A Study On Mutually Unbiased Bases

by

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A dissertation submitted to the

National University of Singapore

in partial fulfilment of

the requirements for the degree of

DOCTOR OF PHILOSOPHY

in

PHYSICS

Singapore,

September 12, 2012

Acknowledgements

I wish to use this oppotunity to express my gratitude to my supervisor Prof. B. -G. Englert and his postdoc Philippe Raynal who generally helped me throughout the project. Without their patience and support, this work is impossible.

Abstract

Various problems of existence of maximal sets of mutually unbiased bases are studied. For finite dimensional spaces, the well-known construction in prime power dimensions is reviewed in a systematic way, followed by an application in quantum dynamics. Next, in dimension six, we perform a numerical search and obtain the analytical expression of the four bases that have the highest "unbiasedness" found in the search. Our result provides another evidence that we can at most have a set of three mutually unbiased bases in dimension six. For infinite dimensional spaces, the continuous degree of freedom of the rotor is studied. A suitable Heisenberg pair of complementary observables is constructed. In this way, we provide a continuous set of mutually unbiased bases for the rotor and show that the rotor degree of freedom is on equal footing with the other continuous degrees of freedom.

Contents

Chapter 1

Introduction

Two orthonormal bases of a Hilbert space are called unbiased if the transition probability from any state of the first basis to any state of the second basis is independent of the two chosen states. In particular, for a finite dimensional Hilbert space $\mathbb{C}^d$, two orthonormal bases $\mathcal{A} = \{|a_1\rangle, |a_2\rangle, \ldots, |a_d\rangle\}$ and $\mathcal{B} = \{|b_1\rangle, |b_2\rangle, \ldots, |b_d\rangle\}$ are unbiased if

$$|\langle a_i|b_j\rangle|^2 = \frac{1}{d} \quad \text{for all } i, j = 1, 2, \ldots, d. \tag{1.0.1}$$

Physically, if the physical system is prepared in a state of the first basis, then all outcomes are equally probable when we conduct a measurement that probes for the states of the second basis.

This maximum degree of incompatibility between two bases [1, 2] states that the corresponding nondegenerate observables are complementary. Indeed, the technical formulation of Bohr's Principle of Complementarity [3] that is given in Ref. [4] relies on the unbiasedness of the pair of bases. Textbook discussions of this matter can be found in Refs. [5, 6].

The concept of unbiasedness can be generalized to more than two bases by defining a set of Mutually Unbiased Bases (MUB) as a set of bases that are pairwise unbiased. Familiar example is the spin states of a spin-1/2 particle for three perpendicular directions.

In addition to playing a central role in quantum kinematics, we note that MUB are important for quantum state tomography [7, 8], for quantifying wave-particle duality in multi-path interferometers [9], and for various tasks in the area of quantum information, such as quantum key distribution [10] or quantum teleportation and dense coding [11, 12, 13].

More specifically, in the context of quantum state tomography, $d+1$ von Neumann measurements provide $d-1$ independent data each in the form of d probabilities with unit sum, so that in total one has the required d^2-1 real numbers that characterize the quantum state. A set of $d+1$ MUB is optimal, in a certain sense [8], for these measurements—if there is such a set. Such a set is termed *maximal*; there cannot be more than $d+1$ MUB. To prove this fact, one may consider the vector space $\mathcal{V}_d$ of d-dimensional traceless Hermitian matrices [8], with inner product defined as the trace of the matrix product. Treating one basis state $|a\rangle$ as the vector $|a\rangle\langle a| - \mathbb{1}/d$, then two orthonormal bases are unbiased if and only if the $(d-1)$-dimensional subspaces spanned by the two bases are orthogonal. Notice that $\mathcal{V}_d$ is a (d^2-1)-dimension real vector space, and one orthonormal basis of $\mathbb{C}^d$ provides $d-1$ linearly independent vectors in $\mathcal{V}_d$. Therefore one can at most have $d+1$ MUB in dimension d.

The existence of maximal sets of MUB, the subject of this dissertation, turns out to be an interesting and difficult problem in both physics and combinatorial mathematics. Ivanovic [7] gave a first construction of maximal sets of MUB if the dimension d is a prime, and Wootters and Fields [8] succeeded in constructing maximal sets when d is the power of a prime. These two cases have been rederived in various ways; see Refs. [14, 15, 16], for example. For other finite values of d, maximal sets of MUB are unknown. Even in the simplest case of dimension six, this is an open problem although there is quite strong evidence that no more than three MUB exist [17, 18, 19, 20]. On the other hand, it is always possible to have at least three MUB in any finite dimensions $d \geq 2$ (see [21] and references therein).

Although mathematically, all infinite separable Hilbert spaces are isomorphic, there are physically or geometrically different ways of taking the limit of $d \to \infty$, which yields physically different continuous degrees of freedom. We may obtain continuous set of MUB for these degrees of freedom by taking the corresponding limit $d \to \infty$ of a maximal set of MUB for prime dimensions, with the only exception of the rotor (Motion along a circle, described by the 2π-periodic angular position, and the angular momentum which takes all integer values. Note that a circle is topologically different from a line). In fact, the rotor is the only physically interesting case where the existence of three MUB has remained unclear.

We consider this problem in dimension six and in the rotor degree of freedom. In dimension six, due to the lack of a finite field, the techniques used in prime power dimensions cannot be applied. On the other hand, the dimensionality is low, therefore a numerical search is possible. We hope that the numerical results may suggest how to handle this problem analytically. For the larger non-prime-power dimensions, a numerical search is beyond current computational power, therefore we hope that the investigation in dimension six is so thorough that one may reach a general theorem. But of course, to really achieve this, it will be extremely difficult. Here we show our attempt in this direction. For the rotor degree of freedom, its discreteness and periodicity prevent us to simply take the limit $d \to \infty$, like in the other continuous degrees of freedom. Here we make use of the discreteness of the familiar number operator in a quantum harmonic oscillator, to map the rotor to the familiar linear motion.

Our main results are

1. In dimension six, we have obtained the analytical expression of the four most distant bases, numerically found in Ref. [20],

2. For the rotor degree of freedom, we have constructed continuous sets of MUB,

which have been summarized in [22, 23]. Besides these two main results, we also review the well-known construction of maximal sets of MUB in prime power dimensions. The freedom of the multiplication of phase factors on the bases is studied in detail. Dimensionality plays an important role in this dissertation, therefore the author fixed the notation to use the letter d for arbitrary dimensionalities, while p for prime dimensionalities. Unfortunately, in Chapter 4, the linear momentum is also denoted by the letter p, but there should not be any confusion.

The contents of the remaining chapters are as follows.

In Chapter 2, one construction of maximal sets of MUB in prime power dimensions is reviewed. We follow the treatment shown in Refs. [11, 16], and focus on the phase factors that cannot be determined by the construction alone. An application of MUB in quantum dynamics for odd prime power dimensions is studied in order to justify a symmetric choice of the phase factors.

In Chapter 3, our numerical study on MUB in dimension six, which verifies the numerical result obtained by by Butterley and Hall [20], is shown. The distance function which is the foundation of our numerical study is discussed in detail followed by the results and analysis of our numerically-found solution, which provides us with a two-parameter family of six dimensional Hadamard matrices and thus the analytical expression of the numerical solution.

Chapter 4 is about MUB for the rotor degree of freedom. We discuss in details the reason why it is fundamentally different from all the other continuous degrees of freedom. Then we show why the continuous set of MUB obtained by a simple change of variable is not fully satisfactory. This motivates us to construct another set of MUB from a suitable Heisenberg pair.

In the Conclusion, we give an overall summary, and also discuss some possible further works on these topics.

Some technical details are presented in two appendices.

Chapter 2

MUB in prime power dimensions

The main objective of this chapter is to give a systematic construction of maximal sets of MUB in prime power dimensions. We follow the treatment suggested in Refs. [11, 16] to regard the numbers $0, 1, 2, \cdots, d-1$ both as elements of a finite field and ordinary integers: Whenever there are some arithmetic operations between them, they are finite field elements; only when there is no need of any arithmetic operations, and we are just taking the numerical values, they are ordinary numbers. A very brief description of finite field is given in the first section. Then based on the shift operators labeled in terms of these finite fields elements, we construct maximal sets of MUB. Next, we focus on the phase factors that cannot be determined completely by the construction. The tool of discrete Wigner functions is used to consider the problem of quantum dynamics. From this physical consideration, we argue that the symmetric choice of the phase factors is favorable in odd prime power dimensions, and after fixing this choice, we derive a discrete analogous of Liouville's theorem.

2.1 Finite fields

It is a basic fact that the number of elements of a finite field is a power of a prime, and for any prime power $d = p^M$, $M \in \mathbb{Z}^+$, there exists one and only one field F (up to isomorphism) with $|F| = d$. In particular, a field P of prime order p can be identified with the field $\mathbb{Z}/p\mathbb{Z}$ of residues modulo p, and a field F with $|F| = p^M$ can be regarded as the splitting field over P of $x^{|F|} - x$ (see Ref. [24] for details).

More explicitly, every element a of F can be represented by a M-tuples $(a_0, a_1, ..., a_{M-1})$ of integers, where each integer runs from 0 to $p-1$, such that

$$a = (a_0, a_1, ..., a_{M-1}) \text{ if } a = \sum_{n=0}^{M-1} a_n p^n, \tag{2.1.1}$$

The field addition operation $\oplus$ is defined as

$$a = b \oplus c \Leftrightarrow a_n = b_n + c_n \pmod{p}. \tag{2.1.2}$$

The inverse of element a relative to the field addition operation is denoted as $\ominus a$, and one may consider the symbol $\ominus$ as the field subtraction operation, just as the familiar case in the field of real numbers.

For the field multiplication operation $\odot$, because of the distributive law obeyed by $\oplus$ and $\odot$, it is sufficient to define $p^j \odot p^k$ as

$$p^j \odot p^k = \begin{cases} p^{j+k} & \text{if } j+k < M\,, \\ \sum_{l=0}^{M-1} \mu_l p^l & \text{if } j+k = M\,, \\ p \odot (p^{j-1} \odot p^k) \text{ recursively,} & \text{if } j+k > M\,, \end{cases} \tag{2.1.3}$$

where the coefficients $\mu_l \in \mathbb{Z}/p\mathbb{Z}$, for $l = 0, 1, \cdots, M-1$ and satisfy

$$x^M - \sum_{l=0}^{M-1} \mu_l x^l \text{ is irreducible over the field with } p \text{ elements.} \tag{2.1.4}$$

As an illustrative example, when $p = M = 2$, in order to make the polynomial $x^2 - \mu_1 x - \mu_0$ irreducible over $\mathbb{Z}/2\mathbb{Z}$, the only possibility to set $\mu_1 = \mu_0 = 1$. And one may check this choice of the μ-coefficients indeed provides us a valid field multiplication operation. Similarly as the addition operation, one may define the inverse of a nonzero element a relative to the operation $\odot$ to be $\oslash a$, and treat the symbol $\oslash$ as the field division operation.

2.2 Construction of MUB

We introduce the shift operators V_j^i, which are the building blocks of the Heisenberg-Weyl group. Then we divide these shift operators into $d+1$ cyclic groups, such that the eigenbases for these groups form one maximal set of MUB. The explicit expression of the MUB is shown in the last part of this section.

2.2.1 Shift operators

For dimension $d = p^M$, throughout this chapter we fix the notation

$$\gamma = \mathrm{e}^{\mathrm{i}2\pi/p}\,, \tag{2.2.1}$$

and select one orthonormal reference basis $\{|i\rangle, i = 0, 1, \cdots, d-1\}$ as the computational basis. With the definition of the field operations, we can define the Fourier transform basis as

$$|\widetilde{j}\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} |k\rangle \gamma^{\ominus k \odot j}\,. \tag{2.2.2}$$

Clearly we have

$$\langle\widetilde{j}|k\rangle = \gamma^{k \odot j}, \tag{2.2.3}$$

which shows that these two bases are unbiased. Define the shift operators for the computational basis,

$$V_l^0 = (V_1^0)^l = \sum_{i=0}^{d-1} |i \oplus l\rangle\langle i| \,, \tag{2.2.4}$$

and the shift operators for the Fourier transform basis

$$V_0^l = (V_0^1)^l = \sum_{i=0}^{d-1} |\widetilde{i}\rangle\langle \widetilde{i \oplus l}| \,, \tag{2.2.5}$$

where $l = 0, 1, \cdots, d-1$. We obtain the relations

$$V_l^0|i\rangle = |i \ominus l\rangle \,, \quad V_l^0|\widetilde{i}\rangle = |\widetilde{i}\rangle\gamma^{i\odot l} \tag{2.2.6}$$

$$\text{and} \quad V_0^l|\widetilde{i}\rangle = |\widetilde{i \oplus l}\rangle \,, \quad V_0^l|i\rangle = |i\rangle\gamma^{i\odot l} \,. \tag{2.2.7}$$

from the definition and the identity

$$\sum_{j=0}^{d-1} \gamma^{j\odot i} = d\delta_{i,0} \,. \tag{2.2.8}$$

Note that Eq. (2.2.8) also allows us to link the projector $|i\rangle\langle i|$ with the shift operator V_0^l as

$$|i\rangle\langle i| = \frac{1}{d}\sum_{n=0}^{d-1}\Bigl(\gamma^{\ominus i\odot l}V_0^l\Bigr)^n . \tag{2.2.9}$$

The operator multiplication of the shift operators V_0^j and V_i^0 gives the building blocks of the Heisenberg-Weyl group

$$V_i^j = V_0^j V_i^0 = \gamma^{i\odot j} V_i^0 V_0^j \,, \tag{2.2.10}$$

with the composition law

$$V_i^j V_k^l = \gamma^{\ominus i\odot l} V_0^j V_0^l V_i^0 V_k^0 = \gamma^{\ominus i\odot l} V_{i\oplus k}^{j\oplus l} \,. \tag{2.2.11}$$

The orthonormality relation for such operators

$$\mathrm{Tr}\bigl\{(V_j^i)^\dagger V_n^m\bigr\} = d\delta_{i,m}\delta_{j,n} \tag{2.2.12}$$

can be derived from the composition law Eq. (2.2.11).

2.2.2 Cyclic groups

Now we have d^2 orthonormal shift operators. We will show that they provide us with a maximal set of MUB. First note that

$$(V_1^i)^l = V_l^{i\odot l} \times \text{some phase factor}, \tag{2.2.13}$$

since every nonzero element has an multiplicative inverse, the d operators $(V_1^i)^l$ with $l = 0, 1, \cdots d-1$ are all different, and together with some proper phase factors, it is possible to make these d operators into a cyclic group. The orthonormality relation Eq. (2.2.12) implies that for any two such groups, the only common element is the identity V_0^0. These d groups together with the group $\{V_0^l, l = 0, 1, \cdots, d-1\}$ divide these d^2 operators into $d+1$ cyclic groups. Denote the common eigenbasis of the operators in the i-th group as $\{|e_j^i\rangle, j = 0, 1, \cdots, d-1\}$, and observe from Eq. (2.2.7) that the eigenbasis of V_0^l is just the computational basis. We make the claim that the following set of bases $\{|j\rangle = |e_j^d\rangle, |e_j^i\rangle, i, j = 0, 1, \cdots, d-1\}$ form a maximal set of MUB.

Before we prove that these bases are really MUB, we want to show that the phase factors which permit us to do such a sorting exist. Eq. (2.2.13) suggests that we set

$$U_l^i = \alpha_l^i V_l^{i\odot l}\,, \tag{2.2.14}$$

where U_l^i denotes the l-th element of the i-th group, and α_l^i is the phase factor we are looking for. Since these phase factors α_l^i make the group cyclic, we have

$$U_l^i = \sum_{k=0}^{d-1} |e_k^i\rangle \gamma^{k\odot l} \langle e_k^i|\,, \tag{2.2.15}$$

and similarly as Eq. (2.2.9), it is possible to express the projector $|e_k^i\rangle\langle e_k^i|$ in terms of the operator U_l^i as

$$|e_k^i\rangle\langle e_k^i| = \frac{1}{d}\sum_{n=0}^{d-1}\left(\gamma^{\ominus k\odot l} U_l^i\right)^n. \tag{2.2.16}$$

When i=0, the operators $(V_1^0)^l = V_l^0, l = 0, 1, \cdots, d-1$ already form a group, therefore we can just set $\alpha_l^0 = 1, l = 0, 1, \cdots, d-1$. When $l = 0$, for any value of i, the element is always the identity. Therefore $\alpha_0^i = 1, i = 0, 1, \cdots, d-1$. For other values of α_j^i, according to the cyclic property,

$$U_l^i = U_1^i (U_{l\ominus 1}^i)^{l\ominus 1}, \tag{2.2.17}$$

which implies the recurrence relation

$$\alpha_l^i = \alpha_1^i \alpha_{l\ominus 1}^i \gamma^{\ominus i \odot (l \ominus 1)}, \tag{2.2.18}$$

or equivalently,

$$\alpha_k^i \alpha_l^i = \alpha_{k\oplus l}^i \gamma^{i\odot k \odot l}. \tag{2.2.19}$$

In summary, the requirements for the phase factors α_j^i are the following

$$\begin{aligned} \alpha_l^0 &= 1, \\ \alpha_0^i &= 1, \\ \alpha_k^i \alpha_l^i &= \alpha_{k\oplus l}^i \gamma^{i\odot k\odot l}, \end{aligned}$$

where i and l run from 0 to $d-1$.

These requirements do not determine the phase factors α_j^i uniquely. It can be easily seen that if α_j^i is a valid choice, and β_j^i are some phase factors satisfying

$$\beta_j^i \beta_k^i = \beta_{j\oplus k}^i, \quad \beta_j^0 = \beta_0^i = 1, \tag{2.2.20}$$

then $\alpha_j^i \beta_j^i$ is also valid. For example, if α_j^i is a valid choice, then for an arbitrary field element b_i, $\alpha_l^i \gamma^{b_i \odot l}$ is also valid. In the next section we will show that the symmetric choice [16]

$$\alpha_l^i = \gamma^{\ominus (i\odot l \odot l)\oslash 2} \tag{2.2.21}$$

is favorable in odd prime power dimensions. Eq. (2.2.19) implies that

$$\alpha_l^i \alpha_{\ominus l}^i = \gamma^{i \odot l \odot l} \,, \tag{2.2.22}$$

therefore for the symmetric choice of α_j^i in Eq. (2.2.21), we have

$$\alpha_l^i = \alpha_{\ominus l}^i \,. \tag{2.2.23}$$

This is why we call such a choice symmetric.

2.2.3 The explicit expression

Explicitly, the 0-th basis is the eigenbasis of V_l^0, namely $|e_i^0\rangle = |\widetilde{i}\rangle$, while the d-th MUB is the computational basis $|e_i^d\rangle = |i\rangle$. Generally the j-th state of the i-th bases $(i = 0, 1, \cdots, d-1)$ can be expressed as

$$|e_j^i\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} |k\rangle \gamma^{\ominus j \odot k} \left(\alpha_{\ominus k}^i\right)^* , \tag{2.2.24}$$

where $\left(\alpha_{\ominus k}^i\right)^*$ is the complex conjugate of the phase factor $\alpha_{\ominus k}^i$, namely

$$\left(\alpha_{\ominus k}^i\right)^* \alpha_{\ominus k}^i = 1 \,. \tag{2.2.25}$$

This can be verified as

$$\begin{aligned} U_l^i |e_j^i\rangle &= \alpha_l^i V_l^{i \odot l} \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} |k\rangle \gamma^{\ominus j \odot k} \left(\alpha_{\ominus k}^i\right)^* \\ &= \frac{1}{\sqrt{d}} \sum_{k \oplus l = 0}^{d-1} |k \oplus l\rangle \gamma^{\ominus j \odot (k \oplus l)} \left(\alpha_l^i \gamma^{i \odot l \odot (k \oplus l)} \left(\alpha_{\ominus k}^i\right)^*\right) \gamma^{l \odot j} \\ &= |e_j^i\rangle \gamma^{l \odot j} \,, \end{aligned} \tag{2.2.26}$$

where Eq. (2.2.19) is needed to show

$$\alpha_l^i \gamma^{i \odot l \odot (k \oplus l)} \left(\alpha_{\ominus k}^i\right)^* = \left(\alpha_{\ominus (k \oplus l)}^i\right)^* . \tag{2.2.27}$$

This explicit expression Eq. (2.2.24) can be used to verify that these bases are indeed mutually unbiased. It is obvious that

$$\langle k|e^i_j\rangle = \frac{1}{\sqrt{d}}\gamma^{\ominus j\odot k}\left(\alpha^i_{\ominus k}\right)^*, \tag{2.2.28}$$

therefore the computational basis is unbiased to all the other bases. Note that if we fix the symmetric choice of the phase factors α^i_j as in Eq. (2.2.21), then

$$\langle k|e^i_j\rangle = \frac{1}{\sqrt{d}}\gamma^{i\odot k\odot k\oslash 2\ominus j\odot k}, \tag{2.2.29}$$

which is just the familiar quadratic complex Gaussian wave function expression of MUB. Generally, we can calculate the transition probabilities directly. Note that for $j, m = 0, 1, \cdots, d-1$,

$$\langle e^i_j|e^m_n\rangle = \frac{1}{d}\sum_{k=0}^{d-1}\gamma^{\ominus k\odot(n\ominus j)}\alpha^i_{\ominus k}\left(\alpha^m_{\ominus k}\right)^*, \tag{2.2.30}$$

therefore

$$\begin{aligned}
\left|\langle e^i_j|e^m_n\rangle\right|^2 &= \frac{1}{d^2}\sum_{k=0}^{d-1}\gamma^{\ominus k\odot(n\ominus j)}\alpha^i_{\ominus k}\left(\alpha^m_{\ominus k}\right)^*\sum_{l=0}^{d-1}\left(\gamma^{\ominus l\odot(n\ominus j)}\alpha^i_{\ominus l}\left(\alpha^m_{\ominus l}\right)^*\right)^* \\
&= \frac{1}{d^2}\sum_{k,l=0}^{d-1}\gamma^{\ominus(k\ominus l)\odot(n\ominus j)}\left(\alpha^i_{k\ominus l}\right)^*\gamma^{\ominus i\odot k\odot(k\ominus l)}\left(\alpha^m_{\ominus(k\ominus l)}\right)^*\gamma^{\ominus m\odot l\odot(k\ominus l)} \\
&= \frac{1}{d}\sum_{k=0}^{d-1}\delta_{i\odot k, m\odot k}\gamma^{\ominus k\odot(n\ominus j)}\left(\alpha^i_k\right)^*\left(\alpha^m_{\ominus k}\right)^*\gamma^{\ominus i\odot k\odot k} \\
&= \frac{1}{d}+\delta_{i,m}\left(\delta_{j,n}-\frac{1}{d}\right)
\end{aligned} \tag{2.2.31}$$

where Eqs. (2.2.8) and (2.2.19) are needed in the calculation. Therefore, the set of bases $\{|j\rangle = |e^d_j\rangle, |e^i_j\rangle, i, j = 0, 1, \cdots, d-1\}$ is indeed a maximal set of MUB for dimension $d = p^M$.

