes \pi)$ for a function*

$$f(g,h) = \mathrm{tr}(\mu g v h \varrho h^{-1} v^{-1} g^{-1})$$

is supported on π_0, π_2 and π_4.

Proof. We already know that Fourier spectrum is supported on $\{\pi_0, \pi_2\}$ for both $f(\square, h)$ and $f(g, \square)$. From this we can then deduce that the support for spectrum on $f(g,h)$ is $\{\pi_0 \otimes \pi_0, \pi_2 \otimes \pi_0, \pi_0 \otimes \pi_2, \pi_2 \otimes \pi_2\}$. Using Clebsch-Gordan formula we obtain the following:

$$\pi_0 \otimes \pi_0 = \bigoplus_{j=0}^{0} \pi_{0-2j} = \pi_0$$

$$\pi_2 \otimes \pi_0 = \pi_2 \otimes \pi_0 = \bigoplus_{j=0}^{0} \pi_{2-2j} = \pi_2$$

$$\pi_2 \otimes \pi_2 = \bigoplus_{j=0}^{2} \pi_{4-2j} = \pi_0 \oplus \pi_2 \oplus \pi_4$$

which proves our initial claim. □

4.4 Convolutions, Kernels and Derivatives

We begin this subsection with some motivation, coming from the commutative analysis. Suppose $\mathcal{F}$ is a set of functions $\mathbb{T}_1 \to \mathbb{C}$, that we want to compute derivatives of. If $\phi : \mathbb{T}_1 \to \mathbb{C}$ is a function, such that for all $f \in \mathcal{F}$

$$\phi * f = f$$

where $*$ denotes a convolution operation, which for all functions $f, g \in \mathcal{F}$ can be defined either as

$$(f * g)(x) = \int f(xy^{-1})g(y)dy$$

or

$$(f * g)(x) = \int f(y)g(y^{-1}x)dy$$

Under the assumptions that ϕ is continuously differentiable, $\partial\phi$ is bounded, f is differentiable and $\phi, f \in L^1(\mathbb{T}_1)$ we can find derivatives in the following way:

$$\partial f(x) = \partial(\phi * f)(x) = (\partial\phi * f)(x)$$

Meaning that we have a way to find derivative of f without calculating it directly (see [The20] and [Fol99] for more details).

Before we proceed with our attempt to generalize this idea for the non-commutative case, we would like to point out, that we are aware of the fact that theory covering this topic has probably been already developed. The reason why we are building it from scratch however, is to specifically focus on the $SU(2)$ case and its direct applications for parameterized quantum circuits.

Definition 4.4.1. Let G be a compact topological group and f, ϕ some arbitrary functions in $L^1(G)$, then for all $g, h \in G$ we define their convolution as follows:

$$(\phi * f)(g) = \int\limits_G \phi(gh^{-1})f(h)dh$$

We immediately get the following property.

Lemma 4.4.1. *For all functions f and ϕ in $L^1(G)$, where G is some compact topological group, the following holds:*

$$\widehat{(\phi * f)}(\pi) = \hat{f}(\pi)\hat{\phi}(\pi)$$

Proof. First of all observe, that compactness of G (in fact local compactness would suffice) ensures that $f * g$ absolutely converges almost everywhere, $f * g \in L^1(G)$ and $||f * g||_1 \leq ||f||_1||g||_1$ (see [Fol16]), thus non-commutative Fourier transform of convolution is well-defined. Moreover this means that conditions for Fubini's theorem are satisfied and we can change the order of integration in $(\widehat{\phi * f})(\pi)$. By definition we have

$$\begin{aligned}(\widehat{\phi * f})(\pi) &= \int_G \pi(g^{-1})(\phi * f)(g)dg \\ &= \int_G \pi(g^{-1}) \int_G \phi(gh^{-1})f(h)dhdg \\ &= \int_G \int_G \pi(g^{-1})\phi(gh^{-1})f(h)dhdg\end{aligned}$$