The explicit expression (2.2.24) also enables us to justify why we call the unitary operator V^i_j the shift operator. Consider the action of V^i_l on the basis ket $|e^i_j\rangle$,

$$V^m_n|e^i_j\rangle = \frac{1}{\sqrt{d}} V^m_0 V^0_n \sum_{k=0}^{d-1} |k\rangle \gamma^{\ominus j \odot k} \left(\alpha^i_{\ominus k}\right)^* \\ = |e^i_{j \oplus i \odot n \ominus m}\rangle \gamma^{j \odot n} \left(\alpha^i_n\right)^* , \tag{2.2.32}$$

which shifts the states of the same basis (if we ignore the phase factor).

2.3 Discrete Wigner function

With the help of the maximal set of MUB $\{|e^i_j\rangle, i, j = 0, 1, \cdots, d\}$ obtained in Sec. 2.2, we define the Hermitian operator $W_{m,n}$ as

$$W_{m,n} = |e^d_m\rangle\langle e^d_m| + \sum_{i=0}^{d-1} |e^i_{i \odot m \ominus n}\rangle\langle e^i_{i \odot m \ominus n}| - \mathbb{1} \,. \tag{2.3.1}$$

By definition, they are normalized,

$$\mathrm{Tr}\{W_{m,n}\} = 1 \,, \tag{2.3.2}$$

and the unbiasedness property (2.2.31) implies the orthonormality relation

$$\mathrm{Tr}\{W_{m,n} W_{m',n'}\} = d \delta_{m,m'} \delta_{n,n'} \,. \tag{2.3.3}$$

These operators can be treated as Wigner-type hermitian basis [25], they are pairwise orthogonal, and we can state the completeness relation

$$G = \frac{1}{d} \sum_{m,n=0}^{d-1} g_{m,n} W_{m,n}, \text{ with } g_{m,n} = \mathrm{Tr}\{G W_{m,n}\} \tag{2.3.4}$$

for any qudit operator G. The coefficients $g_{m,n}$ are just the discrete analogue of Wigner functions [26, 27], we call it discrete Wigner functions [28, 29, 30]. Eq. (2.2.16) allows us to express the $W_{m,n}$ in terms of the shift operators V^i_j as

$$W_{0,0} = \frac{1}{d} \sum_{i=0}^{d-1} \Big(V^i_0 + \sum_{j=1}^{d-1} \alpha^{i \oslash j}_j V^i_j \Big) \,. \tag{2.3.5}$$

Then from Eq. (2.2.32), we obtain

$$W_{m,n} = V_m^n W_{0,0} V_m^{n\dagger} \,. \tag{2.3.6}$$

Particularly, when we restrict ourselves to odd prime power dimensions only, and select the symmetric phase factors (2.2.21), then in Eq. (2.3.5) we have

$$V_0^i + \sum_{j=1}^{d-1} \alpha_j^{i\oslash j} V_j^i = \sum_{j=0}^{d-1} V_{j\oslash 2}^0 V_0^i V_{j\oslash 2}^0 \,, \tag{2.3.7}$$

consequently

$$W_{0,0} = \frac{1}{d} \sum_{i,k=0}^{d-1} V_k^0 V_0^i V_k^0 = \sum_{k=0}^{d-1} |k\rangle\langle \ominus k| \,, \tag{2.3.8}$$

thus in the limit of $p \to \infty$, the $W_{m,n}$ for the symmetric choice of α_j^i converges to the continuous Wigner basis.

Now with the tool of discrete Wigner functions, we consider the problem of quantum dynamics in odd prime power dimensions. The Heisenberg equation of a system in a state with density matrix ρ for under certain Hamiltonian H is

$$\frac{\partial}{\partial t}\rho = i[\rho, H] \,. \tag{2.3.9}$$

We can express the density matrix ρ and the Hamiltonian H in terms of discrete Wigner functions as

$$\rho = \frac{1}{d} \sum_{m,n=0}^{d-1} \rho_{m,n} W_{m,n}, \text{ with } \rho_{m,n} = \mathrm{Tr}\big\{\rho W_{m,n}\big\} \,, \tag{2.3.10}$$

$$H = \frac{1}{d} \sum_{m,n=0}^{d-1} h_{m,n} W_{m,n}, \text{ with } h_{m,n} = \mathrm{Tr}\big\{H W_{m,n}\big\}. \tag{2.3.11}$$

Then, in order to calculate the commutator, we need to express ρH in terms of discrete Wigner functions, that is,

$$(\rho H)_{m_3,n_3} = \frac{1}{d^2} \sum_{m_1,n_1} \sum_{m_2,n_2} \mathrm{Tr}\{\rho_{m_1,n_1} W_{m_1,n_1} h_{m_1,n_1} W_{m_2,n_2} W_{m_3,n_3}\} \,. \tag{2.3.12}$$

Therefore we need to calculate $\mathrm{Tr}\{W_{m_1,n_1}W_{m_2,n_2}W_{m_3,n_3}\}$, the trace of three Wigner bases. This can be easily done in odd prime power dimensions with the symmetric choice of α_i^j. From Eqs. (2.3.6) and (2.3.8), we have

$$W_{m,n} = \sum_{k=0}^{d-1} |m \oplus k\rangle\langle m \ominus k| \gamma^{2\odot k\odot n} \,. \tag{2.3.13}$$

Therefore

$$\begin{aligned}\prod_{i=1}^{3} W_{m_i,n_i} = &\sum_{i,j,k=0}^{d-1} \langle m_1 \ominus i|m_2 \oplus j\rangle\langle m_2 \ominus j|m_3 \oplus k\rangle \\ &\times |m_1 \oplus i\rangle \gamma^{2\odot i\odot n_1 + 2\odot j\odot n_2 + 2\odot k\odot n_3} \langle m_3 \ominus k| \,,\end{aligned} \tag{2.3.14}$$

and consequently

$$\begin{aligned}\mathrm{Tr}\{\prod_{i=1}^{3} W_{m_i,n_i}\} = &\gamma^{2\odot(m_3\ominus m_2)\odot n_1} \gamma^{2\odot(m_1\ominus m_3)\odot n_2} \\ &\times \gamma^{2\odot(m_2\ominus m_1)\odot n_3} \,,\end{aligned} \tag{2.3.15}$$

which is very similar to the result obtained in the continuous case.

Generally, we need to apply Eqs. (2.3.5) and (2.3.6) and obtain

$$W_{m,n} = \frac{1}{d}\sum_{i=0}^{d-1} V_0^i \gamma^{\ominus m\odot i} + \frac{1}{d}\sum_{i=0}^{d-1}\sum_{j=1}^{d-1} \alpha_j^i \gamma^{n\odot j\ominus m\odot i\odot j} V_j^{i\odot j} \,. \tag{2.3.16}$$

The calculation of the trace of three Wigner bases $W_{m_1,n_1}, W_{m_2,n_2}, W_{m_3,n_3}$ is now much more tedious. We use the composition law Eq. (2.2.11) and the fact that except V_0^0 has trace d, all the other V_i^j are traceless. Making use of the symmetry of the three indices, in the end, we have to deal with two kinds of sums:

$$\circ \sum_{i_2,i_3}\sum_{j_2} \gamma^{i_2\odot j_2\odot(m_1\ominus m_2)} \gamma^{i_3\odot j_2\odot(m_3\ominus m_1)} \gamma^{j_2\odot(n_2\ominus n_3)} \alpha_{j_2}^{i_2} \left(\alpha_{j_2}^{i_3}\right)^* \,, \tag{2.3.17}$$

$$\begin{aligned}\circ &\sum_{i_2,i_3}\sum_{j_2,j_3} \gamma^{j_2\odot(n_2\ominus n_1)} \gamma^{j_3\odot(n_3\ominus n_1)} \gamma^{i_2\odot j_2\odot(m_1\ominus m_2)} \gamma^{i_3\odot j_3\odot(m_1\ominus m_3)} \\ &\times \gamma^{j_3\odot i_2\odot j_2} \alpha_{j_1}^{i_1} \left(\alpha_{\ominus j_3}^{i_3}\right)^* \left(\alpha_{\ominus j_2}^{i_2}\right)^* \,.\end{aligned} \tag{2.3.18}$$

We cannot do any further simplification generally. As a check of consistency with Eq. (2.3.15), we fix the symmetric choice, and the two kinds of sums all become Kronecker delta symbols with some proper phase factors, and then we obtain

$$\begin{aligned}
\mathrm{Tr}\{\prod_{i=1}^{3} W_{m_i,n_i}\} = \; & \delta_{m_2,m_3}(1-\delta_{m_1,m_2})\gamma^{2\odot(m_1\ominus m_2)\odot(n_2\ominus n_3)} \\
& +\delta_{m_3,m_1}(1-\delta_{m_2,m_1})\gamma^{2\odot(m_2\ominus m_3)\odot(n_3\ominus n_1)} \\
& +\delta_{m_1,m_2}(1-\delta_{m_3,m_1})\gamma^{2\odot(m_3\ominus m_1)\odot(n_1\ominus n_2)} \\
& +(1-\delta_{m_1,m_2})(1-\delta_{m_2,m_3})\gamma^{2\odot(m_1\ominus m_3)\odot(n_2\ominus n_1)} \\
& \times\gamma^{2\odot(m_2\ominus m_1)\odot(n_3\ominus n_1)} + \delta_{m_1,m_2}\delta_{m_2,m_3}\delta_{m_3,m_1}\,.
\end{aligned}$$

Now there are five possibilities:

$$\begin{aligned}
& 1, m_1 = m_2 = m_3;\; 2, m_1 = m_2 \neq m_3;\; 3, m_1 \neq m_2 = m_3\,; \\
& 4, m_2 \neq m_1 = m_3;\; 5, m_1 \neq m_2,\; m_2 \neq m_3 \text{ and } m_3 \neq m_1\,.
\end{aligned}$$

It can be easily calculated that all the five cases all give us the same result as Eq. (2.3.15), as it should be.

In the end, we get the trace of the three Wigner bases in odd prime power dimensions for the symmetric choice of α_l^i in a particularly simple form (2.3.15), which is also very similar to the continuous case. Now we can use this result to continue our calculation of the Heisenberg's equation through discrete Wigner functions.

2.4 A discrete version of Liouville's theorem

As an application of the construction of MUB and discrete Wigner functions in odd prime power dimensions, we consider the classical approximation of quantum dynamics. Throughout this section, we fix the symmetric choice of the phase factors α_j^i as in Eq. (2.2.21), and therefore have the simple form of the discrete Wigner functions

$$(\rho H)_{m_3,n_3} = \frac{1}{d^2}\sum_{m_1,n_1}\sum_{m_2,n_2}\rho_{m_1,n_1}h_{m_2,n_2}\gamma^{2\odot(m_3\ominus m_2)\odot n_1} \times\gamma^{2\odot(m_1\ominus m_3)\odot n_2}\gamma^{2\odot(m_2\ominus m_1)\odot n_3}\,. \tag{2.4.1}$$

Relabeling the discrete Wigner functions as

$$\begin{cases} m_1 \to m_1 \oplus m_3,\ \ n_1 \to n_1 \oplus n_3, \\ m_2 \to m_2 \oplus m_3,\ \ n_2 \to n_2 \oplus n_3, \end{cases} \tag{2.4.2}$$

provides us a more compact expression

$$(\rho H)_{m_3,n_3} = \frac{1}{d^2}\sum_{m_1,n_1}\sum_{m_2,n_2}\rho_{m_1\oplus m_3,n_1\oplus n_3}h_{m_2\oplus m_3,n_2\oplus n_3}\gamma^{2\odot(m_1\odot n_2\ominus m_2\odot n_1)}\,. \tag{2.4.3}$$

In order to apply the method of Ref. [31], to make a classical approximation, we need to define a discrete version of differentiation. By Eq. (2.2.8), we have

$$a_{m,n} = \frac{1}{d}\sum_{m_1,n_1}\gamma^{(m\ominus m_1)\odot n_1}a_{m_1,n}\,. \tag{2.4.4}$$

Then by analogy of the differentiation in Fourier transform, we can define

$$\frac{\partial}{\partial m}a_{m,n} = \frac{1}{d}\sum_{m_1,n_1}\gamma^{(m\ominus m_1)\odot n_1}a_{m_1,n}\left(\mathrm{i}n_1\frac{2\pi}{p}\right)\,. \tag{2.4.5}$$

The definition (2.4.5) is clearly linear, and we have

$$\frac{\partial}{\partial m}(a_{m,n}b_{m,n}) = \left(\frac{\partial}{\partial m}a_{m,n}\right)b_{m,n} \oplus a_{m,n}\left(\frac{\partial}{\partial m}b_{m,n}\right)\,, \tag{2.4.6}$$

which can be treated as the product rule. To take the continuous limit, it is sufficient to consider only prime dimensions [5], that is, we may set $d = p$. If we relabel the states as

$$m \to \frac{x}{\epsilon},\ n \to \frac{y}{\epsilon},\ \text{with } \epsilon = \sqrt{\frac{2\pi}{p}}\,, \tag{2.4.7}$$

then Eq. (2.4.5) just becomes the normal differentiation in Fourier transform when $\epsilon \to 0$. These facts justify the definition (2.4.5) as a discrete version of differentiation.

Now we can apply the method discussed in Ref. [31] by noticing the discrete displacement

$$
\begin{aligned}
e^{m_1\odot\frac{\partial}{\partial m}} a_{m,n} &= \sum_{k=0}^{\infty} \frac{1}{k!}\Big(m_1 \odot \frac{\partial}{\partial m}\Big)^k a_{m,n} \\
&= \sum_{k=0}^{\infty} \sum_{m',n'} \frac{1}{k!}\Big(\mathrm{i}\frac{2\pi}{p} m_1 \odot n'\Big)^k \frac{1}{d} a_{m',n}\gamma^{n'\odot(m\ominus m')} \\
&= \sum_{m',n'} \frac{1}{d} a_{m',n}\gamma^{n'\odot(m\oplus m_1\ominus m')} = a_{m\oplus m_1,n}\,. \qquad (2.4.8)
\end{aligned}
$$

Substitution of Eq. (2.4.8) into Eq. (2.4.3) yields

$$
\begin{aligned}
(\rho H)_{m_3,n_3} &= \frac{1}{d^2} \sum_{m_1,n_1} \sum_{m_2,n_2} \gamma^{\ominus 2\odot m_2\odot n_1}\gamma^{2\odot m_1\odot n_2} \\
&\quad \times \Big[\exp\Big(m_1\odot\frac{\partial}{\partial m'} \oplus n_2\odot\frac{\partial}{\partial n''} \oplus m_2\odot\frac{\partial}{\partial m''} \\
&\quad \oplus n_1\odot\frac{\partial}{\partial n'}\Big)\rho_{m',n'}h_{m'',n''}\Big]_{m'=m''=m_3,\ n'=n''=n_3} \\
&= \exp\Big(\frac{\mathrm{i}p}{2\pi}\Big\{\frac{\partial}{\partial m_3},\frac{\partial}{\partial n_3}\Big\} \oslash 2\Big)\rho_{m_3,n_3}h_{m_3,n_3}\,. \qquad (2.4.9)
\end{aligned}
$$

Notice that the $\{\partial/\partial m, \partial/\partial n\}$ is the discrete analogue of the Poisson bracket, with the difference that the $\partial/\partial m$ and $\partial/\partial n$ are always referred to the definition (2.4.5). Therefore, we may obtain a compact expression to describe the dynamics of the state ρ in the Hamiltonian H by writing out the commutator using Eq. (2.4.9),

$$
(\rho H)_{m,n} - (H\rho)_{m,n} = 2\mathrm{i}\sin\Big(\frac{p}{2\pi}\Big(\Big\{\frac{\partial}{\partial m},\frac{\partial}{\partial n}\Big\} \oslash 2\Big)\Big)\rho_{m,n}h_{m,n}\,, \qquad (2.4.10)
$$

or

$$
\Big(\frac{\partial}{\partial t}\rho\Big)_{m,n} = -2\sin\Big(\frac{p}{2\pi}\Big(\Big\{\frac{\partial}{\partial m},\frac{\partial}{\partial n}\Big\} \oslash 2\Big)\Big)\rho_{m,n}h_{m,n}\,. \qquad (2.4.11)
$$

Note that the time differentiation on the left hand side of Eq. (2.4.11) is the normal continuous one, while all the other differentiations on the right hand side are referred to the one defined in Eq. (2.4.5), which is discrete. And if we take the limit $p \to \infty$ as in (2.4.7), we just recover the corresponding expression for the continuous Wigner function, which has been reported in Ref. [31]. If we do an approximation on the sine function that only keeps the linear term, then we get the analogous expression to the Poisson bracket in the continuous case as

$$\left(\frac{\partial}{\partial t}\rho\right)_{m,n} \approx -\frac{p}{\pi}\left(\left\{\frac{\partial}{\partial m}, \frac{\partial}{\partial n}\right\} \oslash 2\right)\rho_{m,n}h_{m,n}\,, \tag{2.4.12}$$

which is corresponding to Liouville's theorem. We note that although our final expression (2.4.12) is in a very compact form, and indeed very similar to the continuous case, any real calculation based on it is complicated.

2.5 Summary

We have reviewed the well-known construction in prime power dimensions, such that in dimension $d = p^M$, the $d+1$ bases are the computational basis $\{|k\rangle, k = 0, 1, \cdots, d-1\}$ together with the d bases $\{|e^i_j\rangle, i, j = 0, 1, \cdots, d-1\}$ such that

$$|e^i_j\rangle = \frac{1}{\sqrt{d}}\sum_{k=0}^{d-1} |k\rangle\gamma^{\ominus j\odot k}\left(\alpha^i_{\ominus k}\right)^*,$$

where $i, j = 0, 1, \cdots, d-1$. The phase factors α^i_j should satisfy

$$\begin{aligned} \alpha^0_l &= 1, \\ \alpha^i_0 &= 1, \\ \alpha^i_k\alpha^i_l &= \alpha^i_{k\oplus l}\gamma^{i\odot k\odot l}\,. \end{aligned}$$

These requirements cannot fixed the phase factors α_j^i completely, we have shown that the following symmetric choice

$$\alpha_l^i = \gamma^{\ominus(i \odot l \odot l) \oslash 2}$$

is favorable in odd prime power dimensions, by considering the trace of three Wigner bases. As an direct application, we have obtained the discrete analogous of Liouville's theorem in odd prime power dimensions,

$$\Big(\frac{\partial}{\partial t}\rho\Big)_{m,n} \approx -\frac{p}{\pi}\Big(\Big\{\frac{\partial}{\partial m}, \frac{\partial}{\partial n}\Big\} \oslash 2\Big)\rho_{m,n} h_{m,n}\,.$$

Chapter 3

MUB in dimension six

The smallest non-prime-power number is $d = 6$ and it is a famous open problem whether or not maximal sets of MUB exist in this dimension. In this chapter, we show our numerical search and analysis, which provides another evidence that there can be at most three MUB in dimension six.

Recently, Bengtsson *et al.* [32] introduced a distance between two bases for a quantification of the notion of "unbiasedness." The distance vanishes when the two bases are identical and attains its maximal value of unity when they are unbiased. One can then consider the average squared distance (ASD) between several bases and search for its maximal value. Importantly, this ASD is unity if the bases are pairwise unbiased, and only then. A numerical search for the maximum of the ASD between four bases in dimension six can be performed. Actually, a numerical study on essentially the same quantity was recently carried out by Butterley and Hall [20]. In terms of the ASD, they found the surprisingly large but strictly-less-than-one maximal value of 0.9983. This is strong evidence that no more than three MUB exist in dimension six. However, the set of bases behind this maximum value is not reported in Ref. [20].

It is our objective to close this gap. In Sec. 3.1 we review the notion of Bengtsson *et al.* for the distance between bases. We perform a numerical search for the maximum ASD between four bases in dimension six and report, in Sec. 3.2, our results which confirm the maximum found by Butterley and Hall. We then provide a two-parameter family of three bases which, together with the canonical basis, reaches the numerically-found maximum, for which we give a closed expression. We study this family in detail in Sec. 3.3 and conclude with a summary. The details of the derivation of the two-parameter family are given in the Appendix.

3.1 A distance between bases

Following Bengtsson *et al.* [32], we consider two orthonormal bases of kets of $\mathbb{C}^d$, $a = \{|a_i\rangle\}$ and $b = \{|b_j\rangle\}$, and quantify their squared distance by

$$\begin{aligned} D_{ab}^2 &= 1 - \frac{1}{d-1}\sum_{i,j=1}^{d}\left(|\langle a_i|b_j\rangle|^2 - \frac{1}{d}\right)^2 \\ &= \frac{1}{d-1}\sum_{i,j=1}^{d}|\langle a_i|b_j\rangle|^2\Big(1-|\langle a_i|b_j\rangle|^2\Big) \\ &= \frac{d}{d-1} - \frac{1}{d-1}\sum_{i,j=1}^{d}|\langle a_i|b_j\rangle|^4 \,. \end{aligned} \tag{3.1.1}$$

From the first two expressions of the above Eq. (3.1.1), it is clear that this distance is symmetric and bounded, that is,

$$D_{ab} = D_{ba} \quad \text{and} \quad 0 \le D_{ab} \le 1. \tag{3.1.2}$$

For it to reach its minimum, the value of $|\langle a_i|b_j\rangle|^2$ can be either 0 or 1, which is only the case when the bases are the same, or when the two sets of projectors $\{|a_i\rangle\langle a_i|\}$ and $\{|b_j\rangle\langle b_j|\}$ are identical. For it to reach its maximum, we need

$$|\langle a_i|b_j\rangle|^2 = \frac{1}{d} \quad \text{for all } i, j = 1, 2, \ldots d, \tag{3.1.3}$$

which is exactly the requirement for the two bases to be unbiased.

In the original reasoning by Bengtsson *et al.*, D_{ab} is actually the chordal Grassmanian distance of two planes in the (d^2-1)-dimensional real vector space associated with traceless hermitian operators in the d-dimensional complex Hilbert space. Here, we show another way to see that D_{ab} is indeed a distance function, by using the mapping between one-qudit operators and two-qudit kets.

As discussed in Sec. 3.1 of Ref. [21], for any ket $|\varphi\rangle$ or bra $\langle\phi|$ in a d-dimensional Hilbert space $\mathcal{H}$ or $\mathcal{H}^\dagger$, respectively, there is a conjugate bra or ket

$$\begin{aligned} \mathcal{H} \ni |\varphi\rangle &\longleftrightarrow \langle\varphi^*| \in \mathcal{H}^\dagger\,, \\ \mathcal{H}^\dagger \ni \langle\phi| &\longleftrightarrow |\phi^*\rangle \in \mathcal{H} \end{aligned} \tag{3.1.4}$$

such that

$$\langle\varphi^*|\phi^*\rangle = \langle\varphi|\phi\rangle^* = \langle\phi|\varphi\rangle\,. \tag{3.1.5}$$

This mapping is not unique, but two different realizations differ at most by a unitary transformation. As a rule, $\langle\phi^*|$ and $\langle\phi| = |\phi\rangle^\dagger$ are different bras.

Once a particular choice of mapping has been made, there is a one-to-one correspondence between one-qudit operators and two-qudit kets,

$$|\varphi\rangle\langle\phi| \in B(\mathcal{H}) \longleftrightarrow |\phi^*\rangle \otimes |\varphi\rangle \in \mathcal{H}\otimes\mathcal{H}\,. \tag{3.1.6}$$

In particular, for an orthonormal basis of kets in $\mathcal{H}$, $a = \big\{|a_1\rangle, |a_2\rangle \ldots, |a_d\rangle\big\}$, we have the conjugate basis $a^* = \big\{|a_1^*\rangle, |a_2^*\rangle, \ldots, |a_d^*\rangle\big\}$, and jointly they are used in defining the two-qudit state

$$\rho_a = \frac{1}{d}\sum_{j=1}^{d} |a_j^* a_j\rangle\langle a_j^* a_j|\,, \tag{3.1.7}$$

which has the d-fold eigenvalue $1/d$ and the (d^2-d)-fold eigenvalue zero.

From the last expression of Eq. (3.1.1), we know that this distance is essentially related to

$$\sum_{j,k=1}^{d} |\langle a_j|b_k\rangle|^4 = \sum_{j,k=1}^{d} \mathrm{Tr}\big\{|a_j\rangle\langle a_j|b_k\rangle\langle b_k|a_j\rangle\langle a_j|b_k\rangle\langle b_k|\big\}. \tag{3.1.8}$$

Now we can consider the mapping

$$|a_j\rangle\langle a_j| \leftrightarrow |a_j^* a_j\rangle, \quad |b_k\rangle\langle b_k| \leftrightarrow |b_k^* b_k\rangle. \tag{3.1.9}$$

From the identity

$$\begin{aligned}\langle a_j^* a_j|b_k^* b_k\rangle &= \langle a_j^*|b_k^*\rangle\langle a_k|b_k\rangle \\ &= |\langle a_j|b_k\rangle|^2\end{aligned} \tag{3.1.10}$$

we obtain

$$\begin{aligned}\sum_{j,k=1}^{d} |\langle a_j|b_k\rangle|^4 &= \sum_{j,k=1}^{d} \mathrm{Tr}\big\{|a_j^* a_j\rangle\langle a_j^* a_j|b_k^* b_k\rangle\langle b_k^* b_k|\big\} \\ &= d^2\mathrm{Tr}\big\{\rho_a\rho_b\big\},\end{aligned} \tag{3.1.11}$$

where ρ_a and ρ_b are defined as in Eq. (3.1.7). After normalizing the Hilbert-Schmidt inner product of two-qudit operators in accordance with

$$(A,B) = d\,\mathrm{Tr}\big\{A^\dagger B\big\}\,, \tag{3.1.12}$$

so that $(\rho_a,\rho_a)=1$ and $(\rho_a,\rho_b)=1/d$ for a pair of unbiased bases, we then have

$$(\rho_a,\rho_b) = \frac{1}{d}\sum_{j,k=1}^{d} \big|\langle a_j|b_k\rangle\big|^4 = 1 - \frac{d-1}{d}D_{ab}^2, \tag{3.1.13}$$

or equivalently

$$\begin{aligned}D_{ab}^2 &= \frac{d}{d-1} - \frac{d}{d-1}\,(\rho_a,\rho_b) \\ &= \frac{1}{2}\frac{d}{d-1}\,(\rho_a-\rho_b,\rho_a-\rho_b)\end{aligned} \tag{3.1.14}$$

with the distance D_{ab} of Eq. (3.1.1).

Therefore D_{ab} can be expressed in terms of the Hilbert-Schmidt norm of $\rho_a - \rho_b$,

$$D_{ab} = \sqrt{\frac{1}{2}\frac{d}{d-1}}\,\|\rho_a - \rho_b\| \tag{3.1.15}$$

with $\|A\| = \sqrt{(A,A)}$. This tells something important: If $a \neq b$, then $\rho_a \neq \rho_b$, so that the mapping $a \leftrightarrow \rho_a$ is one-to-one.

For a set of k bases, we have the ASD between the $k(k-1)/2$ pairs of bases, given by

$$\begin{aligned} \overline{D^2} &= \frac{2}{k(k-1)} \sum_{a<b=1}^{k} D_{ab}^2 \\ &= \frac{2}{k(k-1)} \sum_{a<b=1}^{k} \frac{d}{d-1} - \frac{d^2}{d-1}\mathrm{Tr}\big\{\rho_a\rho_b\big\}\,, \end{aligned} \tag{3.1.16}$$

where the prefactor $2/k(k-1)$ is for normalization. As an immediate consequence of Eq. (3.1.2), we have $0 \leq \overline{D^2} \leq 1$ with $\overline{D^2} = 1$ if and only if the k bases are pairwise unbiased. Since the distance D_{ab} vanishes when $a = b$, we can also express $\overline{D^2}$ as

$$\overline{D^2} = \frac{1}{k(k-1)} \sum_{a,b=1}^{k} \frac{d}{d-1} - \frac{d^2}{d-1}\mathrm{Tr}\big\{\rho_a\rho_b\big\}\,. \tag{3.1.17}$$

With this notion of distance at hand, we can numerically search for the maximum ASD between four bases in dimension six and see whether we obtain $\overline{D^2} = 1$, or in other words, if we can find four MUB. This search is the subject matter of the next section.

3.2 Numerical study

We use the steepest-ascent algorithm to find the maximum ASD between four bases in dimension six. The numerical search begins with a randomly chosen initial set of bases, and then changes the bases in each iteration round such that $\overline{D^2}$ is systematically increased.

An infinitesimal variation of a ket in basis a is given by

$$\delta_a|a_j\rangle = \mathrm{i}\epsilon_a|a_j\rangle \quad \epsilon_a = \epsilon_a^\dagger, \tag{3.2.1}$$

where ϵ_a is an infinitesimal hermitian operator acting on the basis a, Accordingly

$$\delta_a\langle a_j| = -\mathrm{i}\langle a_j|\epsilon_a, \quad \text{and} \quad \delta_a|a_j^*\rangle = -\mathrm{i}\epsilon_a^*|a_j^*\rangle, \tag{3.2.2}$$

such that $\epsilon_a^*|a_j^*\rangle \leftrightarrow \langle a_j|\epsilon_a$. For the response of $|a_j^* a_j\rangle$,

$$\begin{aligned}\delta_a|a_j^* a_j\rangle &= (\delta_a|a_j^*\rangle)|a_j\rangle + |a^*\rangle(\delta_a|a_j\rangle)\\ &= \mathrm{i}\left(\mathbb{1}\otimes\epsilon_a - \epsilon_a^*\otimes\mathbb{1}\right)|a_j^* a_j\rangle = \mathrm{i}E_a|a_j^* a_j\rangle,\end{aligned} \tag{3.2.3}$$

where we define $E_a = \mathbb{1}\otimes\epsilon_a - \epsilon_a^*\otimes\mathbb{1}$. Therefore for $|a_j^* a_j\rangle\langle a_j^* a_j|$,

$$\begin{aligned}\delta_a\left(|a_j^* a_j\rangle\langle a_j^* a_j|\right) &= \left(\delta_a|a_j^* a_j\rangle\right)\langle a_j^* a_j| + |a_j^* a_j\rangle\delta_a\left(\langle a_j^* a_j|\right)\\ &= \mathrm{i}[E_a, |a_j^* a_j\rangle\langle a_j^* a_j|].\end{aligned} \tag{3.2.4}$$

Now we are ready to calculate the resulting response of $\overline{D^2}$,

$$\begin{aligned}\delta_a\overline{D^2} &= -\frac{1}{k(k-1)}\frac{d^2}{d-1}\sum_{a=1}^{k}\mathrm{Tr}\big\{(\delta_a\rho_a)\sum_{b=1}^{k}\rho_b\big\}\\ &= -\frac{i}{k(k-1)}\frac{d^2}{d-1}\sum_{a=1}^{k}\mathrm{Tr}\big\{E_a[\rho_a,\sum_{b=1}^{k}\rho_b]\big\}\\ &= -\frac{i}{k(k-1)}\frac{d^2}{d-1}\sum_{a=1}^{k}\mathrm{Tr}\big\{(\mathbb{1}\otimes\epsilon_a - \epsilon_a^*\otimes\mathbb{1})\,[\rho_a,\sum_{b=1}^{k}\rho_b]\big\}\,.\end{aligned} \tag{3.2.5}$$

Notice that

$$\begin{aligned}&(\epsilon_a^*\otimes\mathbb{1})|a_j^* a_j\rangle \leftrightarrow |a_j\rangle\langle a_j|\epsilon_a \leftrightarrow \langle a_j^* a_j|(\mathbb{1}\otimes\epsilon_a)\,,\\ &\langle a_j^* a_j|(\epsilon_a^*\otimes\mathbb{1}) \leftrightarrow \epsilon_a|a_j\rangle\langle a_j| \leftrightarrow (\mathbb{1}\otimes\epsilon_a)|a_j^* a_j\rangle\,,\end{aligned} \tag{3.2.6}$$

thus it is easy to establish that

$$\mathrm{Tr}\big\{(\epsilon_a^* \otimes \mathbb{1})[\rho_a, \rho_b]\big\} = -\mathrm{Tr}\big\{(\mathbb{1} \otimes \epsilon_a)[\rho_a, \rho_b]\big\}. \tag{3.2.7}$$

Therefore we have

$$\begin{aligned}\delta_a \overline{D^2} &= -\frac{2\mathrm{i}}{k(k-1)} \frac{d^2}{d-1} \sum_{a=1}^{k} \mathrm{Tr}\big\{(\mathbb{1} \otimes \epsilon_a)[\rho_a, \sum_{b=1}^{k} \rho_b]\big\} \\ &= -\frac{2\mathrm{i}}{k(k-1)} \frac{d^2}{d-1} \sum_{a=1}^{k} \mathrm{Tr}\big\{\epsilon_a \mathrm{Tr}_1\{[\rho_a, \sum_{b=1}^{k} \rho_b]\}\big\}. \end{aligned} \tag{3.2.8}$$

Eq. (3.2.8) makes it clear that if we choose

$$\begin{aligned}\epsilon_a &= \mathrm{i}\kappa \sum_{b=1}^{k} \mathrm{Tr}_1\{[\rho_a, \rho_b]\} \\ &= \mathrm{i}\kappa \sum_{b=1}^{k} \sum_{i,j=1}^{d} |\langle a_i | b_j \rangle|^2 [|a_i\rangle\langle a_i|, |b_j\rangle\langle b_j|] \end{aligned} \tag{3.2.9}$$

where κ is one sufficiently small positive number, then the variation $\delta_a \overline{D^2}$ is always positive, and therefore the value of $\overline{D^2}$ is systematically increased, until it reaches its local maximums.

In practice, the finite unitary change of basis a, $|a_j\rangle \to U_a |a_j\rangle$ is accomplished by

$$U_a = (1 + \mathrm{i}\epsilon_a) \prod_{n=0}^{\infty} \Big[1 + e^{\mathrm{i}2\pi/3} \big(\epsilon_a^2\big)^{3^n}\Big] \tag{3.2.10}$$

Notice this U_a equals $1 + \mathrm{i}\epsilon_a$ to first order in ϵ_a, and that a high-precision evaluation of the infinite product of U_a requires very few terms.

The iteration is terminated, when all components of the gradient vanish (in the numerical sense specified by the machine precision). We repeat this steepest-ascent search many times to ensure that we find the global maximum.

Table 1: Rate of success and CPU time (in seconds) for the steepest ascent search for the maximum ASD. The absolute maximum of $\overline{D^2} = 1$ is always reached for $d+1$ bases in dimensions $d = 2$, 3, 4, and 5. As the seven-dimensional case illustrates, the difficulty of finding the global maximum increases rapidly with the dimension because there are many local maxima at which the steepest-ascent search can get stuck. We have also looked for the largest ASD between four bases in dimensions two to seven. We could not find four MUB in dimensions two and six. The CPU time refers to a Intel®Core™2 Duo CPU E6550 processor at 2.33 GHz, supported by 3.25 GB of RAM.

	$d+1$ bases			4 bases		
d	$\overline{D^2}_{\max}$	Success rate (%)	CPU time	$\overline{D^2}_{\max}$	Success rate (%)	CPU time
2	1	100	0.049	8/9	100	0.108
3	1	99.9	0.272	1	99.9	0.272
4	1	100	1.268	1	100	0.976
5	1	99.7	4.432	1	59.8	10.995
6	0.9849	39.2	188.407	0.9983	69.6	20.158
7	1	3.8	467.157	1	1.1	101.002

A similar numerical study was recently performed by Butterley and Hall [20] who minimized $1 - \overline{D^2}$ with the so-called Levenberg-Marquadt algorithm. Our approach confirms the extremal value they found, and we also exhibit the structure of the four bases that maximize $\overline{D^2}$ for $d = 6$. We have used our code not only in dimension $d = 6$ but also for other d values as a mean of benchmarking. We have run our code 2,500 times for the dimensions two to five, 10,000 times for the dimension six and 300 times for the dimension seven, both for $k = d + 1$ bases and for four bases. Our results are summarized in Table 1. Only in two cases, the maximum ASD does not

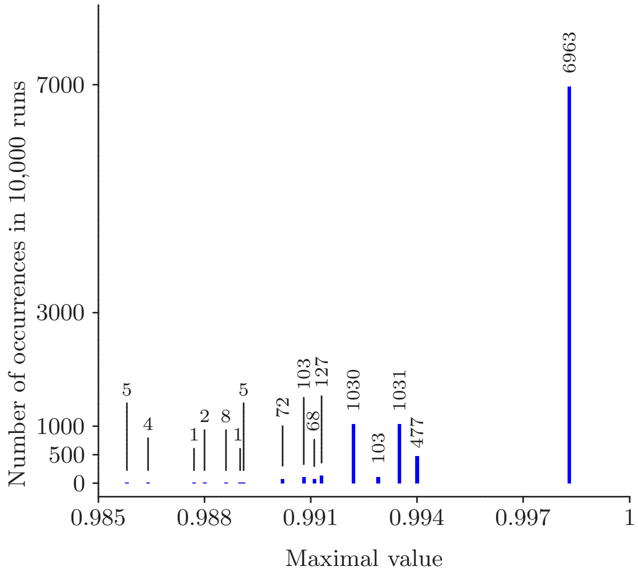

Figure 3.1: Histogram of the maximum values of the ASD found during a numerical search for 10,000 randomly chosen initial four bases. The search converges to one of the local maxima in about 30% of all runs, and to the global maximum of $\overline{D^2}_{\max} = 0.9983$ for the other 70% of initial bases.

reach the upper bound of $\overline{D^2} = 1$. They are the cases of four bases in dimension two and six. At most three MUB can be constructed in dimension two. Thus the maximum ASD between four bases has to be less than one. This example is interesting because it can be analytically solved. In $\mathbb{R}^3$, the four bases correspond to the tetrahedron, where each edge represents a basis.

Importantly, we have searched for the maximum ASD between four bases in dimension six. We have found the largest value to be $\overline{D^2}_{\max} = 0.9983$. In the search for the global maximum, we have also found a few other local maxima whose frequencies of occurrence are reported in Figure 3.1. These results are consistent with those reported by Butterley and Hall [20]. We find the same local and global maxima with very similar frequencies. This is as expected because we have generated the four random bases from which the search proceeds in the same way as Butterley and Hall, using the same dedicated Matlab command. The two numerical methods are different, however. We use the steepest-ascent algorithm while they employ the Levenberg-Marquadt algorithm for a nonlinear least-squares optimization.

Since we consider four bases, there are six pairs of bases and their respective distances are not without interest. Indeed, it turns out that one basis is unbiased with the three remaining bases. And these three remaining bases are themselves equidistant. The immediate implication is that the privileged basis can be chosen to be the computational basis while the three remaining bases are Hadamard bases, that is: the unitary matrices composed of the columns that represent the basis kets with reference to the computational basis are complex Hadamard matrices divided by $\sqrt{6}$. We recall here that a complex Hadamard matrix is a d-dimensional square matrix satisfying the two conditions of unimodularity and orthogonality [33]

$$\begin{aligned} |H_{ij}| &= 1 \quad \text{for } i,j = 1,\dots,d\,, \\ HH^\dagger &= d\;. \end{aligned} \tag{3.2.11}$$

Therefore, the unitary matrix $H/\sqrt{d}$ has matrix elements that can be related to a pair of unbiased bases: $\langle a_i|b_j\rangle = H_{ij}/\sqrt{d}$.

In addition to maximizing $\overline{D^2}$, our code also returns the four bases for which the maximum is achieved. After a bit of polishing—the set of four bases is not unique, since global unitary transformations yield equivalent sets, and the order of kets in each basis is arbitrary—this allows us to seek for the structure hidden behind the maximum ASD. In the next section we will present a two-parameter family of three bases. The two parameters are two phases while the three bases are three Hadamard bases. We study in detail the properties of this family and show that, for some definite values of the two parameters, these three bases together with the canonical basis reach the numerically-found maximum ASD of 0.9983. This definite structure of the optimal four bases is our main result, with a closed expression for $\overline{D^2}_{\max}$ as a most-welcome bonus; see Eq. (3.3.30) below.

Harking back to Table 1, we note that the best set of seven bases in dimension six has an ASD of 0.9849, short of unity by a mere one-and-a-half percent. For all practical purposes—those of state tomography, say—these seven bases are marginally worse than the imaginary seven MUB that no one has managed to find.