Now observe that $g^{-1} = h^{-1}hg^{-1} = h^{-1}(gh^{-1})^{-1}$, hence $\pi(g^{-1}) = \pi(h^{-1})\pi((gh^{-1})^{-1})$ and we have the following expression

$$\begin{aligned}\int_G \int_G \pi(g^{-1})\phi(gh^{-1})f(h)dhdg &= \int_G \int_G \pi(h^{-1})\pi((gh^{-1})^{-1})\phi(gh^{-1})f(h)dhdg \\ &= \int_G \int_G \pi(h^{-1})f(h)\pi((gh^{-1})^{-1})\phi(gh^{-1})dhdg \\ &= \int_G \pi(h^{-1})f(h) \int_G \pi((gh^{-1})^{-1})\phi(gh^{-1})dgdh \\ &= \hat{f}(\pi)\hat{\phi}(\pi)\end{aligned}$$

□

As a matter of fact, when we differentiate convolutions of functions on $SU(2)$, there is a similar property to the one, that we have in the commutative scenario. The next theorem illustrates that:

Theorem 4.4.2. *Let G be a compact Lie group and $\mathfrak{g}$ its associated Lie algebra. For $X \in \mathfrak{g}$ and continuously differentiable functions $f, \phi \in L^1(G)$, the following equality holds:*

$$\partial_X(\phi * f)(g) = (\partial_X \phi * f)(g)$$

where ∂_X is a right Lie derivative.

Proof. By definition

$$\partial_X(\phi * f)(g) = \partial_X\left(\int_G \phi(\Box h^{-1})f(h)dh\right)(g)$$
$$= \frac{d}{dt}\left(\int_G (\phi(\Box e^{tX}h^{-1})f(h))\Big|_{t=0} dh\right)(g)$$

Due to compactness of G and continuous differentiability of f and ϕ we can move derivative under the integral sign, therefore we get:

$$\partial_X(\phi * f)(g) = \left(\int_G \frac{d}{dt}(\phi(\Box e^{tX}h^{-1})f(h))\Big|_{t=0} dh\right)(g)$$
$$= \left(\int_G \frac{d}{dt}\phi(\Box e^{tX}h^{-1})\Big|_{t=0} f(h)dh\right)(g)$$
$$= (\partial_X\phi * f)(g)$$

□

Remark. It is easy to see, that the same property holds if we take ∂_X to be left Lie derivative. Besides, all the facts that we shall be showing up until the end of this subsection for right derivatives will also be true for the left ones.

Our next goals are to find a proper non-commutative kernel K and a class of functions such that the expectation value function on $SU(2)$ for parameterized quantum circuits falls in this class, with a property that when this kernel is convoluted with any function f from the class it gives us

$$K * f = f$$

This property together with theorem 4.4.2 will provide us with a tool that will reduce calculation of derivatives for the whole class of functions to just finding the derivative of the kernel.

Definition 4.4.2. Let G be a compact Hausdorff group and $\alpha \in \mathbb{N}$ – some fixed natural number. We shall call $f \in L^1(G)$ a function with *α-bounded spectrum* if for all irreducible representations π_j of G for which $\alpha < d_{\pi_j}$, it holds that $\hat{f}(\pi_j) = 0$. Additionally f will be called a function with *α-minimal bounded spectrum* if α is of the minimal value for which f has α-bounded spectrum.

The definition above comes in handy when we want to describe functions on compact Hausdorff groups similar to those with finite support of Fourier spectrum in the classical commutative case. The next theorem illustrates, that there exists a suitable analogy for the case of compact Hausdorff groups.

Theorem 4.4.3. *Let G be a compact Hausdorff group and denote*

$$K_m := \sum_{j=1}^{m} d_{\pi_j} \chi_{\pi_j}$$

Then for all $g \in G$ and $f \in L^1(G)$ the convolution $(K_m * f)(g)$ approximates the non-commutative Fourier spectrum of f up to d_{π_m}-dimensional irreducible representation, meaning $(K_m * f)(g)$ is a partial Fourier expansion. Additionally if f is a function with d_{π_m}-bounded spectrum, then

$$(K_m * f)(g) = f(g)$$

Proof. Denote a partial Fourier expansion of f up to d_{π_m}-dimensional irreducible representation as $\mathfrak{F}_m(f)$. We now have the following:

$$\begin{aligned}
\mathfrak{F}_m(f(g)) &= \sum_{j=0}^{m} d_{\pi_j} \operatorname{tr}(\hat{f}[\pi_j(h)]\pi_j(g)) \\
&= \sum_{j=0}^{m} d_{\pi_j} \sum_{k,l=1}^{d_{\pi_j}} \hat{f}[\pi_j(h)]_{k,l} \pi_j(g)_{l,k} \\
&= \sum_{j=0}^{m} d_{\pi_j} \sum_{k,l=1}^{d_{\pi_j}} \left(\int\limits_G \pi_j(h^{-1})_{k,l} f(h) dh \cdot \pi_j(g)_{l,k} \right)
\end{aligned}$$

Representing trace function of a product as a sum of products of respective matrix elements and expanding $\hat{f}(\pi_j(h))_{k,l}$ clearly shows that we can move the integral sign out of the double sum. Expression above can then be rewritten in the following way:

$$\begin{aligned}
\mathfrak{F}_m(f(g)) &= \int\limits_G \sum_{j=0}^{m} d_{\pi_j} \sum_{k,l=1}^{d_{\pi_j}} \pi_j(h^{-1})_{k,l} f(h) \pi_j(g)_{l,k} dh \\
&= \int\limits_G \sum_{j=0}^{m} d_{\pi_j} \sum_{k,l=1}^{d_{\pi_j}} \pi_j(g)_{l,k} \pi_j(h^{-1})_{k,l} f(h) dh \\
&= \int\limits_G \sum_{j=0}^{m} d_{\pi_j} \mathrm{tr}[\pi_j(g)\pi_j(h^{-1})] f(h) dh \\
&= \int\limits_G \sum_{j=0}^{m} d_{\pi_j} \mathrm{tr}[\pi_j(gh^{-1})] f(h) dh \\
&= \Big[\Big(\sum_{j=0}^{m} d_{\pi_j} \mathrm{tr}(\pi_j(\Box))\Big) * f\Big](g) \\
&= \Big[\Big(\sum_{j=0}^{m} d_{\pi_j} \chi_{\pi_j}(\Box)\Big) * f\Big](g) \\
&= (K_m * f)(g)
\end{aligned}$$

Finally if f has a d_{π_m}-bounded spectrum, then

$$\sum_{j=m+1}^{\infty} d_{\pi_j} \mathrm{tr}(\hat{f}[\pi_j(h)]\pi_j(g)) = 0$$

and therefore

$$\begin{aligned}
(K_m * f)(g) &= \sum_{j=0}^{m} d_{\pi_j} \mathrm{tr}(\hat{f}[\pi_j(h)]\pi_j(g)) \\
&= \sum_{j=0}^{\infty} d_{\pi_j} \mathrm{tr}(\hat{f}[\pi_j(h)]\pi_j(g)) \\
&= f(g)
\end{aligned}$$

□

Indeed, theorems 4.4.2 and 4.4.3 provide us with a useful tool for computing derivatives of functions with d_{π_m}-bounded spectrum. The whole computation then comes down to finding $\partial_X K_m$ for a suitable m and convoluting it with the function. Notice, that for a function $f(g)$ we then have:

$$\partial_X f(g) = (\partial_X K_m * f)(g)$$

Our next goal is to find $\partial_X K_m$.

Proposition 4.4.4. *Let G be a matrix Lie group, then for all $g \in G$*

$$(\partial_X K_m)(g) = \sum_{j=0}^{m} d_{\pi_j} \mathrm{tr}(\pi_j(g)\Pi_j(X))$$

Proof.

$$\begin{aligned}(\partial_X K_m)(g) &= \partial_X\Big(\sum_{j=0}^{m} d_{\pi_j} \mathrm{tr}(\pi_j(g))\Big)\\ &= \sum_{j=0}^{m} d_{\pi_j} \frac{d}{dt}\mathrm{tr}(\pi_j(ge^{tX}))\Big|_{t=0}\\ &= \sum_{j=0}^{m} d_{\pi_j} \frac{d}{dt}\mathrm{tr}(\pi_j(g)\pi_j(e^{tX}))\Big|_{t=0}\end{aligned}$$

We can now look at each summand separately.