3.3 The two-parameter family

Following Karlsson [34], we express the two-parameter family in terms of 2×2 block matrices where each of the nine blocks is itself a complex Hadamard matrix. Such 2×2 block matrices are called H_2-reducible. The two-parameter family contains three bases, the fourth basis being the canonical basis. We will see that these three Hadamard bases are equidistant, that their determinants are identical, and that they belong to the so-called Fourier transposed family F_6^T. Finally, we will show that together with the canonical basis they reach the numerically-found maximum of the ASD.

3.3.1 Parametrization

We begin by defining a few quantities. We will need the third root of unity $\omega = \exp(\mathrm{i}\,2\pi/3)$ as well as the following 2×2 matrices:

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} , \quad X = \begin{bmatrix} x^* & 0 \\ 0 & x \end{bmatrix} , \quad F_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

and

$$T = \begin{bmatrix} 1 & \omega t^2 \\ 1 & -\omega t^2 \end{bmatrix} \tag{3.3.1}$$

where $t = \exp(\mathrm{i}\theta_t)$ and $x = \exp(\mathrm{i}\theta_x)$ are two phases. Let us notice that T and F_2 are themselves Hadamard matrices.

The Hadamard matrices for the three bases are given by

$$\begin{aligned} M_1 &= \begin{bmatrix} X & 0 & 0 \\ 0 & \mathrm{i}\omega^* t Z X^{*2} & 0 \\ 0 & 0 & X \end{bmatrix} \frac{1}{\sqrt{6}} \begin{bmatrix} F_2 & F_2 & F_2 \\ F_2 & \omega F_2 & \omega^* F_2 \\ T & \omega^* T & \omega T \end{bmatrix} \\ &= \frac{1}{\sqrt{6}} X_1 N_1 \,, \end{aligned}$$

$$M_2 = \frac{1}{\sqrt{6}} \begin{bmatrix} F_2 & F_2 & F_2 \\ T & \omega T & \omega^* T \\ T & \omega^* T & \omega T \end{bmatrix} = \frac{1}{\sqrt{6}} N_2 \,,$$

and

$$\begin{aligned} M_3 &= \begin{bmatrix} X^* & 0 & 0 \\ 0 & \omega^* X^* & 0 \\ 0 & 0 & -\mathrm{i} t Z X^2 \end{bmatrix} \frac{1}{\sqrt{6}} \begin{bmatrix} F_2 & F_2 & F_2 \\ T & \omega T & \omega^* T \\ F_2 & \omega^* F_2 & \omega F_2 \end{bmatrix} \\ &= \frac{1}{\sqrt{6}} X_3 N_3 \,. \end{aligned} \tag{3.3.2}$$

In the above parameterization, we have introduced the matrices X_i and N_i, $i = 1, 2, 3$, which we will address as dephasing and central matrices, respectively. The derivation of this parameterization is explained in Appendix A.

3.3.2 Properties

This section is devoted to proving the three properties earlier mentioned.

Equidistance

A significant property of the three proposed Hadamard matrices is their equidistance. The relevant terms that appear in the distance between the two bases M_a and M_b (i.e., $|\langle a_i|b_j\rangle|$) are the elements of the product matrix $M_a^\dagger M_b$ (i.e., $\langle a_i|b_j\rangle$) in absolute value. Therefore, if the three product matrices $M_1^\dagger M_2$, $M_2^\dagger M_3$ and $M_3^\dagger M_1$ have equal coefficients in absolute value, then the three bases M_1, M_2 and M_3 are equidistant.

Direct calculation shows that this is exactly what happens here. To simplify the notation, denote $\mathrm{i}ZX^{*2}$ as $\bar{X}$, that is,

$$\bar{X} = \mathrm{i}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} \mathrm{e}^{\mathrm{i}2\theta_x} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}2\theta_x} \end{bmatrix} = \mathrm{i}\begin{bmatrix} \mathrm{e}^{\mathrm{i}2\theta_x} & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}2\theta_x} \end{bmatrix} \tag{3.3.3}$$

It is easy to see that in the product matrix of

$$6M_1^\dagger M_2 = \begin{bmatrix} F_2 & F_2 & T^\dagger \\ F_2 & \omega^2 F_2 & \omega T^\dagger \\ F_2 & \omega F_2 & \omega^2 T^\dagger \end{bmatrix}\begin{bmatrix} X^* & 0 & 0 \\ 0 & \omega^2 t^* \bar{X}^* & 0 \\ 0 & 0 & X^* \end{bmatrix}\begin{bmatrix} F_2 & F_2 & F_2 \\ T & \omega T & \omega^2 T \\ T & \omega^2 T & \omega T \end{bmatrix} \tag{3.3.4}$$

there are only three different forms of the nine block elements

$$\alpha^{(k)} = F_2 X^* F_2 + \omega^k t^* F_2 \bar{X}^* T + \omega^{2k+1} T^\dagger X^* T, \quad k = 1, 2, 3\,. \tag{3.3.5}$$

Similar observation shows that

$$\beta^{(k)} = F_2 X^* F_2 + \omega^k T^\dagger X^* T + \omega^{2k-1} t F_2 \bar{X}^* T \text{ for } M_2^\dagger M_3\,, \tag{3.3.6}$$

$$\gamma^{(k)} = F_2 X^2 F_2 + \omega^{k-1} t T^\dagger X \bar{X} F_2 + \omega^{2k+1} t^* F_2 \bar{X} X T \text{ for } M_3^\dagger M_1\,, \tag{3.3.7}$$

with $k = 1, 2, 3$, are the corresponding forms of the block elements in the other two products. Therefore, we only need to calculate the terms like $F_2 X^* F_2$, and then combine them accordingly. As the result, we have the following cyclic structure:

$$M_1^\dagger M_2 = \frac{1}{6}\begin{bmatrix} \alpha^{(1)} & \alpha^{(2)} & \alpha^{(3)} \\ \alpha^{(3)} & \alpha^{(1)} & \alpha^{(2)} \\ \alpha^{(2)} & \alpha^{(3)} & \alpha^{(1)} \end{bmatrix}, \quad M_2^\dagger M_3 = \frac{1}{6}\begin{bmatrix} \beta^{(1)} & \beta^{(2)} & \beta^{(3)} \\ \beta^{(3)} & \beta^{(1)} & \beta^{(2)} \\ \beta^{(2)} & \beta^{(3)} & \beta^{(1)} \end{bmatrix},$$

and

$$M_3^\dagger M_1 = \frac{1}{6}\begin{bmatrix} \gamma^{(1)} & \gamma^{(2)} & \gamma^{(3)} \\ \gamma^{(3)} & \gamma^{(1)} & \gamma^{(2)} \\ \gamma^{(2)} & \gamma^{(3)} & \gamma^{(1)} \end{bmatrix}. \tag{3.3.8}$$

More precisely, for the matrix elements $\alpha_{ij}^{(k)}$ of the 2×2 matrice $\alpha^{(k)}$, we have

$$\begin{aligned} \alpha_{11}^{(k)} &= 2\omega^{k-1}\left(2\cos(\theta_x)\cos\left(\tfrac{2k}{3}\pi\right) - (\omega^2 t)^*\sin(2\theta_x)\right), \\ \alpha_{22}^{(k)} &= 2\omega^{k-1}\left(2\cos(\theta_x)\cos\left(\tfrac{2k}{3}\pi\right) - (\omega^2 t)\sin(2\theta_x)\right), \\ \alpha_{12}^{(k)} &= 2\mathrm{i}\omega^{k+1}t\Big(2\cos\left(\theta_t + \tfrac{2k+2}{3}\pi\right)\sin(\theta_x) - \cos(2\theta_x)\Big), \\ \alpha_{21}^{(k)} &= 2\mathrm{i}\omega^{k}t^*\Big(2\cos\left(\theta_t - \tfrac{2k}{3}\pi\right)\sin(\theta_x) - \cos(2\theta_x)\Big). \end{aligned} \tag{3.3.9}$$

For the matrices $\beta^{(k)}$, we have (where the symbol $\check{}$ stands for swapping the two diagonal elements)

$$\beta^{(1)} = \check{\alpha}^{(2)}, \quad \beta^{(2)} = \check{\alpha}^{(1)} \quad \text{and} \quad \beta^{(3)} = \check{\alpha}^{(3)}. \tag{3.3.10}$$

And lastly for the matrices $\gamma^{(k)}$,

$$\begin{aligned} \gamma_{11}^{(k-1)} &= \gamma_{22}^{(k+1)} = \mathrm{i}\omega^{-k}t\alpha_{21}^{(k)}, \\ \gamma_{12}^{(k)} &= \mathrm{i}\omega^{-k-1}t^*\alpha_{22}^{(k)}, \\ \gamma_{21}^{(k)} &= \mathrm{i}\omega^{-k+1}t\alpha_{11}^{(k)}. \end{aligned} \tag{3.3.11}$$

Therefore, the corresponding elements have the same absolute value, which shows that the equidistance property of the two-parameter family.

Determinant

A direct calculation shows that

$$\mathrm{Det}(X_1) = \mathrm{Det}(N_1) = \mathrm{Det}(X_3) = \mathrm{Det}(N_3) = wt^2. \tag{3.3.12}$$

Accordingly, the three Hadamard bases share the same determinant

$$\mathrm{Det}(M_1) = \mathrm{Det}(M_2) = \mathrm{Det}(M_3) = w^* t^4 \,. \tag{3.3.13}$$

However, although the determinants are equal, there seems to be no simple relation between the three matrices M_1, M_2, and M_3. In particular, they do not have the same spectrum and are, therefore, not related by unitary transformations.

Fourier transposed family

The Fourier transposed family, first studied by Haagerup, is parameterized by Karlsson in the form [34]

$$F_6^T \sim \begin{bmatrix} F_2 & F_2 & F_2 \\ Z_1 & \omega Z_1 & \omega^* Z_1 \\ Z_2 & \omega^* Z_2 & \omega Z_2 \end{bmatrix} , \tag{3.3.14}$$

where the matrices Z_1 and Z_2 are given by

$$Z_i = \begin{bmatrix} 1 & z_i \\ 1 & -z_i \end{bmatrix} , \quad |z_i| = 1 \,. \tag{3.3.15}$$

The equivalence relation in Eq. (3.3.14) means equality up to left and right dephasing and left and right permutations. In other words, the central matrix is the fundamental object that specifies the equivalence class. In the form of Eq. (3.3.2), it is clear that the three matrices N_1, N_2, and N_3 belong to the Fourier transposed family. As a result, the two-parameter family itself belongs to the Fourier transposed family. Actually, we have already used the property of the Fourier transposed family to simplify the above calculation of $M_a^\dagger M_b$.

Let us note here that only the right equivalence is natural for more than two bases as it only states that bases are defined up to permutations and global phases of their basis states. In particular, the distance between bases is invariant under right equivalence but not under left equivalence.

3.3.3 Average distance

Let us now compute the global maximum of the ASD between the three bases. Since the three bases are equidistant, we only have to compute the distance between, say, M_1 and M_2. We need to sum up the fourth power of the absolute value of all the elements of the matrix $M_1^\dagger M_2$. Due to its cyclic structure, we know that this desired sum can be calculated as

$$\text{sum} = \sum_{i,j=1}^{2} \sum_{k=1}^{3} 3 \left(|\alpha_{ij}^{(k)}|/6 \right)^4 . \tag{3.3.16}$$

Then from Eq. (3.1.1), the squared distance is

$$D_{12}^2(\theta_x, \theta_t) = \frac{6}{5} - \frac{\text{sum}}{5} = \frac{6}{5} - \sum_{i,j} \sum_{k} \frac{|\alpha_{ij}^{(k)}|^4}{2160} . \tag{3.3.17}$$

From the result in Eq. (3.3.9), we have to deal with the following terms

$$\begin{aligned}
|\alpha_{11}^{(k)}| &= 2 \left| 2\cos(\theta_x) \cos\left(\tfrac{2k+1}{3}\pi\right) + (\omega^2 t)^* \sin(2\theta_x) \right| , \\
|\alpha_{22}^{(k)}| &= 2 \left| 2\cos(\theta_x) \cos\left(\tfrac{2k+1}{3}\pi\right) + (\omega^2 t) \sin(2\theta_x) \right| , \\
|\alpha_{12}^{(k)}| &= 4\cos\left(\theta_t + \tfrac{2k+2}{3}\pi\right) \sin(\theta_x) - 2\cos(2\theta_x) , \\
|\alpha_{21}^{(k)}| &= 4\cos\left(\theta_t - \tfrac{2k}{3}\pi\right) \sin(\theta_x) - 2\cos(2\theta_x) .
\end{aligned} \tag{3.3.18}$$

It is clear that $|\alpha_{11}^{(k)}|^2 = |\alpha_{22}^{(k)}|^2$ and the difference between $|\alpha_{12}^{(k)}|$ and $|\alpha_{21}^{(k)}|$ is just the labeling k. Therefore, the squared terms are only of two kinds: $|\alpha_{11}^{(k)}|^2$ and $|\alpha_{21}^{(k+1)}|^2$. Direct calculation shows

$$\begin{aligned}
\frac{1}{4}|\alpha_{11}^{(k)}|^2 &= 4\cos(\tfrac{2k\pi}{3})^2 \cos(\theta_x) + \sin(2\theta_x)^2 \\
&\quad +4\cos(\tfrac{2k\pi}{3}) \cos(\theta_x) \sin(2\theta_x) \cos(\theta_t + \tfrac{\pi}{3}) , \\
\frac{1}{4}|\alpha_{21}^{(k+1)}|^2 &= 4\cos(\theta_t + \tfrac{\pi}{3} - \tfrac{2k\pi}{3})^2 \sin(\theta_x)^2 + \cos(2\theta_x)^2 \\
&\quad +4\cos(\theta_t + \tfrac{\pi}{3} - \tfrac{2k\pi}{3}) \sin(\theta_x) \cos(2\theta_x) ,
\end{aligned} \tag{3.3.19}$$

where we have used

$$\cos(\theta_t - \tfrac{2\pi}{3}) = -\cos(\theta_t + \tfrac{\pi}{3})\,. \tag{3.3.20}$$

Eq. (3.3.19) also suggests that we do the change of variable as

$$\theta_t' = \theta_t + \frac{\pi}{3}. \tag{3.3.21}$$

Now we are ready to calculate the summation of the fourth powers. Notice the following identities

$$\begin{aligned}
&\sum_{k=1}^{3} \cos(x + \frac{2k\pi}{3}) = 0, \quad \sum_{k=1}^{3} \cos(x + \frac{2k\pi}{3})^2 = \frac{3}{2}\,, \\
&\sum_{k=1}^{3} \cos(x + \frac{2k\pi}{3})^3 = 3\cos(x)^3 - \frac{9}{4}\cos(x)\,, \\
&\sum_{k=1}^{3} \cos(x + \frac{2k\pi}{3})^4 = \frac{9}{8}\,,
\end{aligned} \tag{3.3.22}$$

it is not difficult to obtain

$$\begin{aligned}
\frac{1}{16}\sum_{k=1}^{3} |\alpha_{11}^{(k)}|^4 &= 18\cos(\theta_x)^4 + 3\sin(2\theta_x)^4 + 12\cos(\theta_x)^2\sin(2\theta_x)^2 \\
&\quad +24\cos(\theta_x)^2\sin(2\theta_x)^2\cos(\theta_t')^2 \\
&\quad +24\cos(\theta_x)^3\sin(2\theta_x)\cos(\theta_t')\,, \\
\frac{1}{16}\sum_{k=1}^{3} |\alpha_{21}^{(k)}|^4 &= 18\sin(\theta_x)^4 + 3\cos(2\theta_x)^4 + 36\sin(\theta_x)^2\cos(2\theta_x)^2 \\
&\quad +32\sin(\theta_x)^3\cos(2\theta_x)\big(3\cos(\theta_t')^3 - \frac{9}{4}\cos(\theta_t')\big)\,.
\end{aligned} \tag{3.3.23}$$

Notice that it is possible to express all the terms in our result (3.3.23) in terms of $\sin(\theta_x)$ and $\cos(\theta_t')$, this suggests that we are able to express the squared distance, which is related to the summation of the fourth order by Eq. (3.3.17), as a polynomial function in two variables. After some straightforward calculation, we arrive at the following compact expression

$$D_{12}^2(\theta_x, \theta_t) = \frac{8}{45}\big[5 - P\big(\sin(\theta_x), \cos(\theta_t + \tfrac{1}{3}\pi)\big)\big]\,, \tag{3.3.24}$$

with the polynomial

$$
\begin{aligned}
P(p,q) = 8p^8 &+ 8q^2p^6 - 16q^3p^5 \\
&+ 16qp^5 - 16q^2p^4 + 8q^3p^3 \\
&- 7p^4 - 14qp^3 + 8q^2p^2 \\
&+ 2p^2 + 4qp\,.
\end{aligned}
\tag{3.3.25}
$$

We denote by $(p_{\text{opt}}, q_{\text{opt}})$ the (p,q) pair for which $P(p,q)$ is minimal and, therefore, $D_{12}(\theta_x, \theta_t)$ is maximal. It turns out that q_{opt} is related to p_{opt} by

$$
\cos(\theta_t^{\text{opt}} + \tfrac{1}{3}\pi) = q_{\text{opt}} = \frac{1 - 2p_{\text{opt}}^2}{p_{\text{opt}}}\,, \tag{3.3.26}
$$

or explicitly

$$
\cos\bigl(\theta_t^{\text{opt}} + \tfrac{1}{3}\pi\bigr) = \frac{\cos(2\theta_x^{\text{opt}})}{\sin(\theta_x^{\text{opt}})}\,. \tag{3.3.27}
$$

This reduces the two-parameter family to a single-parameter family, and p_{opt}^2 is therefore found to be the unique real solution of a cubic equation,

$$
112p_{\text{opt}}^6 - 192p_{\text{opt}}^4 + 111p_{\text{opt}}^2 = 22\,, \tag{3.3.28}
$$

that is,

$$
\sin(\theta_x^{\text{opt}})^2 = p_{\text{opt}}^2 = \frac{3 + 16r - r^2}{28r} = 0.6946 \tag{3.3.29}
$$

with $r = (21\sqrt{3} - 36)^{1/3} = 0.7199$. It follows that there are eight optimal pairs of phases $(\theta_x^{\text{opt}}, \theta_t^{\text{opt}})$ for which the maximal distance $D_{12}^{\max}$ is reached.

The above expressions for θ_x^{opt} and θ_t^{opt} can be injected back into the formula of the distance to obtain first $D_{12}^{\max}$ and then

$$
\begin{aligned}
\overline{D^2}_{\max} &= \frac{1}{70}\bigl[71 - 12\cos(\theta_x^{\text{opt}})^4\bigr] \\
&= \frac{1}{70}\left[71 - 3\left(\frac{r^2 + 12r - 3}{14r}\right)^2\right] = 0.9983\,,
\end{aligned}
\tag{3.3.30}
$$

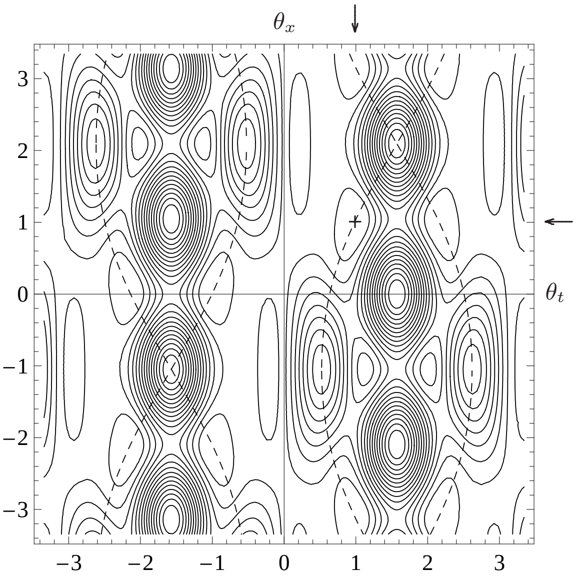

Figure 3.2: Contour plot of the ASD for the two-parameter family. Along the dashed curves, relation (3.3.27) holds. The four single-parameter families—one for each dashed curve—are equivalent to the two-parameter family in the sense that the maximal and minimal value of the ASD can be found by searching along one of the dashed lines only. The arrows point to the location of one of the eight maxima at $(\theta_x, \theta_t) = (0.9852, 1.0094)$, marked by a cross.

which agrees with the numerically-found maximum ASD within the machine precision. Furthermore, the distance D_{12} vanishes for

$$\begin{aligned} &\theta_x = \pi/2\,, \qquad \theta_t = 0 \ (\mathrm{mod}\ 2\pi/3) \\ \text{and}\ \ &\theta_x = -\pi/2\,, \quad \theta_t = \pi/3 \ (\mathrm{mod}\ 2\pi/3)\,. \end{aligned} \tag{3.3.31}$$

As can be verified from the parameterization (3.3.2) or from the matrix products (3.3.8), the bases are indeed identical up to global phases and permutations for these values of the two phases θ_x and θ_t.

The single-parameter family that we obtain when eliminating θ_t by using Eq. (3.3.27) can also be considered. Since Eq. (3.3.26) is equivalent to Eq. (3.3.27), this single-parameter family reaches both the minimum and maximum of the ASD. This is illustrated in Fig. 3.2, a contour plot of $\overline{D^2}$ for the two-parameter family of Hadamard bases, with the location of the (θ_x, θ_t) values of the single-parameter family indicated. The location of one of the eight maxima is marked, and the locations of the other seven follow from the symmetry properties of the contours.