$$\begin{aligned}\frac{d}{dt}\mathrm{tr}(\pi_j(g)\pi_j(e^{tX}))\Big|_{t=0} &= \mathrm{tr}(\pi_j(g)\frac{d}{dt}\pi_j(e^{tX}))\Big|_{t=0}\\ &= \mathrm{tr}(\pi_j(g)\Pi_j(X))\end{aligned}$$

□

Thus for a function $f(g) \in L^1(G)$ with a d_{π_m}-bounded spectrum we have

$$(\partial_X f)(g) = \int_G \sum_{j=0}^{m} d_{\pi_j} \mathrm{tr}(\pi_j(gh^{-1})\Pi_j(X)) f(h) dh$$

We will finish this subsection with computing Π_m in the matrix form for the basis elements of Lie algebra $\mathfrak{sl}(2, \mathbb{C})$. Recall that the basis for $\mathfrak{sl}(2, \mathbb{C})$ is as follows:

$$H = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\ X_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ X_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

We know that for any $X \in \mathfrak{sl}(2, \mathbb{C})$

$$(\Pi_m(X)f)(z_1, z_2) = -\frac{\partial f}{\partial z_1}(X_{11}z_1 + X_{12}z_2) - \frac{\partial f}{\partial z_2}(X_{21}z_1 + X_{22}z_2)$$

Applying this formula to H, X_+ and X_- yields

$$\begin{aligned}\Pi_m(H) &= -z_1\frac{\partial}{\partial z_1} + z_2\frac{\partial}{\partial z_2}\\ \Pi_m(X_+) &= -z_2\frac{\partial}{\partial z_1}\\ \Pi_m(X_-) &= -z_1\frac{\partial}{\partial z_2}\end{aligned}$$

By applying these operators to the basis elements of $\mathcal{P}_m$, we get

$$\begin{aligned}\Pi_m(H)(z_1^{m-k}z_2^k) &= -(m+2k)z_1^{m-k}z_2^k \\ \Pi_m(X_+)(z_1^{m-k}z_2^k) &= -(m-k)z_1^{m-k-1}z_2^{k+1} \\ \Pi_m(X_-)(z_1^{m-k}z_2^k) &= -kz_1^{m-k+1}z_2^{k-1}\end{aligned}$$

Finally we get the following matrices for Π_m

$$\Pi_m(H) = \begin{pmatrix} -m & & & & 0 \\ & -m+2 & & & \\ & & \ddots & & \\ & & & m-2 & \\ 0 & & & & m \end{pmatrix}$$

$$\Pi_m(X_+) = \begin{pmatrix} 0 & -m & & & 0 \\ & 0 & -m+1 & & \\ & & 0 & \ddots & \\ & & & \ddots & -1 \\ 0 & & & & 0 \end{pmatrix}$$

$$\Pi_m(X_-) = \begin{pmatrix} 0 & & & & 0 \\ -1 & \ddots & & & \\ & \ddots & 0 & & \\ & & -m+1 & 0 & \\ 0 & & & -m & 0 \end{pmatrix}$$

4.5 Integrals and Derivatives of Functions on $SU(2)$ as Finite Sums

In the previous subsection we have showed that finding derivative of the expectation function for a parameterized quantum circuit can be reduced to computing an integral of specific form. More importantly in order for a quantum computer to perform such a computation, it is essential that such computation can be made within a finite amount of operations while knowing only finite amount of circuit outputs.
In the commutative case for functions $f, \phi : \mathbb{T}_1 \to \mathbb{C}$ if for all ϕ it holds that

$$\phi * f = f$$

We can find derivative of f via

$$\partial f(x) = ((\partial\phi) * f)(x)$$

We have already seen, that we can utilize a similar approach for functions on compact Hausdorff groups with an α-bounded spectrum. For functions f and ϕ on one-torus however, if their Fourier spectrum is contained for example in a finite set of the form $\{-K, \ldots, K\} \subset \mathbb{Z}$ then the convolution at point x can be found in the following way

$$\partial f(x) = \frac{1}{K+1} \sum_{j=0}^{2K} \frac{d}{dt} \phi(x e^{2\pi i t} e^{\frac{2\pi i j}{2K}}) f(e^{\frac{2\pi i j}{2K}}) \Big|_{t=0}$$

which makes it computationally useful (see [The20] for more details).
Our hope for the $SU(n)$ case is to develop a similar approach to the one, that already exists for the unitary groups $U(n)$.