3.4 Summary

We have performed a numerical search for the maximum ASD between four bases in dimension six. We have found that it is strictly smaller than unity and so confirmed the study recently performed by Butterley and Hall [20]. We regard this result as strong evidence that no four MUB exist in dimension six.

Next, we have gone beyond this numerical result by providing the four bases behind the numerically-found maximum. More specifically, we have found a two-parameter family of three bases, which together with the canonical basis, reaches the maximum of the ASD. We have characterized this two-parameter family in full. We have proved its inclusion in the Fourier transposed family and shown that the three bases are equidistant. Furthermore, we have analytically computed the maximum ASD between these three Hadamard bases and the canonical basis to show that it reproduces the numerical result. This is a first analytical result on the way to a proof that no more than three MUB exist in dimension six.

Chapter 4

MUB for the rotor degree of freedom

Now we turn our attention to the continuous degrees of freedom, or the limit of $d \to \infty$, actually it is sufficient to consider prime dimensions only [5], or the limit of $p \to \infty$. This limit is taken by considering a basic pair of complementary unitary operators with conjugated eigenbases (Fourier transforms of each other), or the so-called Weyl pair [2] (we refer Weyl pair to unitary operators, while Heisenberg pair to observables). Note that conjugated eigenbases are unbiased, and as a manifestation of Bohr's principle of complementarity [2, 3], the Weyl pair is algebraically complete as it suffices for a complete parameterization of the degree of freedom.

Since there exist different ways of taking the $d \to \infty$ (or practically $p \to \infty$) limit [5, 6, 21], different basic pairs corresponding to different continuous degrees of freedom can be obtained. If we treat the Weyl pair symmetrically when taking the limit, as in Eq. (2.4.7), then we will obtain the basic pair of complementary observables of the linear motion, that is, the Heisenberg pair of position observable Q and momentum observable P. We can also take this limit asymmetrically. Using the same notation as in Eq. (2.4.7), if we do the relabeling such that

$$m \to 2\pi\phi/p \text{ and } n \to l \tag{4.0.1}$$

then at the $p \to \infty$ limit, the parameters ϕ and l are just the 2π-periodic angular position, and the discrete angular momentum describing circular motion, or the rotor. Similarly, if we set

$$m \to \log r/\epsilon,\ n \to s/\epsilon \text{ with } \epsilon = \sqrt{2\pi/p}, \tag{4.0.2}$$

then at the $p \to \infty$ limit, the parameters r and s describe the radial motion, where r denotes the nonnegative radial position, while s the momentum. Another possibility is to consider the spherical coordinates, that is, parameterize the position as $(r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta)$. If we fix the value of r- and φ-coordinates, and let the polar angle θ varies from 0 to π, then the trajectory represents the motion within a segment (in the same vein, the rotor can be treated as varying the azimuthal angle, while the radial motion as varying the radial length). If we set $\tan(\theta/2) = r$ and $\omega = s$ in Eq. (4.0.2), then the parameters θ and ω are just the right parameters describing this continuous degree of freedom.

In summary, taking the $d \to \infty$ limit produce four kinds of continuous degrees of freedom:

1. the degree of freedom of the linear motion
2. the degree of freedom of the rotor (described by the 2π-periodic angular position, and the angular momentum which takes all integer values),
3. the degree of freedom of the radial motion (position limited to positive values, and the momentum takes all real values),

4. the degree of freedom of the motion within a segment (position limited to a finite range, but without periodicity, and the momentum takes all real values).

And the corresponding limit $d \to \infty$ of a maximal set of MUB for prime dimensions yields a continuous set of MUB for any continuous degree of freedom except for the rotor. Furthermore, these continuous sets of MUB are related to an underlying Heisenberg pair of complementary observables. This matter is reviewed in section 1.1.7-1.1.11 of Ref. [21].

In fact, all of the standard methods of constructing a maximal set of MUB fail for the rotor. For example, the technique of expressing the MUB as quadratic complex Gaussian wave functions does not generate more than two MUB. Moreover, it is impossible to supplement the two unbiased bases of the Weyl pair of the rotor with a third unbiased basis. The rotor is a very peculiar degree of freedom: It is the only case where the existence of three MUB has remained unclear.

The question of the existence of more than two MUB for the rotor was raised in Ref. [21], and the aim of this chapter is to give an affirmative answer by constructing a satisfactory continuous set of MUB. Indeed, by a rather simple procedure, a first continuous set can be constructed. However, this set is not fully satisfactory since it cannot be related to an underlying Heisenberg pair of complementary observables as it is the case for the three other continuous degrees of freedom. To get around this discrepancy, we construct a Heisenberg pair of complementary observables and use it to obtain a second and more suitable continuous set of MUB. This shows that the rotor degree of freedom really is on equal footing with all the other continuous degrees of freedom. The two sets of MUB are found by mapping — in two different ways — the rotor problem onto the well-studied case of linear motion so that the known method of constructing a continuous set of mutually unbiased bases can then be applied.

Here is a brief outline of this chapter. In Sec. 4.1, we describe the rotor degree of freedom and repeat the argument of Ref. [21] that shows explicitly that the two bases corresponding to the Weyl pair cannot be supplemented with a third unbiased basis. In Sec. 4.2, we provide a first but unsatisfactory continuous set of MUB for the rotor degree of freedom. This motivates us to find a Heisenberg pair of complementary observables for the rotor in Sec. 4.3. In Sec. 4.4, another continuous set of MUB is constructed from this Heisenberg pair, and its wave functions is presented explicitly. Technical details of the approximation of the wave functions for this set of MUB in the φ-basis are presented in the appendix.

4.1 The rotor degree of freedom

A quantum rotor is parameterized by the 2π-periodic angular position and the angular momentum. We denote the hermitian angular-momentum operator by L, its integer eigenvalues by l, and the corresponding eigenkets and eigenbras by $|l\rangle$ and $\langle l|$, such that [1]

$$L|l\rangle = |l\rangle l \quad \text{for } l = 0, \pm 1, \pm 2, \dots \tag{4.1.1}$$

with the orthogonality and completeness relations

$$\langle l|l'\rangle = \delta_{l,l'} \quad \text{and} \quad \sum_{l=-\infty}^{\infty} |l\rangle\langle l| = 1. \tag{4.1.2}$$

[1]Throughout this chapter, operators are denoted by letters in the upper case, while letters in the lower case corresponds to numbers.

We call the angular-momentum eigenbasis the l-basis. Its Fourier transform is the $\varphi-$basis

$$|\varphi\rangle = \sum_{l=-\infty}^{\infty} |l\rangle \mathrm{e}^{-\mathrm{i}l\varphi}. \tag{4.1.3}$$

Since $l \in \mathbb{Z}$, we have $\mathrm{e}^{\mathrm{i}l2\pi} = 1$ and the φ-basis is 2π-periodic. The orthogonality and completeness of the φ-basis follow from Eqs. (4.1.2) and (4.1.3), namely

$$\langle\varphi|\varphi'\rangle = 2\pi\delta^{(2\pi)}(\varphi-\varphi') \quad \text{and} \quad \int\limits_{(2\pi)} \frac{\mathrm{d}\varphi}{2\pi}|\varphi\rangle\langle\varphi| = 1, \tag{4.1.4}$$

where $\delta^{(2\pi)}(\cdot)$ is the 2π-periodic delta function and the integration covers any 2π-interval. By construction, the l-basis and the φ-basis are unbiased: $|\langle\varphi|l\rangle|^2 = 1$ does not depend on the quantum numbers φ and l.

We can now introduce the unitary shift operator E on the l-basis,

$$E|l\rangle = |l+1\rangle. \tag{4.1.5}$$

Since the l-basis and the φ-basis are conjugate, the latter is the eigenbasis of E,

$$\begin{aligned} E|\varphi\rangle &= E\sum_{l=-\infty}^{\infty} |l\rangle \mathrm{e}^{-\mathrm{i}l\varphi} \\ &= |\varphi\rangle \mathrm{e}^{\mathrm{i}\varphi}. \end{aligned} \tag{4.1.6}$$

As the continuous limit of Eq. (2.2.9), we have

$$|\varphi\rangle\langle\varphi| = \frac{1}{2\pi}\sum_{l=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}l\varphi}E^{l}\,. \tag{4.1.7}$$

And similarly the operator $\mathrm{e}^{\mathrm{i}aL}$ is the shift operator for the φ-basis,

$$\langle\varphi|\mathrm{e}^{\mathrm{i}\phi L} = \langle\varphi+\phi|\,. \tag{4.1.8}$$

This follows from the action of the angular-momentum operator L on the eigenbra $\langle\varphi|$

$$\langle\varphi|L = -\mathrm{i}\frac{\partial}{\partial\varphi}\langle\varphi|\,. \tag{4.1.9}$$

The shift operator E and the angular-momentum operator L are therefore algebraically complete [5, 6]; their algebraic properties follow from the commutation relation

$$[L, E] = E\,, \tag{4.1.10}$$

which follows from

$$\begin{aligned}(LE - EL)|l\rangle &= |l+1\rangle(l+1-l) \\ &= E|l\rangle\,. \end{aligned} \tag{4.1.11}$$

We mentioned in the beginning of this chapter that, despite the similarities with the linear motion, there is a fundamental difference: It is impossible to construct a third basis that is unbiased to both the l-basis and the φ-basis. The nonexistence of a third basis can be seen as follows. Assume that there is a ket $|x\rangle$ belonging to such a basis, then the property of being mutually unbiased implies

$$|\langle\varphi|x\rangle|^2 = \lambda \text{ for all } \varphi, \text{ and } |\langle l|x\rangle|^2 = \mu \text{ for all } l. \tag{4.1.12}$$

It then follows from the completeness relation in Eq. (4.1.4) that

$$\langle x|x\rangle = \langle x|\left(\int\limits_{(2\pi)} \frac{\mathrm{d}\varphi}{2\pi}|\varphi\rangle\langle\varphi|\right)|x\rangle = \int\limits_{(2\pi)} \frac{\mathrm{d}\varphi}{2\pi}\lambda = \lambda. \tag{4.1.13}$$

The other completeness relation in Eq. (4.1.2), however, implies

$$\langle x|x\rangle = \langle x|\left(\sum_{l=-\infty}^{\infty}|l\rangle\langle l|\right)|x\rangle = \sum_{l=-\infty}^{\infty}\mu = \infty. \tag{4.1.14}$$

The discrete spectrum of L makes the series diverge and thus leads to a contradiction.

Therefore it remains unclear whether it is possible at all to obtain more than two MUB for the rotor. In addition, we may wonder whether there is a continuous set of MUB as it naturally obtains for all the other continuous degrees of freedom and whether it is related to an underlying Heisenberg pair of complementary observables. Furthermore, if a continuous set of MUB exists, we know that the φ-basis and the l-basis cannot be both included.

We will examine two mappings. The first mapping is a stereographic mapping, which is not fully satisfactory: Geometrically, it provides a continuous set of MUB for the rotor, however, physically, there is no underlying Heisenberg pair (Q, P). The second mapping exploits the one-to-one correspondence between nonnegative integers and integers, or in physical terms, between the Fock basis and the angular momentum basis. This mapping satisfies all the geometrical and physical requirements. Correspondingly, we obtain two continuous sets of MUB for the rotor. It will turn out that the φ-basis is contained in the first set, whereas it is not contained in the second set of Sec. 4.4 below. We note that the second mapping does not have an intuitive physical significance, and the functional form of the wave fucntions of the resulting MUB is extremely complicated.

4.2 A first continuous set of MUB

We consider the first mapping between the line and the rotor. Regarding to the wave functions of the MUB, this mapping is just a change of variable, which allows us to express the first set of MUB for the rotor as 2π-periodic wave functions of the angular position φ. Then, we show that it is impossible to express the Weyl-Heisenberg pair (E, L) for the rotor in terms of the Heisenberg pair (Q, P) arising from this mapping. Therefore there is not a valid underlying Heisenberg pair for this mapping and this set of MUB is not fully satisfactory. Or from a topologically point of view, this simple change of variable which links a circle and a line cannot be one-to-one, therefore one expects some weaknesses in the resulting MUB. And we observe that the lack of an underlying Heisenberg pair is one of them.

4.2.1 The wave functions of the MUB

The continuous degree of freedom of linear motion admits a continuous set of MUB. Geometrically, these MUB correspond to rotations of the position basis by an angle θ, which therefore labels the bases. Their wave functions take the simple form of a quadratic complex Gaussian function

$$\Phi_y^{(\theta)}(q) = \frac{1}{\sqrt{\pi(1-\mathrm{e}^{2\mathrm{i}\theta})}} \exp\left(\mathrm{i}\frac{qy}{\sin\theta} - \frac{\mathrm{i}}{2}\frac{q^2+y^2}{\tan\theta}\right), \tag{4.2.1}$$

where $0 \leq \theta < \pi$ and the real parameter y labels the basis element [2]. One may check that the $\theta \to 0$ limit of the right hand side of Eq. (4.2.1) is indeed $\delta(q-y)$.

First of all, for a given θ, two wave functions $\Phi_y^{(\theta)}(q)$ and $\Phi_{y'}^{(\theta)}(q)$ are orthogonal,

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}q\, \Phi_y^{(\theta)}(q)^* \Phi_{y'}^{(\theta)}(q) &= \frac{\exp\left(\mathrm{i}\frac{y^2-y'^2}{2\tan\theta}\right)}{2\pi\sin\theta} \int_{-\infty}^{\infty} \mathrm{d}q\, \mathrm{e}^{-\mathrm{i}q(y-y')/\sin\theta} \\ &= \delta(y-y'), \end{aligned} \tag{4.2.2}$$

and we also have the completeness relation

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}y\, \Phi_y^{(\theta)}(q)^* \Phi_y^{(\theta)}(q') &= \frac{\exp\left(\mathrm{i}\frac{q^2-q'^2}{2\tan\theta}\right)}{2\pi\sin\theta} \int_{-\infty}^{\infty} \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}y(q-q')/\sin\theta} \\ &= \delta(q-q'). \end{aligned} \tag{4.2.3}$$

[2] Up to a q-independent phase factor, these wave functions are the ones used by Wootters [28].

Indeed, for a given θ, the wave functions $\Phi_y^{(\theta)}(q)$ form a basis. Second, calculation of the modulus of the inner product between any wave function in the θ_1 basis and any wave function in the θ_2 basis shows that

$$\left|\int_{-\infty}^{\infty} \mathrm{d}q\, \Phi_{y_1}^{(\theta_1)}(q)^* \Phi_{y_2}^{(\theta_2)}(q)\right|^2 = \int_{-\infty}^{\infty} \mathrm{d}q\, \Phi_{y_1}^{(\theta_1)}(q)^* \Phi_{y_2}^{(\theta_2)}(q) \int_{-\infty}^{\infty} \mathrm{d}q'\, \Phi_{y_1}^{(\theta_1)}(q') \Phi_{y_2}^{(\theta_2)}(q')^*$$
$$= \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \mathrm{d}\alpha\, \mathrm{d}\beta \exp\Big(\mathrm{i}(y_1 \sin\theta_2 - y_2 \sin\theta_1)\alpha\Big) \exp\Big(\mathrm{i}\sin(\theta_1 - \theta_2)\alpha\beta\Big)\,,$$

where we did the change of variables

$$\alpha = \frac{q' - q}{\sin\theta_1 \sin\theta_2}, \quad \beta = \frac{q' + q}{2}\,. \tag{4.2.4}$$

The β-integral gives the delta function, therefore we have

$$\left|\int_{-\infty}^{\infty} \mathrm{d}q\, \Phi_{y_1}^{(\theta_1)}(q)^* \Phi_{y_2}^{(\theta_2)}(q)\right|^2 = \frac{1}{2\pi\,|\sin(\theta_1 - \theta_2)|}, \tag{4.2.5}$$

which implies that any two bases θ_1 and θ_2, with $\theta_1 \neq \theta_2$, are unbiased: The modulus of the inner product between any wave function in the θ_1 basis and any wave function in the θ_2 basis is independent of the two basis elements y_1 and y_2.

Now, a simple change of variable readily provides a continuous set of MUB for the rotor as specified by their wave functions in φ. For, the substitution $q = \tan(\varphi/2)$ allows us to write

$$\int_{-\infty}^{\infty} \mathrm{d}q\, \Phi_{y_1}^{(\theta_1)}(q)^*\, \Phi_{y_2}^{(\theta_2)}(q) = \int_{(2\pi)} \frac{\mathrm{d}\varphi}{2\pi}\, \Gamma_{y_1}^{(\theta_1)}(\varphi)^*\, \Gamma_{y_2}^{(\theta_2)}(\varphi) \tag{4.2.6}$$

upon defining the 2π-periodic wave functions

$$\begin{aligned} \Gamma_y^{(\theta)}(\varphi) &= \sqrt{2\pi \frac{\mathrm{d}q}{\mathrm{d}\varphi}}\, \Phi_y^{(\theta)}\big(\tan(\varphi/2)\big) \\ &= \sqrt{\frac{2\pi}{1 + \cos\varphi}}\, \Phi_y^{(\theta)}\big(\tan(\varphi/2)\big). \end{aligned} \tag{4.2.7}$$

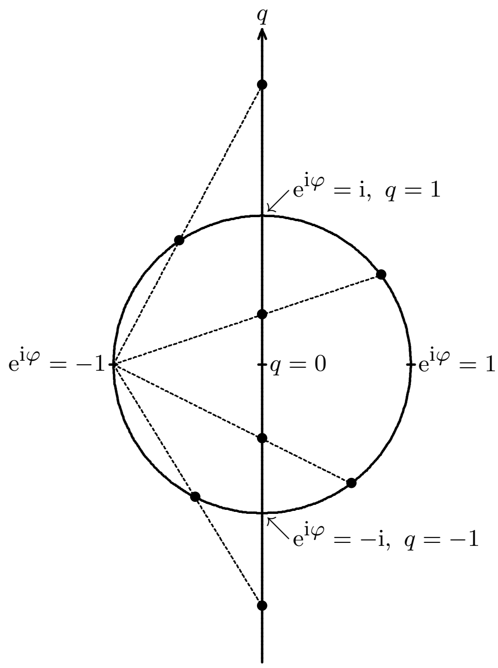

Figure 4.1: Graphical representation of the change of variable $q = \tan(\varphi/2)$. This substitution is an example of stereographic projection: The unit circle is projected from the point $e^{i\varphi} = -1$ onto the real line which intersects the circle at the two points $e^{i\varphi} = \pm i$. The origin $q = 0$ of the real line corresponds to the point $e^{i\varphi} = 1$ on the circle. The dots • represent points on the circle and their stereographic projection onto the real line. The dashed lines illustrate the imaginary line joining the origin of the projection, the point on the circle to be projected and its projection onto the real line.

By construction, we conserve the important properties of orthogonality and completeness as expressed in Eq. (4.1.4) for being orthonormal bases, and also the unbiasedness. It follows that the wave functions $\Gamma_y^{(\theta)}(\varphi)$ form a continuous set of MUB for the rotor degree of freedom.

We note for completeness that the basis for $\theta = 0$ is essentially the φ-basis of Eqs. (4.1.3) and (4.1.4), inasmuch as

$$\int_{(2\pi)} \frac{d\varphi}{2\pi} |\varphi\rangle \Gamma_y^{(0)}(\varphi) = \frac{|\varphi = 2\arctan(y)\rangle}{\sqrt{\pi(1+y^2)}}. \tag{4.2.8}$$

Furthermore, when $\theta \neq 0$, the wave functions $\Gamma_y^{(\theta)}(\varphi)$ of Eq. (4.2.7) have a pole at $\varphi = \pi$ and rapidly oscillate in the vicinity of that pole. The wave functions of the second continuous set of MUB of Sec. 4.4 below have similar singularities where, however, the angular position of the pole will depend on the basis θ.

4.2.2 The lack of an underlying Heisenberg pair

Consistent with the change of variable $q = \tan(\varphi/2)$, as illustrated in Fig. 4.1, we would like to express the Weyl–Heisenberg pair (E, L) of the circular motion and the Heisenberg pair (Q, P) of the linear motion in terms of each others. As noted in Ref. [21], such a relation with the linear motion exists for the two other continuous degrees of freedom of radial motion and motion within a segment.

First, let us find the expressions of the two hermitian operators Q and P in terms of E and L. According to Eq. (4.2.7), we express the 2π-periodic eigenbras $\langle\varphi|$ of E in terms of the eigenbras $\langle q|$ of Q as

$$\langle q = \tan(\varphi/2)| = \sqrt{\frac{1+\cos\varphi}{2\pi}}\langle\varphi|. \tag{4.2.9}$$

The position operator Q is given by $\langle q|Q = q\langle q|$, or after changing the variable, $\langle\varphi|Q = \tan(\varphi/2)\langle\varphi|$, or equivalently

$$\langle\varphi|Q = \mathrm{i}\frac{1-\mathrm{e}^{\mathrm{i}\varphi}}{1+\mathrm{e}^{\mathrm{i}\varphi}}\langle\varphi|\,. \tag{4.2.10}$$

Note that the operator Q is non-degenerate and the φ-basis is complete, therefore we can establish that

$$Q = \mathrm{i}\frac{1-E}{1+E}\,, \tag{4.2.11}$$

and reciprocally

$$E = \frac{1+\mathrm{i}Q}{1-\mathrm{i}Q}\,. \tag{4.2.12}$$

Next we want to find its conjugate operator P. To do so, we consider the unitary shift operator $\mathrm{e}^{\mathrm{i}aP}$ with real a, such that

$$\langle q|\mathrm{e}^{\mathrm{i}aP} = \langle q+a|. \tag{4.2.13}$$

To obtain its expression in terms of E and L, we look at its action on a bra $\langle\varphi|$. It reads

$$\begin{aligned}\langle\varphi|\mathrm{e}^{\mathrm{i}aP} &= \sqrt{\frac{\mathrm{d}\varphi'}{\mathrm{d}\varphi}}\langle\varphi'| \\ &= \sqrt{\frac{1+\cos\varphi'}{1+\cos\varphi}}\langle\varphi|\mathrm{e}^{\mathrm{i}(\varphi'-\varphi)L}\,,\end{aligned} \tag{4.2.14}$$

where $\varphi' = 2\arctan(\tan(\varphi/2)+a)$, or equivalently $\tan(\varphi'/2) = \tan(\varphi/2)+a$. From Eqs. (4.2.11) and (4.2.12), it is not difficult to arrive at

$$\langle\varphi|\mathrm{e}^{\mathrm{i}aP} = \frac{1}{|1-\mathrm{i}\frac{a}{2}(1+\mathrm{e}^{\mathrm{i}\varphi})|}\langle\varphi|\left(\frac{1+\mathrm{i}\frac{a}{2}(1+\mathrm{e}^{-\mathrm{i}\varphi})}{1-\mathrm{i}\frac{a}{2}(1+\mathrm{e}^{\mathrm{i}\varphi})}\right)^{L} \tag{4.2.15}$$

Therefore the resulting $E;L$-ordered form of the shift operator is

$$\mathrm{e}^{\mathrm{i}aP} = \frac{1}{|1-\mathrm{i}\frac{a}{2}(1+E)|}\left(\frac{1+\mathrm{i}\frac{a}{2}(1+E^\dagger)}{1-\mathrm{i}\frac{a}{2}(1+E)}\right)^{L}. \tag{4.2.16}$$

Now considering the $a\to 0$ limit of $\mathrm{e}^{\mathrm{i}aP}$, we have

$$\begin{aligned}1+\mathrm{i}aP &= 1+\mathrm{i}a\Big(\frac{1}{2}(1+E^\dagger)(L-\frac{1}{2})+\frac{1}{2}(1+E)(L+\frac{1}{2})\Big) \\ &= 1+\mathrm{i}a\Big(L+\frac{1}{2}(E^\dagger+E)L+\frac{1}{4}(E-E^\dagger)\Big) \\ &= 1+\mathrm{i}a\frac{1}{2}|1+E|\,L\,|1+E|\,,\end{aligned} \tag{4.2.17}$$

which implies that

$$P = \frac{1}{2}|1+E|\,L\,|1+E|, \tag{4.2.18}$$

where $|A| = \sqrt{A^\dagger A}$ for any operator A.

As required, P is hermitian and we verify that the commutation relation between Q and P, that is,

$$\begin{aligned}[Q,P] &= \Big[\mathrm{i}\frac{1-E}{1+E}, \frac{1}{2}|1+E|\,L\,|1+E|\Big] \\ &= \frac{1}{2}|1+E|\,\Big[\mathrm{i}\frac{1-E}{1+E}, L\Big]\,|1+E|\,. \end{aligned} \tag{4.2.19}$$

Note that

$$\begin{aligned}\langle\varphi|\Big[\mathrm{i}\frac{1-E}{1+E}, L\Big] &= \mathrm{i}\Big(\frac{\partial}{\partial\varphi}\tan(\varphi/2)\Big)\langle\varphi| \\ &= 2\mathrm{i}\langle\varphi|\frac{1}{|1+E|^2}\,, \end{aligned} \tag{4.2.20}$$

therefore we have indeed $[Q,P]=\mathrm{i}$.

It remains to look at the spectral properties of P to conclude that we have constructed a well-defined Heisenberg pair of complementary observables (Q,P). This can be done by considering

$$\begin{aligned}\langle\varphi|P|p\rangle &= \mathrm{i}\Big(\frac{1}{2}\sin\varphi-(1+\cos\varphi)\frac{\partial}{\partial\varphi}\Big)\langle\varphi|p\rangle \\ &= \langle\varphi|p\rangle p\,. \end{aligned} \tag{4.2.21}$$

Therefore the eigenfunctions of P have the form

$$\sqrt{1+\cos\varphi}\langle\varphi|p\rangle = c\,\mathrm{e}^{\mathrm{i}p\tan(\varphi/2)}, \tag{4.2.22}$$

where c is a normalization constant. The choice $c=1$ together with the definition (4.2.9) imply the expected Fourier coefficient

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}pq}. \tag{4.2.23}$$

Therefore the two operators Q and P, expressed in terms of the Weyl–Heisenberg pair (E,L), represent a valid Heisenberg pair of complementary observables: They have the right Heisenberg commutation relation as well as the right properties.

Let us now focus on the two operators E and L in terms of Q and P. We already know E as in Eq. (4.2.12), and inverting Eq. (4.2.18) gives

$$L = \frac{1}{2}\sqrt{1+Q^2}P\sqrt{1+Q^2}. \tag{4.2.24}$$

These two operators yield the commutation relation $[L, E] = E$, since

$$\begin{aligned}\langle q|\Big[P, \frac{1+\mathrm{i}Q}{1-\mathrm{i}Q}\Big] &= -\mathrm{i}\Big(\frac{\partial}{\partial q}\frac{1+\mathrm{i}q}{1-\mathrm{i}q}\Big)\langle q| \\ &= 2\frac{1}{1+q^2}\langle q|E\,. \end{aligned} \tag{4.2.25}$$

As earlier, we must check that these two operators have the required spectrum. By construction, the eigenvalues of E are phases and, upon inverting Eq. (4.2.9), its 2π-periodic eigenbras are [cf. Eq. (4.2.8)]

$$\langle\varphi = 2\arctan q| = \sqrt{\pi(1+q^2)}\langle q|. \tag{4.2.26}$$

Let us now investigate the spectral properties of the seemingly unproblematic hermitian operator L that is defined by the (Q, P) function in Eq. (4.2.24). Again, considering the differential equation provided by

$$\begin{aligned}\langle q|L|\lambda\rangle &= \frac{1}{2\mathrm{i}}\Big(q + (1+q^2)\frac{\partial}{\partial q}\Big)\langle q|\lambda\rangle \\ &= \langle q|\lambda\rangle\lambda\,. \end{aligned} \tag{4.2.27}$$

We find its eigenfunctions are

$$\langle q|\lambda\rangle = \frac{c'}{\sqrt{1+q^2}}\Big(\frac{1+\mathrm{i}q}{1-\mathrm{i}q}\Big)^{\lambda}, \tag{4.2.28}$$

where the eigenvalue λ is *any* real number, not restricted to integers, and c' is a normalization constant. The fact that all real numbers can be eigenvalues of the hermitian operator L is also evident as soon as one realizes that the unitary transformation

$$Q \to Q, \quad P \to P + 2x/(1+Q^2)\,, \tag{4.2.29}$$

transforms the pair (E, L),

$$E \to E, \quad L \to L + x\,, \tag{4.2.30}$$

where x can be any real number. It follows that the L operator of Eq. (4.2.24) is not the L operator of Sec. 4.1, the generator of the unitary cyclic shift $\langle\varphi| \to \langle\varphi + \alpha|$.

The choice $c' = 1/\sqrt{\pi}$ together with the definition (4.2.26) imply the inner product

$$\langle\varphi|\lambda\rangle = \left(\mathrm{e}^{\mathrm{i}\varphi}\right)^{\lambda} = \mathrm{e}^{\mathrm{i}\lambda\left(\varphi - 2\pi\lfloor\frac{\varphi}{2\pi}\rceil\right)}, \tag{4.2.31}$$

where $\lfloor x\rceil$ denotes the integer that is nearest to x. Furthermore, the eigenvectors of the L of Eq. (4.2.24) are not all orthogonal. Indeed we have

$$\begin{aligned}
\langle\lambda|\lambda'\rangle &= \int\limits_{-\infty}^{\infty} \mathrm{d}q\, \frac{1}{\pi}\frac{1}{1+q^2}\Bigl(\frac{1+\mathrm{i}q}{1-\mathrm{i}q}\Bigr)^{\lambda'-\lambda} \\
&= \frac{\mathrm{i}}{2\pi}\frac{1}{\lambda'-\lambda}\Bigl(\frac{1+\mathrm{i}q}{1-\mathrm{i}q}\Bigr)^{\lambda'-\lambda}\Bigg|_{q=-\infty}^{\infty} \\
&= \mathrm{sinc}\bigl(\pi(\lambda-\lambda')\bigr),
\end{aligned} \tag{4.2.32}$$

so that only the eigenvectors whose eigenvalues differ by an integer are orthogonal. Consequently, the λ-basis is overcomplete: There are many completeness relations, such as

$$\sum_{l=-\infty}^{\infty} |l+\lambda_0\rangle\langle l+\lambda_0| = 1, \tag{4.2.33}$$

with $0 \le \lambda_0 < 1$, say. Mathematically speaking, the operator L of Eq. (4.2.24) is hermitian but not self-adjoint.

We may wonder whether the above issues remain if we start from the unitary shift operator $\mathrm{e}^{\mathrm{i}\alpha L}$ instead of inverting Eq. (4.2.18). We proceed from the expression of the 2π-periodic eigenbras $\langle\varphi|$ in terms of the eigenbras $\langle q|$ in Eq. (4.2.26). The unitary shift $\mathrm{e}^{\mathrm{i}\alpha L}$ acts on $\langle\varphi|$ as

$$\langle\varphi|\mathrm{e}^{\mathrm{i}\alpha L} = \langle\varphi+\alpha|. \tag{4.2.34}$$

On a bra $\langle q|$, it then reads

$$\langle q|\mathrm{e}^{\mathrm{i}\alpha L} = \sqrt{\frac{\mathrm{d}q'}{\mathrm{d}q}}\langle q'|, \tag{4.2.35}$$

where

$$q' = \frac{q\cos(\alpha/2)+\sin(\alpha/2)}{\cos(\alpha/2)-q\sin(\alpha/2)}. \tag{4.2.36}$$

From Eqs. (4.2.35) and (4.2.36), we derive the $Q;P$-ordered form of the shift operator $\mathrm{e}^{\mathrm{i}\alpha L}$, which is

$$\begin{aligned}\mathrm{e}^{\mathrm{i}\alpha L} = &\frac{1}{|\cos(\alpha/2)-Q\sin(\alpha/2)|} \\ &\times\exp\left(\mathrm{i}\frac{(1+Q^2)\sin(\alpha/2)}{\cos(\alpha/2)-Q\sin(\alpha/2)}P\right).\end{aligned} \tag{4.2.37}$$

It does not admit a uniform $\alpha\to 0$ limit and, therefore, it does not have a self-adjoint generator.

The origin of the problem is the conflict between the 2π-periodicity of the rotor degree of freedom and the substitution $q=\tan(\varphi/2)$. In particular, the limits $q\to\infty$ and $q\to-\infty$ both correspond to $\mathrm{e}^{\mathrm{i}\varphi}\to -1$ although the ranges $q\gg 1$ and $-q\gg 1$ are not adjacent on the q line. Or topologically, the line is simply connected while the circle is not. Therefore the stereographic projection cannot be fully satisfactory. This eventually leads to an ill-defined Weyl–Heisenberg pair (E,L) expressed in terms of the Heisenberg pair (Q,P), while the inverse relation does not present any issue.

Although we obtained the present set (4.2.7) of MUB in a rather straightforward manner, we seek for another continuous set of MUB which would not suffer from the lack of an underlying Heisenberg pair of complementary observables. The primary reason is the following: Not only do we want to find a continuous set of MUB for the rotor but we also want to settle the question whether the rotor degree of freedom is on equal footing with the three other continuous degrees of freedom. To do so, we must find an alternative set of MUB which arises from a bona fide Heisenberg pair of complementary observables. This goal will be achieved by starting the construction from the angular momentum instead of the angular position.

4.3 A Heisenberg pair for the rotor

The construction of continuous MUB for the other continuous degrees of freedom, given in Ref. [21], relies on the respective Heisenberg pairs of complementary hermitian observables, the analogs of position and momentum for motion along a line. The procedure could be applied to the rotor degree of freedom as well if we had a Heisenberg pair for it, but that has been lacking, and the construction of Sec. 4.2 does not provide it.

Owing to the discreteness of l and the periodicity of φ, there is no Heisenberg pair (Q, P) for the rotor such that, say, L is an invertible function of Q and E is an invertible function of P. We need to construct the Heisenberg pair in a different way. One strategy is as follows.

For position operator Q and momentum operator P, we have the familiar Fock basis of kets $|n\rangle$ with $n = 0, 1, 2, \ldots$, the eigenkets of the number operator $N = \frac{1}{2}(Q^2 + P^2 - 1)$,

$$N|n\rangle = |n\rangle n. \tag{4.3.1}$$

We identify the Fock basis with the l basis in accordance with

$$|n\rangle = |l\rangle \quad \text{if} \quad 2n + 1 = |4l + 1|, \tag{4.3.2}$$

or more explicitly,

$$n = \begin{cases} 2l & \text{if } l \geq 0, \\ -2l-1 & \text{if } l < 0\,, \end{cases} \quad \text{and } l = \begin{cases} n/2 & \text{for even n}, \\ -(n+1)/2 & \text{for odd } n\,. \end{cases}$$

This mapping is illustrated in Fig. 4.2. Considering the operators L and N, from Eq. (4.3.2), we have the following relation between them

$$L = \frac{2N+1}{4}(-1)^N - \frac{1}{4}, \tag{4.3.3}$$

$$N = \frac{1}{2}\big|4L+1\big| - \frac{1}{2}. \tag{4.3.4}$$

The unitary shift operator

$$\begin{aligned} E &= \sum_{l=-\infty}^{\infty} |l+1\rangle\langle l| \\ &= \sum_{n \text{ even}} |n+2\rangle\langle n| + \sum_{n \text{ odd}} |n\rangle\langle n+2| \\ &\quad + |n=0\rangle\langle n=1| \end{aligned} \tag{4.3.5}$$

can then be expressed with the aid of the isometric ladder operator for the Fock states,

$$A = \frac{1}{\sqrt{2N+2}}(Q + \mathrm{i}P) = \sum_{n=0}^{\infty} |n\rangle\langle n+1|, \tag{4.3.6}$$

and its adjoint, for which $AA^\dagger = 1$. We have

$$E = A^{\dagger 2}\frac{1+(-1)^N}{2} + \frac{1-(-1)^N}{2}A^2 + A - A^\dagger A^2. \tag{4.3.7}$$

This expression (4.3.7) can be verified by considering the action of E on $\langle n|$. In summary, in Eqs. (4.3.3) and (4.3.7) we have the basic rotor observables E and L expressed in terms of N, A, and $A^\dagger$ which are functions of the Heisenberg pair (Q, P).

From Eqs. (4.3.2) and (4.3.6), we have

$$\frac{1}{\sqrt{|4L+1|+1}}\big(Q + \mathrm{i}P\big) = \sum_{l=0}^{\infty} |l\rangle\langle -l-1| + \sum_{l=-\infty}^{-1} |l\rangle\langle -l|\,, \tag{4.3.8}$$

which helps us to find the reciprocal relations that operator Q and P as functions of E and L. The above Eq. (4.3.8) is expressed in terms of projectors, notice that we can express the projector $|l\rangle\langle l|$ in terms of L as

$$|l\rangle\langle l| = \int_{(2\pi)} \frac{\mathrm{d}\alpha}{2\pi}\, \mathrm{e}^{\mathrm{i}(L-l)\alpha}\,. \tag{4.3.9}$$

Then introduce the following projectors

$$\Pi_+ = \sum_{l=0}^{\infty} |l\rangle\langle l|, \qquad \Pi_- = \sum_{l=-\infty}^{-1} |l\rangle\langle l|, \tag{4.3.10}$$

and the hermitian and unitary reflection operator

$$R = \sum_{l=-\infty}^{\infty} |l\rangle\langle -l| = \sum_{l=-\infty}^{\infty} |l\rangle\langle l| E^{2l} = \sum_{l=-\infty}^{\infty} E^{-2l}|l\rangle\langle l|, \tag{4.3.11}$$

such that for any operator function $f(E, L)$,

$$Rf(E,L)R^{\dagger} = f(RER^{\dagger}, RLR^{\dagger}) = f(E^{\dagger}, -L)\,. \tag{4.3.12}$$

It is then easy to establish

$$\begin{aligned} \Pi_+ RE &= \sum_{l=0}^{\infty} |l\rangle\langle l| \sum_{l'=-\infty}^{\infty} |l'\rangle\langle -l'|E \\ &= \sum_{l=0}^{\infty} |l\rangle\langle -l-1|, \end{aligned} \tag{4.3.13}$$

and similarly

$$\begin{aligned} \Pi_- R &= \sum_{l=-\infty}^{-1} |l\rangle\langle l| \sum_{l'=-\infty}^{\infty} |l'\rangle\langle -l'| \\ &= \sum_{l=-\infty}^{-1} |l\rangle\langle -l|. \end{aligned} \tag{4.3.14}$$

Compare with Eq. (4.3.8), we have the following result

$$Q + \mathrm{i}P = \sqrt{4L+2}\,\Pi_+ RE + \sqrt{-4L}\,\Pi_- R, \tag{4.3.15}$$

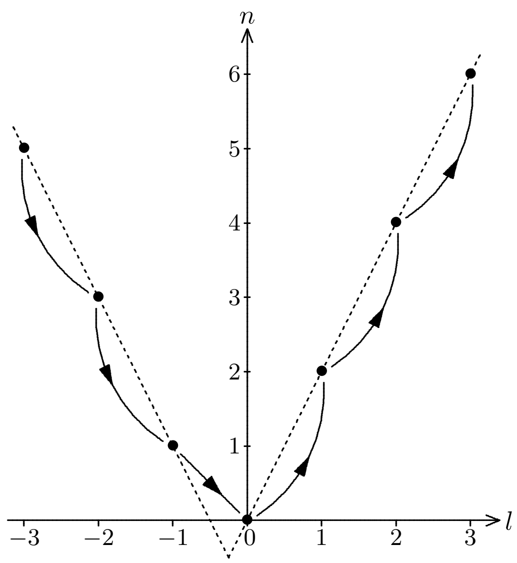

Figure 4.2: Graphical representation of Eqs. (4.3.2)–(4.3.5). The dashed line shows the relation of Eq. (4.3.2) between the quantum numbers l and n, with the dots $\bullet$ indicating the integer pairs (l, n) of physical significance. Negative l values are mapped one-to-one onto odd n values, whereas nonnegative l values are mapped onto even n values. The arrowed lines that connect them symbolize the mapping $|l\rangle \to |l+1\rangle$ associated with the unitary shift operator E of Eq. (4.3.5).

It is a matter of inspection to verify that $[Q, P] = \mathrm{i}$ for the hermitian (Q, P) pair defined by Eq. (4.3.15).

The fundamental difference between the construction here and that in Sec. 4.2 should be obvious: In Sec. 4.2, we are employing the one-to-one mapping of Fig. 4.1 between the circle with one point removed and the real line, whereas we are now relying on the one-to-one mapping of Fig. 4.2 between integers and natural numbers, which has nothing to do with the mapping of a circle to a line. The shortcoming of this mapping is that it lacks a physical significance, we are not aware of another rotor problem in which these operators would appear naturally and thus reveal their physical significance.

4.4 A second continuous set of MUB

With the Heisenberg pair of Eq. (4.3.15) at hand, we follow the usual procedure and note that any two linear combinations $\alpha Q + \beta P$ and $\alpha' Q + \beta' P$ are a pair of complementary observables if $\alpha\beta' \neq \alpha'\beta$ holds for the real coefficients; see, for instance, Sec. 1.1.8 in Ref. [21]. We restrict ourselves to the one-parameter set with $\alpha = \cos\theta$ and $\beta = \sin\theta$ for $0 \leq \theta < \pi$,

$$Y_\theta \equiv Q\cos\theta + P\sin\theta = \mathrm{e}^{\mathrm{i}\theta N} Q\,\mathrm{e}^{-\mathrm{i}\theta N}. \tag{4.4.1}$$

The eigenkets $|\theta; y\rangle$ of Y_θ are then given in terms of the eigenkets $|q\rangle$ of Q,

$$Y_\theta|\theta; y\rangle = |\theta; y\rangle y \quad \text{for} \quad |\theta; y\rangle = \mathrm{e}^{\mathrm{i}\theta N}|q = y\rangle, \tag{4.4.2}$$

since

$$Y_\theta \mathrm{e}^{\mathrm{i}\theta N}|q\rangle = \mathrm{e}^{\mathrm{i}\theta N}|q\rangle q\,. \tag{4.4.3}$$

For each θ, the $|\theta; y\rangle$s make up a continuous basis of kets. In fact, for the wave function defined in Eq. (4.2.1), we have $\Phi_y^{(\theta)}(q) = \langle q|\theta; y\rangle$, since the wave function $\Phi_y^{(\theta)}(q)$ just solves the differential equation determined by

$$\begin{aligned}\langle q|Y_\theta|\theta; y\rangle &= \Big(q\cos\theta - i\sin\theta\frac{\partial}{\partial q}\Big)\langle q|\theta; y\rangle \\ &= \langle q|\theta; y\rangle y\,,\end{aligned} \tag{4.4.4}$$

and the boundary condition for $\theta = 0$, while of course the geometrical meaning of the q-basis here is quite different from that of the q-basis in Sec. 4.2. As established already in Sec. 4.2, the bases for different θ values are unbiased: For $\theta_1 \neq \theta_2$, the transition probability density

$$\big|\langle\theta_1; y_1|\theta_2; y_2\rangle\big|^2 = \frac{1}{2\pi\,|\sin(\theta_1 - \theta_2)|} \tag{4.4.5}$$

does not depend on the quantum numbers y_1 and y_2.