Definition 4.5.1. For an element $u \in U(n)$ consider a polynomial $P_{t,t}(u)$ of degree at most t which is homogeneous in the matrix elements of u and additionally has degree at most n in the complex conjugates of these elements. A *unitary t-design* is a set of unitary matrices $X := \{u_k\}_{j=1}^{K}$ such that for every polynomial $P_{t,t}(u)$

$$\frac{1}{|X|} \sum_{u_j \in X} P_{t,t}(u_j) = \int_{U(n)} P_{t,t}(u) d\mu(U)$$

where $d\mu(U)$ is Haar measure on $U(n)$.

A function $f(g) = \mathrm{tr}(\mu g \varrho g^{-1})$, if we take $g \in U(2)$, turns into $P_{2,2}(g)$, so our problem would reduce to finding a proper unitary 2-design. This case has actually been studied well, as a matter of fact the Clifford group is a 2-design (see [Mat14]).

Theorem 4.5.1. *Consider an epimorphism $\pi : U(n) \twoheadrightarrow PU(n)$ onto projective unitary group, such that for any $\psi \in L^1(PU(n))$ and for any $g \in PU(n)$ and $u \in U(n)$*

$$\int_{PU(n)} \psi(g) d\mu(PU(n)) = \int_{U(n)} (\psi \circ \pi)(u) d\mu(U(n))$$

Let $\widetilde{P}_{t,t}$ be such, that $P_{t,t} = \widetilde{P}_{t,t} \circ \pi$. Then

$$\int_{PU(n)} \widetilde{P}_{t,t}(g) d\mu(PU(n)) = \frac{1}{|X|} \sum_{g_j \in \pi(X)} \widetilde{P}_{t,t}(g_j)$$

Proof. First of all we have

$$\begin{aligned}\frac{1}{|X|}\sum_{u_j\in X} P_{t,t}(u_j) &= \int\limits_{U(n)} P_{t,t}(u)d\mu(U)\\ &= \int\limits_{U(n)} (\widetilde{P}_{t,t}\circ\pi)(u)d\mu(U)\\ &= \int\limits_{PU(n)} \widetilde{P}_{t,t}(g)d\mu(PU(n))\end{aligned}$$

On the other hand

$$\begin{aligned}\frac{1}{|X|}\sum_{u_j\in X} P_{t,t}(u_j) &= \frac{1}{|X|}\sum_{u_j\in X}(\widetilde{P}_{t,t}\circ\pi)(u_j)\\ &= \frac{1}{|X|}\sum_{g_j\in\pi(X)} \widetilde{P}_{t,t}(g_j)\end{aligned}$$

which finishes the proof. □

We hope that that similarly to $PU(n)$ it is possible to find a proper connection between integrals over $SU(n)$ and unitary t-designs.

5 Conclusion

In this thesis we proposed a new approach for the study of parameterized quantum circuits, that employs abstract harmonic analysis techniques. Our core target was an expectation value function of parameterized quantum circuits.
We have showed that

- The expectation value function of a single qubit gate can be reduced to the study of specific type functions on a Lie group $SU(2)$.
- We have found the non-commutative Fourier transforms of an expectation function.
- Knowing the properties of non-commutative Fourier spectrum of expectation value function, we have developed a means to reduce the problem of finding derivative of this function to the study of another simpler function, which we thoroughly analyzed.
- We have developed a method for the study of expectation function of a multiple qubit gate and proved that many essential properties of this function are preserved when we extend the case from a single to multiple qubit gate.

These results can be used in quantum machine learning for maximizing the expectation function of quantum neural networks. Just as in case of classic computers, this is one of the essential tools to build efficient machine learning algorithms.

In order to make our approach computationally valuable it is important to be able to compute or estimate derivatives of the expectation functions in finite amount of steps, meaning we need a method that would allow us to perform these computations while only having access to finite amount of circuit outputs. While we have already presented some ideas on how to approach this problem, we leave it for our future research in this area.

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Appendix

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