The well-known position wave functions for the Fock states,

$$\langle q|n\rangle = \pi^{-\frac{1}{4}}\left(2^n n!\right)^{-\frac{1}{2}} \mathrm{e}^{-\frac{1}{2}q^2} H_n(q) \equiv f_n(q), \tag{4.4.6}$$

where $H_n(q)$ denotes the nth Hermite polynomial, translate into the wave function of $|\theta; y\rangle$ in the l-basis. When l is nonnegative, we have $2l = n$, therefore

$$\begin{aligned}\langle 2l = n|\theta; y\rangle &= \langle 2l = n|\mathrm{e}^{\mathrm{i}N\theta}|y\rangle \\ &= \mathrm{e}^{\mathrm{i}2l\theta} f_{2l}(q).\end{aligned} \tag{4.4.7}$$

When l is negative, we have $-2l - 1 = n$, therefore

$$\begin{aligned}\langle -2l - 1 = n|\theta; y\rangle &= \langle -2l - 1 = n|\mathrm{e}^{\mathrm{i}N\theta}|y\rangle \\ &= \mathrm{e}^{-\mathrm{i}(2l+1)\theta} f_{-2l-1}(y).\end{aligned} \tag{4.4.8}$$

Or more compactly, we can write

$$\langle l|\theta; y\rangle = \mathrm{e}^{\mathrm{i}n\theta} f_n(y)\Big|_{n\,=\,\frac{1}{2}|4l+1|\,-\,\frac{1}{2}}. \tag{4.4.9}$$

The periodic wave function in the φ-basis is then available in terms of the Fourier sum

$$\begin{aligned}\psi_y^{(\theta)}(\varphi) \equiv \langle\varphi|\theta; y\rangle &= \sum_{l=0}^{\infty}\langle\varphi|l\rangle\langle l|\theta; y\rangle \\ &= \sum_{l=0}^{\infty}\Big[\mathrm{e}^{\mathrm{i}l(\varphi+2\theta)} f_{2l}(y) + \mathrm{e}^{-\mathrm{i}\theta}\mathrm{e}^{-\mathrm{i}(l+1)(\varphi-2\theta)} f_{2l+1}(y)\Big]\end{aligned} \tag{4.4.10}$$

that is implied by Eqs. (4.1.2) and (4.1.3). From the above Eq. (4.4.10), and after noting that the Hermite polynomial is even for even index and odd for odd index, we can establish the identity

$$\begin{aligned}\psi_y^{(\theta)}(\varphi) = \frac{1}{2}\bigg(&\psi_y^{(0)}(\varphi + 2\theta) + \psi_{-y}^{(0)}(\varphi + 2\theta) \\ &+ \mathrm{e}^{-\mathrm{i}\theta}\Big[\psi_y^{(0)}(\varphi - 2\theta) - \psi_{-y}^{(0)}(\varphi - 2\theta)\Big]\bigg),\end{aligned} \tag{4.4.11}$$

which expresses the wave functions of the θ-basis in terms of those for $\theta = 0$. Therefore one needs to evaluate the series in Eq. (4.4.10) only for $\theta = 0$.

Figs. 4.3(a) and 4.4(a) show $\psi_y^{(0)}(\varphi)$ for $y = 0$ and $y = 1/2$. These wave functions are singular at $\varphi = \pi$: $\psi_0^{(0)}(\varphi)$ has a pole there, whereas $\psi_{\frac{1}{2}}^{(0)}(\varphi)$ is finite but oscillates arbitrarily rapidly in the vicinity of $\varphi = \pi$, which is a common feature of all wave functions $\psi_y^{(0)}(\varphi)$ with $y \neq 0$. The pole and the rapidly oscillating factors are exhibited in the even-in-y and odd-in-y parts of $\psi_y^{(0)}(\varphi)$,

$$\begin{aligned}\frac{1}{2}\Big[\psi_y^{(0)}(\varphi) + \psi_{-y}^{(0)}(\varphi)\Big] &= \sum_{l=0}^{\infty} \mathrm{e}^{\mathrm{i}l\varphi} f_{2l}(y) \\ &= \frac{\mathrm{e}^{\frac{\mathrm{i}}{2}y^2 \tan\frac{\varphi}{2}}}{\sqrt{1+\cos\varphi}}\chi_y^{(+)}(\varphi)\end{aligned} \tag{4.4.12}$$

and

$$\begin{aligned}\frac{1}{2}\Big[\psi_y^{(0)}(\varphi) - \psi_{-y}^{(0)}(\varphi)\Big] &= \sum_{l=0}^{\infty} \mathrm{e}^{-\mathrm{i}(l+1)\varphi} f_{2l+1}(y) \\ &= \frac{\mathrm{e}^{-\frac{\mathrm{i}}{2}y^2 \tan\frac{\varphi}{2}}}{\sqrt{1+\cos\varphi}}\chi_y^{(-)}(\varphi)\,,\end{aligned} \tag{4.4.13}$$

where the factors $\chi_y^{(\pm)}(\varphi)$ are smooth functions of φ with remaining low-amplitude oscillations around $\varphi = \pi$ but no poles at $\varphi = \pi$. For $y = 0$, we have $\chi_0^{(-)}(\varphi) = 0$. Figure 4.3(b) is a plot of $\chi_0^{(+)}(\varphi)$ while Figures 4.4(b) and (c) are plots of $\chi_{\frac{1}{2}}^{(\pm)}(\varphi)$. Details of the calculation of $\psi_y^{(0)}(\varphi)$ are shown in the appendix.

4.5 Summary

We provided two continuous sets of MUB for the rotor degree of freedom. We thus answered the question of whether there are more than two MUB for the rotor degree of freedom by providing explicit continuous sets. These

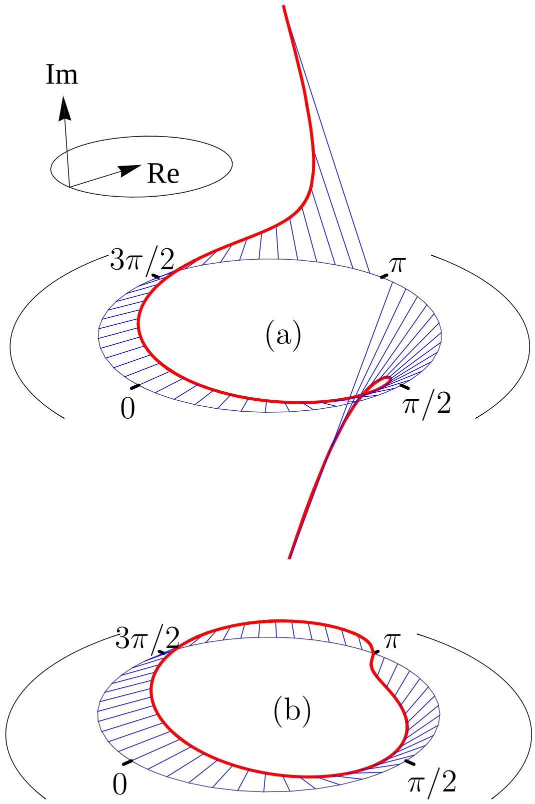

Figure 4.3: (color online) The wave functions $\psi_y^{(0)}(\varphi)$ for $y = 0$. One 2π-period of φ is represented by a circle. At each point on the circle, we have a complex plane perpendicular to the plane of the circle, with the real axis toward the center of the φ circle. In these complex planes we mark the values of the wave functions by thin blue lines, whose end points make up the thick red lines. The unit distance in the complex planes is indicated by the outside arcs for $\pi/2 < \varphi < \pi$ and $3\pi/2 < \varphi < 2\pi$, which mark points with $\psi = -1$. Plot (a) shows $\psi_0^{(0)}(\varphi)$ which has a simple pole at $\varphi = \pi$. After removing the pole $1/\sqrt{1 + \cos\varphi}$, plot (b) shows the smooth function $\chi_0^{(+)}(\varphi)$ of Eq. (4.4.12).

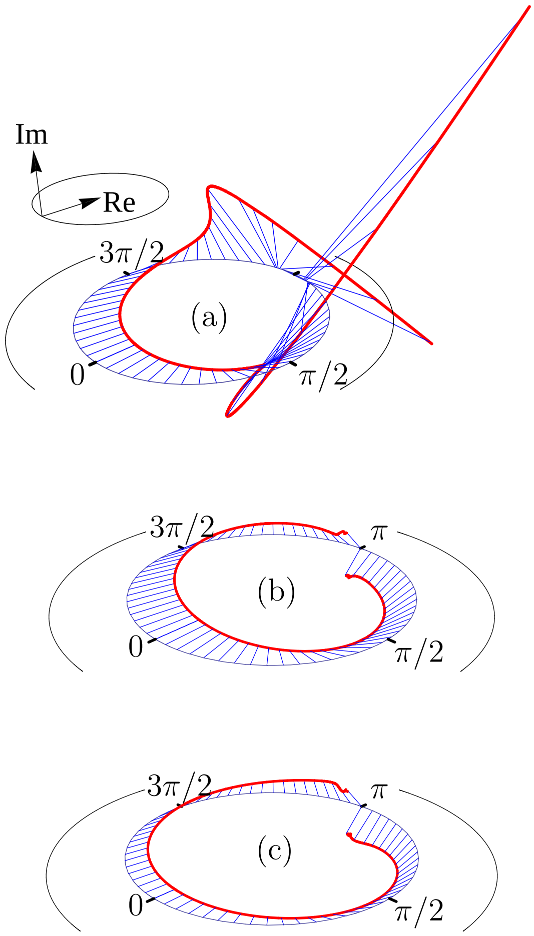

Figure 4.4: (color online) Plot (a) shows the wave function $\psi_{\frac{1}{2}}^{(0)}(\varphi)$. The vicinity of $\varphi = \pi$ is excluded because this wave function is oscillating very rapidly there. After removing the pole $1/\sqrt{1+\cos\varphi}$ and the rapidly oscillating factors $\mathrm{e}^{\pm\frac{\mathrm{i}}{8}\tan\frac{\varphi}{2}}$, we have the even-in-$y$ and odd-in-y parts $\chi_{\frac{1}{2}}^{(\pm)}(\varphi)$ of Eqs. (4.4.12) and (4.4.13), which are shown in plots (b) and (c). These functions have remaining low-amplitude oscillations in the vicinity of $\varphi = \pi$ but no poles at $\varphi = \pi$ However, the imaginary part of $\chi_{1/2}^{(\pm)}(\varphi)$ is discontinuous at $\varphi = \pi$.

two sets of MUB are found by mapping the problem of finding MUB for the rotor onto that of the linear motion, for which a method of constructing a continuous set of MUB is known. The first continuous set is specified by simple wave functions but is not satisfactory as it does not relate to an underlying Heisenberg pair. So, we established such a Heisenberg pair of complementary observables for the rotor to construct a second and more suitable continuous set of MUB. In summary, the rotor degree of freedom is on equal footing with the other continuous degrees of freedom: For all of them there are continuous sets of MUB which are related to an underlying Heisenberg pair of complementary observables.

Chapter 5

Conclusion

We have focused our attention on the existence of maximal sets of MUB in dimension six and for the continuous degree of freedom of the rotor. We have found four most distant bases in dimension six and constructed two continuous sets of MUB for the rotor, and therefore provided some analytical insight into the famous problem of MUB in dimension six and solved the problem for the rotor mathematically.

In dimension six, it is still a long way to analytically prove that we can at most have three MUB. Nevertheless, we believe that the four bases we provided are really optimal in the sense of maximizing the distance function defined in Eq. (3.1.1), and we have proved this fact analytically within the two-parameter family defined in Sec. 3.3. Two directions might be relevant for an extension of the present study. First, it would be interesting to see if the optimality of our solution can be extended to a larger family of bases, for example, to the whole Fourier transposed family. Second and complementarily, there might exist an argument to restrict the search for the maximum ASD between the canonical basis and three Hadamard bases to the Fourier transposed family, instead of the entire Hadamard family which, so far, has not been fully parameterized. In this context, however, it should be noted that—as follows from the findings of Jaming *et al.* [35]—there are no four MUB if one restricts the search to members of the Fourier family.

For the rotor degree of freedom, the problem has been settled in a mathematical sense. We can view the difficulty of the rotor degree of freedom both geometrically (a circle is a compact manifold and does not admit global charts) and algebraically (the angular momentum parameter is discrete), and actually the complicated functional form of the wave function in the φ-basis is expected. But we are still looking for a physically intuitive understanding of the resulting MUB. Or in another word, it remains to understand the physical significance of the unitary operator of Eq. (4.3.7), regarded as an observable for a linear degree of motion. Also, it is possible that one can find an alternative construction.

Appendix A

Derivation of the two-parameter family

We start from four bases U_i, $i = 0, 1, 2, 3$, in matrix form, i.e. a unitary matrix whose columns represent the basis states. These four bases are the optimal solution to our numerical search for the maximum ASD between four bases in dimension six. From the numerics, we know that one basis, say U_0, is unbiased with the remaining three bases U_1, U_2, and U_3. Therefore, we first single out this preferred basis such that

$$\begin{aligned} \mathbb{1} &= U_0^\dagger U_0\,, \\ M_1 &= U_0^\dagger U_1\,, \\ M_2 &= U_0^\dagger U_2\,, \\ M_3 &= U_0^\dagger U_3\,. \end{aligned} \tag{A.1}$$

When multiplied by $\sqrt{6}$, the matrices M_1, M_2, and M_3 are Hadamard matrices since they are unbiased to the identity matrix.

The second step is to use Karlsson's parameterization [34] to simplify our solution. His parameterization applies to H_2-reducible Hadamard matrices that can be written in the form $H = X_L P_L N P_R X_R$, where the left and right X matrices only contain phases on the diagonal, the P matrices are permutation matrices and the central matrix has the form

$$N = \begin{bmatrix} F_2 & Z_1 & Z_2 \\ Z_3 & \frac{1}{2}Z_3 A Z_1 & \frac{1}{2}Z_3 B Z_2 \\ Z_4 & \frac{1}{2}Z_4 B Z_1 & \frac{1}{2}Z_4 A Z_2 \end{bmatrix}, \tag{A.2}$$

where the 2×2 Z matrices are

$$Z_i = \begin{bmatrix} 1 & z_i \\ 1 & -z_i \end{bmatrix} \quad \text{with} \quad |z_i| = 1\,, \tag{A.3}$$

and

$$\begin{aligned} A &= F_2\Big(-\frac{1}{2}\mathbb{1} + \mathrm{i}\frac{\sqrt{3}}{2}\Lambda\Big), \\ B &= F_2\Big(-\frac{1}{2}\mathbb{1} - \mathrm{i}\frac{\sqrt{3}}{2}\Lambda\Big) \end{aligned} \tag{A.4}$$

with a unitary and hermitian 2×2 matrix Λ. Our Hadamard matrices are indeed H_2-reducible since they can be written as $M_i = X_{L_i} P_{L_i} N_i P_{R_i} X_{R_i}$ with the central matrices given by

$$\begin{aligned} N_1 &= \frac{1}{\sqrt{6}} \begin{bmatrix} F_2 & F_2 & F_2 \\ F_2 & \omega F_2 & \omega^* F_2 \\ T & \omega^* T & \omega T \end{bmatrix}, \\ N_2 &= \frac{1}{\sqrt{6}} \begin{bmatrix} F_2 & F_2 & F_2 \\ T & \omega T & \omega^* T \\ T & \omega^* T & \omega T \end{bmatrix}, \\ N_3 &= \frac{1}{\sqrt{6}} \begin{bmatrix} F_2 & F_2 & F_2 \\ T & \omega T & \omega^* T \\ F_2 & \omega^* F_2 & \omega F_2 \end{bmatrix}. \end{aligned} \tag{A.5}$$

We choose to express the matrix T with factors of $\omega = \exp(\mathrm{i}2\pi/3)$,

$$T = \begin{bmatrix} 1 & \omega t^2 \\ 1 & -\omega t^2 \end{bmatrix} , \tag{A.6}$$

to exhibit the crucial dependence on the phase factor t. The left permutation matrices are all equal, $P_{L_1} = P_{L_2} = P_{L_3} = P_L$.

Third, we notice that only the left dephasing and permutation matrices are relevant for the distance. Indeed the right dephasing matrices only add global phases to the basis vectors while the right permutation only permute the basis vectors. In other words, two bases B and BP_RX_R are equivalent in terms of distance. Therefore we can choose to conserve only the relevant structure for our bases, that is, $M_i = X_{L_i}P_{L_i}N_i$.

The fourth step is to use the fact that only relative dephasing and permutations of the rows are relevant to the distance. Therefore we define new bases as

$$\begin{aligned} M_1 &\mathrel{\widehat{=}} P_L^\dagger X_2^\dagger X_1 P_L N_1 \, , \\ M_2 &\mathrel{\widehat{=}} N_2 \, , \\ M_3 &\mathrel{\widehat{=}} P_L^\dagger X_2^\dagger X_3 P_L N_3 \, . \end{aligned} \tag{A.7}$$

To simplify the notations, we again denote the two new diagonal matrices in $P_L^\dagger X_2^\dagger X_1 P_L$ and $P_L^\dagger X_2^\dagger X_3 P_L$ by X_1 and X_3, respectively. We further observe that

$$X_1 = \begin{bmatrix} A_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & A_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & A_1 \end{bmatrix} \quad \text{and} \quad X_3 = \begin{bmatrix} B_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & B_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B_3 \end{bmatrix} . \tag{A.8}$$

Next we add a suitable global phase to X_1 and X_3. We multiply X_1 by $\exp(-\mathrm{i}\mathrm{Arg}(A_1[1,1]A_1[2,2]/2))$ and X_3 by $\exp(-\mathrm{i}\mathrm{Arg}(B_1[1,1]B_1[2,2]/2))$

such that A_1 and B_1 take the simple form

$$\begin{bmatrix} \exp(-\mathrm{i}\phi) & 0 \\ 0 & \exp(\mathrm{i}\phi) \end{bmatrix}, \tag{A.9}$$

for some phase ϕ. We end up with the remarkable form

$$X_1 = \begin{bmatrix} A_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & A_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & A_1 \end{bmatrix} \quad \text{and} \quad X_3 = \begin{bmatrix} A_1^* & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \omega^* A_1^* & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B_3 \end{bmatrix} \tag{A.10}$$

where

$$A_1 = \begin{bmatrix} x^* & 0 \\ 0 & x \end{bmatrix}. \tag{A.11}$$

So far, we have found that

$$\begin{aligned} A_3 &= A_1\,, \\ B_1 &= A_1^*\,, \\ B_2 &= \omega^* A_1^*\,, \end{aligned} \tag{A.12}$$

and it only remains to find the structure behind the two 2×2 dephasing matrices A_2 and B_3.

To do so, we now consider the products $M_i^\dagger M_j$. We obtain

$$M_1^\dagger M_2 = \begin{bmatrix} a_1 & a_2 & a_3 \\ a_3 & a_1 & a_2 \\ a_2 & a_3 & a_1 \end{bmatrix} \quad \text{with} \quad \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = F_3 \begin{bmatrix} F_2 & A_1^* & F_2 \\ F_2 & A_2^* & T \\ T^\dagger & A_3^* & T \end{bmatrix} \tag{A.13}$$

and F_3 is the standard (unnormalized) 3-dimensional Fourier matrix

$$F_3 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^* \\ 1 & \omega^* & \omega \end{bmatrix}. \tag{A.14}$$

Similarly we have

$$M_2^\dagger M_3 = \begin{bmatrix} b_1 & b_2 & b_3 \\ b_3 & b_1 & b_2 \\ b_2 & b_3 & b_1 \end{bmatrix} \quad \text{with} \quad \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = F_3 \begin{bmatrix} F_2 & B_1 & F_2 \\ T^\dagger & B_2 & T \\ T^\dagger & B_3 & F_2 \end{bmatrix} \tag{A.15}$$

and

$$M_3^\dagger M_1 = \begin{bmatrix} c_1 & c_2 & c_3 \\ c_3 & c_1 & c_2 \\ c_2 & c_3 & c_1 \end{bmatrix} \quad \text{with} \quad \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = F_3 \begin{bmatrix} F_2 & Y_1 & F_2 \\ T^\dagger & Y_2 & F_2 \\ F_2 & Y_3 & T \end{bmatrix} \tag{A.16}$$

where

$$Y = X_3^* X_1 = \begin{bmatrix} Y_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & Y_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & Y_3 \end{bmatrix} = \begin{bmatrix} A_1^2 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \omega A_1 A_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & B_3^* A_1 \end{bmatrix} . \tag{A.17}$$

The seventh step is to look once more at the numerics. With respect to the product $M_1^\dagger M_2$, we see that

$$a_2 = \omega^* Z a_3 Z \,. \tag{A.18}$$

Thus we are lead to define the matrix equation

$$E_1 \widehat{=} a_2 - \omega^* Z a_3 Z = 0 \,. \tag{A.19}$$

This only represents a system of three equations since $E_1[1,1] = E_1[2,2]$. In the same manner, we have for $M_2^\dagger M_3$

$$E_2 \widehat{=} b_1 - \omega^* Z b_3 Z = 0 \,, \tag{A.20}$$

and $E_2[1,1] = E_2[2,2]$ so that, here too, only three equations are relevant. Finally, for $M_3^\dagger M_1$, we obtain

$$E_3 \widehat{=} c_1 + Zc_2Z = 0 \tag{A.21}$$

and, owing to $(\omega^* - 1)E_3[1,2] = t(1-\omega)E_3[2,1]$, again only three equations are relevant. We should mention here that there are other interesting identities within the products $M_i^\dagger M_j$, such as $b_2 = [a_1 + a_1^\dagger + Z(a_1 - a_1^\dagger)Z]/2$, but they are much more complicated to handle and will not be necessary to achieve our parameterization.

The eighth steps is to solve the above nine equations. We obtain

$$\begin{aligned}
E_1[1,1] &: \ \mathrm{tr}\big\{A_1\big\} = \mathrm{tr}\big\{A_3\big\}\,, \\
E_1[1,2] &: \ A_1 - 2\omega^* t^{*2} A_2 + \omega^* t^{*2} A_3 = r\mathbb{1}\,, \\
E_1[2,1] &: \ \omega^* t^{*2} A_1 - 2\omega^* t^{*2} A_2 + A_3 = r'\mathbb{1}\,.
\end{aligned} \tag{A.22}$$

From the numerics, we know that $r = r'$ and thus $A_1 = A_3$, which we already found by looking at the dephasing matrix X_1. Note also that the expression of the complex number r is not required. Furthermore we find

$$\begin{aligned}
E_2[1,1] &: \ \mathrm{tr}\big\{B_1\big\} = \omega\mathrm{tr}\big\{B_2\big\}\,, \\
E_2[1,2] &: \ \omega^* t^{*2} B_1 + \omega B_2 - 2\omega t^{*2} A_3 = s\mathbb{1}\,, \\
E_2[2,1] &: \ B_1 + t^{*2} B_2 - 2\omega t^{*2} B_3 = s'\mathbb{1}\,.
\end{aligned} \tag{A.23}$$

From the numerics, we know that $s = s'(= r)$ and thus $B_1 = \omega B_2$, which we already obtained by looking at the dephasing matrix X_3. The next three equations are much more interesting. Indeed we have

$$\begin{aligned}
E_3[1,1] &: \ 2\mathrm{tr}\big\{Y_1\big\} - \omega^*\mathrm{tr}\big\{Y_2\big\} - \omega\mathrm{tr}\big\{Y_3\big\} = 0\,, \\
E_3[2,2] &: \ 2\mathrm{tr}\big\{Y_1\big\} - \omega t^{*2}\mathrm{tr}\big\{Y_2\big\} - \omega^* t^2\mathrm{tr}\big\{Y_3\big\} = 0\,, \\
E_3[1,2] &: \ t^{*2} Y_2 - Y_3 = u\mathbb{1}\,.
\end{aligned} \tag{A.24}$$

From the numerics, we know that $u = 0$ and the last equation reduces to

$$Y_3 = t^{*2} Y_2. \tag{A.25}$$

Since $Y_2 = \omega A_1 A_2$ and $Y_3 = B_3^* A_1$, the above equation directly translates into

$$B_3 = \omega^* t^2 A_2^* \,. \tag{A.26}$$

This last relation can be inserted in $E_3[1,1]$ and $E_3[2,2]$, which become identical and can be written as

$$2\mathrm{tr}\{Y_1\} - (\omega^* + \omega t^{*2})\mathrm{tr}\{Y_2\} = 0\,. \tag{A.27}$$

This equation will soon become Eq. (3.3.27).

A last hint from the numerics is needed. We actually notice that

$$Y_1 Y_2 Y_3 = -\mathbb{1}\,. \tag{A.28}$$

As $Y_3 = t^{*2} Y_2$, we arrive at $t^{*2} Y_1 Y_2^2 = -\mathbb{1}$ so that $\omega t^* A_1^2 A_2 = \pm \mathrm{i} U$, where $U^2 = \mathbb{1}$, that is, $U = \mathbb{1}$ or $U = Z$ since it has to be diagonal. With the help of the numerics, we conclude that

$$A_2 = \mathrm{i}\omega^* t Z A_1^{*2} \tag{A.29}$$

and consequently

$$B_3 = -\mathrm{i} t Z A_1^2\,. \tag{A.30}$$

The final parametrization of the dephasing matrices is therefore given by

$$X_1 = \begin{bmatrix} A_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathrm{i}\omega^* t Z A_1^{*2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & A_1 \end{bmatrix},$$
$$X_3 = \begin{bmatrix} A_1^* & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \omega^* A_1^* & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathrm{i} t Z A_1^2 \end{bmatrix}. \tag{A.31}$$

Let us finally come back to Eq. (A.27). We can now substitute $Y_1 = A_1^2$ and $Y_2 = (\mathrm{i}\omega^* t Z A_1^{*2})(\omega A_1) = \mathrm{i} t Z A_1^*$ in Eq. (A.27) and, upon defining $x = \exp(\mathrm{i}\theta_x)$ and $t = \exp(\mathrm{i}\theta_t)$, we arrive at

$$\cos(\theta_t - 2\pi/3) = -\frac{\cos(2\theta_x)}{\sin(\theta_x)}\,, \tag{A.32}$$

which is Eq. (3.3.27).

Appendix B

Approximation of $\psi_y^{(0)}(\varphi)$

Our approximation for the wave function $\psi_y^{(0)}(\varphi)$ in the φ-basis is presented, which enables us to justify the remark made in the end of Sec. 4.4 that the even part and odd part of this wave function can be factored out as the functions $\chi_y^{(\pm)}(\varphi)$ multiplying a prefactor that oscillates arbitrarily rapidly in the vicinity of $\varphi = \pi$.

We consider the even-in-y and odd-in-y parts of $\psi_y^{(0)}(\varphi)$ separately, that is, $\psi_y^{(0)}(\varphi) = \text{even part} + \text{odd part}$, where

$$\begin{aligned}\text{even part} &= \sum_{l=0}^{\infty} \mathrm{e}^{\mathrm{i}l\varphi} f_{2l}(y) \\ &= \mathrm{e}^{-y^2/2} \sum_{l=0}^{\infty} \frac{\pi^{-1/4}}{2^l \sqrt{(2l)!}} \mathrm{e}^{\mathrm{i}l\varphi} H_{2l}(y),\end{aligned} \tag{B.1}$$

$$\begin{aligned}\text{odd part} &= \sum_{l=0}^{\infty} \mathrm{e}^{-\mathrm{i}(l+1)\varphi} f_{2l+1}(y) \\ &= \mathrm{e}^{-y^2/2} \mathrm{e}^{-\mathrm{i}\varphi} \sum_{l=0}^{\infty} \frac{\pi^{-1/4}}{2^{l+1/2} \sqrt{(2l+1)!}} \mathrm{e}^{-\mathrm{i}l\varphi} H_{2l+1}(y).\end{aligned} \tag{B.2}$$

The difficulty in calculating the wave function $\psi_y^{(0)}(\varphi)$ is that the two infinite series in Eqs. (B.1) and (B.2) converge extremely slowly. Here our approach is to express a slowly convergent series as a sum of integral and a rapidly convergent series. This is accomplished in two steps.

First, the troublesome term $1/\sqrt{(2l)!}$ in Eq. (B.1) is treated by considering the infinite product representation of $\cos\alpha$:

$$\begin{aligned}\cos\alpha &= \prod_{k=0}^{\infty}\Big(1-\frac{4\alpha^2}{(2k+1)^2\pi^2}\Big)\\ &= \big(1-(2\alpha/\pi)^2\big)\prod_{k=1}^{\infty}\Big(1-\frac{(2\alpha/\pi)^2}{(2k+1)^2}\Big).\end{aligned} \tag{B.3}$$

Note the limit

$$\lim_{\alpha=\pi/2}\frac{\cos\alpha}{1-(2\alpha/\pi)^2}=\frac{\pi}{4}\,. \tag{B.4}$$

Therefore substituting $\alpha=\pi/2$ into Eq. (B.3) gives

$$\begin{aligned}\frac{\pi}{4} &= \prod_{k=1}^{\infty}\Big(1-\frac{1}{(2k+1)^2}\Big)\\ &= \Big(\prod_{k=1}^{l-1}\frac{2k(2k+2)}{(2k+1)^2}\Big)\Big(\prod_{k=l}^{\infty}\Big(1-\frac{1}{(2k+1)^2}\Big)\Big)\\ &= \frac{2^{4l}(l!)^4}{((2l)!)^2}\frac{1}{4l}\prod_{k=l}^{\infty}\Big(1-\frac{1}{(2k+1)^2}\Big),\end{aligned} \tag{B.5}$$

or equivalently

$$\begin{aligned}\frac{\pi^{-1/4}2^l l!}{\sqrt{(2l)!}} &= l^{1/4}\prod_{k=l}^{\infty}\Big(1-\frac{1}{(2k+1)}\Big)^{-1/4}\\ &= \big(l+\frac{1}{4}\big)^{1/4}\big(1+\frac{1}{4l}\big)^{-1/4}\prod_{k=l}^{\infty}\Big(1-\frac{1}{(2k+1)^2}\Big)^{-1/4}.\end{aligned} \tag{B.6}$$

We are interested in the situation that l is large, therefore it is possible to approximate the above Eq. (B.6) in a simple form, with the higher order terms of $1/l$ discarded. In order to do this, we leave the term $(1+1/(4l))^{1/4}$ in Eq. (B.6) untouched, and perform the approximation in the remaining expression, which we denote as

$$L\text{-Rest}=\big(1+\frac{1}{4l}\big)^{-1/4}\prod_{k=l}^{\infty}\Big(1-\frac{1}{(2k+1)^2}\Big)^{-1/4}. \tag{B.7}$$

The approximation is accomplished by considering

$$\begin{aligned}
-4\log(L\text{-Rest}) &= \log(1+\frac{1}{4l}) + \sum_{k=l}^{\infty}\log\bigl(1-\frac{1}{(2k+1)^2}\bigr) \\
&= \log(1+\frac{1}{4l}) + \int_l^{\infty}\mathrm{d}\lambda\,\log(1-\frac{1}{4\lambda^2}) \\
&\quad - \sum_{k=l}^{\infty}\int_k^{k+1}\mathrm{d}\lambda\,\log\Bigl((1-\frac{1}{4\lambda^2})/(1-\frac{1}{(2k+1)^2})\Bigr)\,,
\end{aligned} \tag{B.8}$$

where the last term can be approximated by discarding fourth or higher order terms in its Taylor series expansion around $\lambda = k+1/2$, and we arrive at the following expression

$$\begin{aligned}
-4\log(L\text{-Rest}) &\approx \log(1+\frac{1}{4l}) - (l+\frac{1}{2})\log(1+\frac{1}{2l}) - (l-\frac{1}{2})\log(1-\frac{1}{2l}) \\
&\quad - \sum_{k=l}^{\infty}\int_k^{k+1}\mathrm{d}\lambda\,\frac{1}{2}(\lambda-k-\frac{1}{2})^2\Bigl[\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2}\log(1-\frac{1}{4\lambda^2})\Bigr]_{\lambda=k+\frac{1}{2}}\,.
\end{aligned}$$

Discarding terms of order $1/l^4, 1/l^5\cdots$, we obtain

$$\log(L\text{-Rest}) \approx \frac{1}{128}\bigl(l+\frac{1}{4}\bigr)^{-2}. \tag{B.9}$$

Therefore

$$L\text{-Rest} \approx 1 + \frac{1}{128}\bigl(l+\frac{1}{4}\bigr)^{-2}. \tag{B.10}$$

Substitute Eq. (B.10) into Eq. (B.6), we have

$$\frac{\pi^{-1/4}2^l l!}{\sqrt{(2l)!}} = \bigl(l+\frac{1}{4}\bigr)^{1/4} + \frac{1}{128}\bigl(l+\frac{1}{4}\bigr)^{-7/4} + a_l\,, \tag{B.11}$$

where $a_l \propto l^{-5/4}$ for large l, which implies

$$\begin{aligned}
\text{even part} = \mathrm{e}^{-y^2/2}\sum_{l=0}^{\infty}\Bigl((l+\frac{1}{4})^{1/4} + \frac{1}{128}(l+\frac{1}{4})^{-7/4} \\
+ a_l\Bigr)\frac{\mathrm{e}^{\mathrm{i}l\varphi}}{4^l l!}H_{2l}(y)\,.
\end{aligned} \tag{B.12}$$

For the odd part, we have

$$\begin{aligned}\frac{\pi^{-1/4}2^{l+\frac{1}{2}}l!}{\sqrt{(2l+1)!}} &= \frac{\pi^{-1/4}2^l l!}{\sqrt{(2l)!}}\big(l+\frac{1}{2}\big)^{-1/2}\\ &= \big(l+\frac{3}{4}\big)^{-1/4}\Big(\frac{(l+1/4)(l+3/4)}{(l+1/2)^2}\Big)^{1/4}\\ &\quad\times\Big(1+\frac{1}{128}\big(l+\frac{1}{4}\big)^{-2}+\cdots\Big)\,. \end{aligned} \tag{B.13}$$

Discarding terms of order $1/l^4, 1/l^5\cdots$, we obtain

$$\frac{\pi^{-1/4}2^{l+\frac{1}{2}}l!}{\sqrt{(2l+1)!}} = \big(l+\frac{3}{4}\big)^{-1/4} - \frac{1}{128}\big(l+\frac{3}{4}\big)^{-9/4} + b_l\,, \tag{B.14}$$

where $b_l \propto l^{-17/4}$ for large l. Therefore, similarly as the even part, we have

$$\begin{aligned}\text{odd part} = \mathrm{e}^{-y^2/2}\sum_{l=0}^{\infty}\Big((l+\frac{3}{4})^{-1/4} - \frac{1}{128}(l+\frac{3}{4})^{-9/4}\\ + b_l\Big)\frac{\mathrm{e}^{-\mathrm{i}l\varphi}}{4^{l+1/2}l!}H_{2l+1}(y)\,. \end{aligned} \tag{B.15}$$

Numerically, a_l and b_l are found as

$$a_l \approx -0.00158(l+\tfrac{1}{4})^{-15/4}\,, \tag{B.16}$$

$$b_l \approx 0.00166(l+\tfrac{3}{4})^{-17/4}\,. \tag{B.17}$$

It is clear that the infinite sums involving a_l and b_l converge quickly.

The next step is to find the integrals. Note that

$$\begin{aligned}\Big(l+\frac{1}{4}\Big)^{1/4}\mathrm{e}^{\mathrm{i}l\varphi} &= \Big(\frac{1}{\mathrm{i}}\frac{\partial}{\partial\varphi}+\frac{1}{4}\Big)^{1/4}\mathrm{e}^{\mathrm{i}l\varphi}\\ &= \Big(\frac{1}{\mathrm{i}}\frac{\partial}{\partial\varphi}+\frac{1}{4}\Big)^{1/4}\int_0^\infty\frac{\mathrm{d}t}{(-\frac{1}{4})!}\,t^{-1/4}\mathrm{e}^{-t}\mathrm{e}^{\mathrm{i}l\varphi}\Big|_{t=(\frac{1}{\mathrm{i}}\frac{\partial}{\partial\varphi}+\frac{1}{4})x^4}\\ &= \Big(\frac{1}{\mathrm{i}}\frac{\partial}{\partial\varphi}+\frac{1}{4}\Big)\frac{4}{(-\frac{1}{4})!}\int_0^\infty\mathrm{d}x\,x^2\mathrm{e}^{-\frac{1}{4}x^4}\Big(\mathrm{e}^{\mathrm{i}\varphi}\mathrm{e}^{-x^4}\Big)^l\,, \end{aligned} \tag{B.18}$$

And similarly,

$$\left(l+\frac{1}{4}\right)^{-7/4} \mathrm{e}^{\mathrm{i}l\varphi} = \frac{4}{\frac{3}{4}!} \int_0^\infty \mathrm{d}x\, x^6 \mathrm{e}^{-\frac{1}{4}x^4} \left(\mathrm{e}^{\mathrm{i}\varphi}\mathrm{e}^{-x^4}\right)^l . \tag{B.19}$$

Eqs. (B.18) and (B.19) suggest that we need to consider the l-summation of the terms in the form of $z^l H_{2l}(y)/(4^l l!)$. This can be done by noting the relation between the Hermite polynomials and the laguerre polynomials,

$$H_{2l}(y) = (-1)^l 4^l l! L_l^{(-1/2)}(y^2) . \tag{B.20}$$

The identity for the laguerre polynomials

$$\sum_{l=0}^\infty (-z)^l L_l^{(-1/2)}(y^2) = (1+z)^{-1/2} \mathrm{e}^{y^2 \frac{z}{1+z}} , \tag{B.21}$$

immediately implies that

$$\sum_{l=0}^\infty \frac{z^l}{4^l l!} H_{2l}(y) = (1+z)^{-1/2} \mathrm{e}^{y^2 \frac{z}{1+z}} . \tag{B.22}$$

Finally, Eqs. (B.18), (B.19) and (B.22) help us to express the even part in Eq. (B.12) as an integral and a rapidly convergent series as

$$\text{even part} = \text{even integral} + \text{even rest} , \tag{B.23}$$

where

$$\begin{aligned} \text{even integral} = \frac{\mathrm{e}^{y^2/2}}{(-\frac{1}{4})!} \int_0^\infty \mathrm{d}x\, x^2 \mathrm{e}^{-\frac{1}{4}x^4} \Big[1 &+ \frac{1}{24} x^4 z^2 \\ &+ (z-1)(4y^2+1-z) \Big] z^{-\frac{5}{2}} \mathrm{e}^{-\frac{y^2}{z}} , \end{aligned} \tag{B.24}$$

with $z = 1 + \mathrm{e}^{\mathrm{i}\varphi}\mathrm{e}^{-x^4}$, and

$$\text{even rest} = \mathrm{e}^{-\frac{1}{2}y^2} \sum_{l=0}^\infty a_l \frac{\mathrm{e}^{\mathrm{i}l\varphi}}{4^l l!} H_{2l}(y) . \tag{B.25}$$

The treatment for the odd part is similar. We have

$$\text{odd part} = \text{odd integral} + \text{odd rest}\,, \tag{B.26}$$

where

$$\text{odd integral} = y\mathrm{e}^{-y^2/2}\mathrm{e}^{-\mathrm{i}\varphi}\frac{1}{\frac{1}{4}!}\int_0^\infty \mathrm{d}x\,\mathrm{e}^{-\frac{3}{4}x^4}(1-\tfrac{x^8}{40})z^{-\frac{3}{2}}\mathrm{e}^{-\frac{y^2}{z}}\,, \tag{B.27}$$

with $z = 1 + \mathrm{e}^{-\mathrm{i}\varphi}\mathrm{e}^{-x^4}$, and

$$\text{odd rest} = \mathrm{e}^{-\frac{1}{2}y^2}\mathrm{e}^{-\mathrm{i}\varphi}\sum_{l=0}^{\infty} b_l \frac{\mathrm{e}^{-\mathrm{i}l\varphi}}{4^{l+\frac{1}{2}}\,l!}H_{2l+1}(y)\,. \tag{B.28}$$

For the even integral in Eq. (B.24), we have the factor

$$\exp\Big(-\frac{y^2}{z}+\frac{y^2}{2}\Big) = \exp\Big(\frac{y^2}{2}-\frac{y^2}{1+\mathrm{e}^{\mathrm{i}\varphi}}\Big)\exp\Big(-y^2\big(\frac{1}{z}-\frac{1}{1+\mathrm{e}^{\mathrm{i}\varphi}}\big)\Big), \tag{B.29}$$

since $z = 1 + \mathrm{e}^{\mathrm{i}\varphi}\mathrm{e}^{-x^4}$. Now we can put the factor

$$\exp\Big(\frac{y^2}{2}-\frac{y^2}{1+\mathrm{e}^{\mathrm{i}\varphi}}\Big) = \exp\Big(\frac{y^2}{2}\frac{\mathrm{e}^{\mathrm{i}\varphi}-1}{\mathrm{e}^{\mathrm{i}\varphi}+1}\Big) = \exp\Big(\frac{\mathrm{i}}{2}y^2\tan\tfrac{\varphi}{2}\Big)\,, \tag{B.30}$$

out as the prefactor of the integral. Similarly for the odd part, we have the prefactor $\exp\big(-\mathrm{i}(y^2/2)\tan(\varphi/2)\big)$. The term $\tan(\varphi/2)$ makes the prefactors oscillate arbitrarily rapidly in the vicinity of $\varphi = \pi$, as already mentioned in Sec. 4.4.

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