

THE ROLE OF FRAME FORCE IN QUANTUM DETECTION

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ABSTRACT. A method is given to construct tight frames that minimize an error term, which in quantum physics has the interpretation of the probability of a detection error. The method converts the frame problem into a set of ordinary differential equations using concepts from classical mechanics and orthogonal group techniques. The minimum energy solutions of the differential equations are proven to correspond to the tight frames that minimize the error term. Because of this perspective, several numerical methods become available to compute the tight frames. Beyond the applications of quantum detection in quantum mechanics, solutions to this frame optimization problem can be viewed as a generalization of classical matched filtering solutions. As such, the methods we develop are a generalization of fundamental detection techniques in radar.

1. INTRODUCTION

We shall define a *frame optimization problem* which resembles classical mean square error (MSE) optimization, but is generally only equivalent to MSE in geometrically structured problems, see the Appendix (Section A.5). In fact, our technical goal is to construct a so-called tight frame that minimizes an error term, which in quantum physics has the interpretation of the probability of a detection error. As such, we shall also refer to our frame optimization problem as a *quantum detection problem*. Our setting is tight frames because of the emerging applicability of such objects in dealing with the robust transmission of data over erasure channels such as the internet [14, 30, 40], multiple antenna code design for wireless communications [39], A/D conversion in a host of applications [8, 7, 32], quantum measurement and encryption schemes [49, 50, 10, 25, 24], and multiple description coding [31, 54], among others. The complexity of some of these applications goes beyond MSE, cf., matched filtering in the quantum detection setting [6], matched filtering in applied general relativity [1, 2, 59], and minimization for multiscale image decompositions [55], see also [28] for orthogonal MSE matched filter detection. Furthermore, quantum detection has applications

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in optical communications, including the detection of coherent light signals such as radio, radar, and laser signals [38, 45, 44, 43], and applications in astronomy as a means of detecting light from distant sources [38, 56].

The frame optimization problem is defined in Section 1.2 along with the definition of frames. Section 1.1 includes background material for the problem from the quantum mechanics point of view. Section 1.3 is devoted to an outline of our solution, as well as an outline of the structure of the paper.

1.1. Background. In quantum mechanics, the definition of a von Neumann measurement [33, 52, 58] can be generalized using positive-operator-valued measures (POMs) and tight frames [38, 22, 25], see the Appendix (Section A.1) for POMs and Section 1.2 for tight frames. This generalized definition of a quantum measurement allows one to distinguish more accurately among elements of a set of nonorthogonal quantum states. We can formulate our frame optimization problem of Section 1.2 in terms of quantum measurement. In this case the frame optimization problem becomes a quantum detection problem for a physical system whose state is limited to be in only one of a countable number of possibilities, see Appendix (Section A.2). These possible states are not necessarily orthogonal. We want to find the best method of measuring the system in order to distinguish which state the system is in. Mathematically, we want to find a tight frame that minimizes an error term P_e . In the context of quantum detection in quantum mechanics, P_e is in fact the probability of a detection error, see the Appendix (Sections A.1 - A.4) for details.

The quantum detection problem we consider has not been solved analytically in quantum mechanics. Kennedy, Yuen, and Lax [61] gave necessary and sufficient conditions on a POM so that it minimizes P_e . In fact, they show that P_e is minimized if and only if the corresponding POM satisfies a particular operator inequality. Wooteer [37] gave a construction of a tight frame that seems to have a small probability of a detection error, but he did not completely justify his construction. Helstrom [38] solved the problem completely for the case in which the quantum system is limited to be in one of two possible states. Peres and Terno [49] solved a slightly different problem where they optimized two quantities. They constructed a POM that maximized an expression representing the information gain and minimized another expression representing the probability of an inconclusive measurement.

1.2. Definitions and problem. A frame can be considered as a generalization of an orthonormal basis [17, 20, 60, 18, 9]. Let H be a separable Hilbert space, let $K \subseteq \mathbb{Z}$, and let $\{e_i\}_{i \in K}$ be an orthonormal basis for H . An orthonormal basis has the property that

$$\forall x \in H, \quad \|x\|^2 = \sum_{i \in K} |\langle x, e_i \rangle|^2.$$

We use this property to motivate the definition of a frame.

Definition 1.1. Let H be a separable Hilbert space and let $K \subseteq \mathbb{Z}$. A set $\{e_i\}_{i \in K} \subseteq H$ is a *frame* for H with *frame bounds* A and B , $0 < A < B$, if

$$\forall x \in H, \quad A\|x\|^2 \leq \sum_{i \in K} |\langle x, e_i \rangle|^2 \leq B\|x\|^2.$$

A frame $\{e_i\}_{i \in K}$ for H is a *tight frame* if $A = B$. A tight frame with frame bound A is an *A-tight frame*.

Problem 1.2. Let H be a d -dimensional Hilbert space. Given a sequence $\{x_i\}_{i=1}^N \subseteq H$ of unit normed vectors and a sequence $\{\rho_i\}_{i=1}^N \subseteq \mathbb{R}$ of positive weights that sums to 1. The *frame optimization problem* is to *construct* a 1-tight frame $\{e_i\}_{i=1}^N$ that minimizes the quantity,

$$P_e(\{e_i\}_{i=1}^N) = 1 - \sum_{i=1}^N \rho_i |\langle x_i, e_i \rangle|^2, \quad (1.1)$$

taken over all N -element 1-tight frames. Such a tight frame exists by a compactness argument, see Theorem A.7 in the Appendix (Appendix A.4) for a proof. Our goal is to quantify this existence.

We have taken $\sum_{i=1}^N \rho_i = 1$ because of the probabilistic interpretation in the Appendix. This condition is not required in the main body of the paper, even though we use it as a technical convenience in Section 3.

1.3. Outline. The frame optimization problem (1.1) has many applications as implied in the first paragraph of the Introduction. To illustrate the connection between the frame optimization problem and quantum mechanics, beyond Section 1.1, and as a background for some of our technology, we have included an Appendix, as mentioned in Section 1.1. In Section A.1 we present quantum measurement theory in terms of POMs; and then motivate a quantum detection problem in Sections A.2 - A.4. In particular, Section A.4 expounds the remarkable and elementary relationship between POMs and tight frames. Using this relationship, we formulate this quantum detection problem as the frame optimization problem of Section 1.2. Figure 1 describes our solution to these equivalent problems; and, in particular, it highlights some of the various techniques that we require.

We begin in Section 2 with preliminaries from classical Newtonian mechanics [46] and the recent characterization of finite unit normed tight frames as minimizers of a frame potential [5] associated with the notion of frame force.

In Section 3 we use Naimark's theorem to simplify the frame optimization problem by showing that we only need to consider orthonormal sets in place of 1-tight frames. We then use the concept of the frame force [5] to construct a corresponding force for the frame optimization problem. In Section 4 we use the orthogonal group $O(N)$ as a means to parameterize orthonormal sets. With this parameterization, we construct a set of differential equations on $O(N)$ and show that the minimum energy solutions correspond exactly to

Frame optimization problem = Section A.4 = Quantum mechanical quantum detection problem

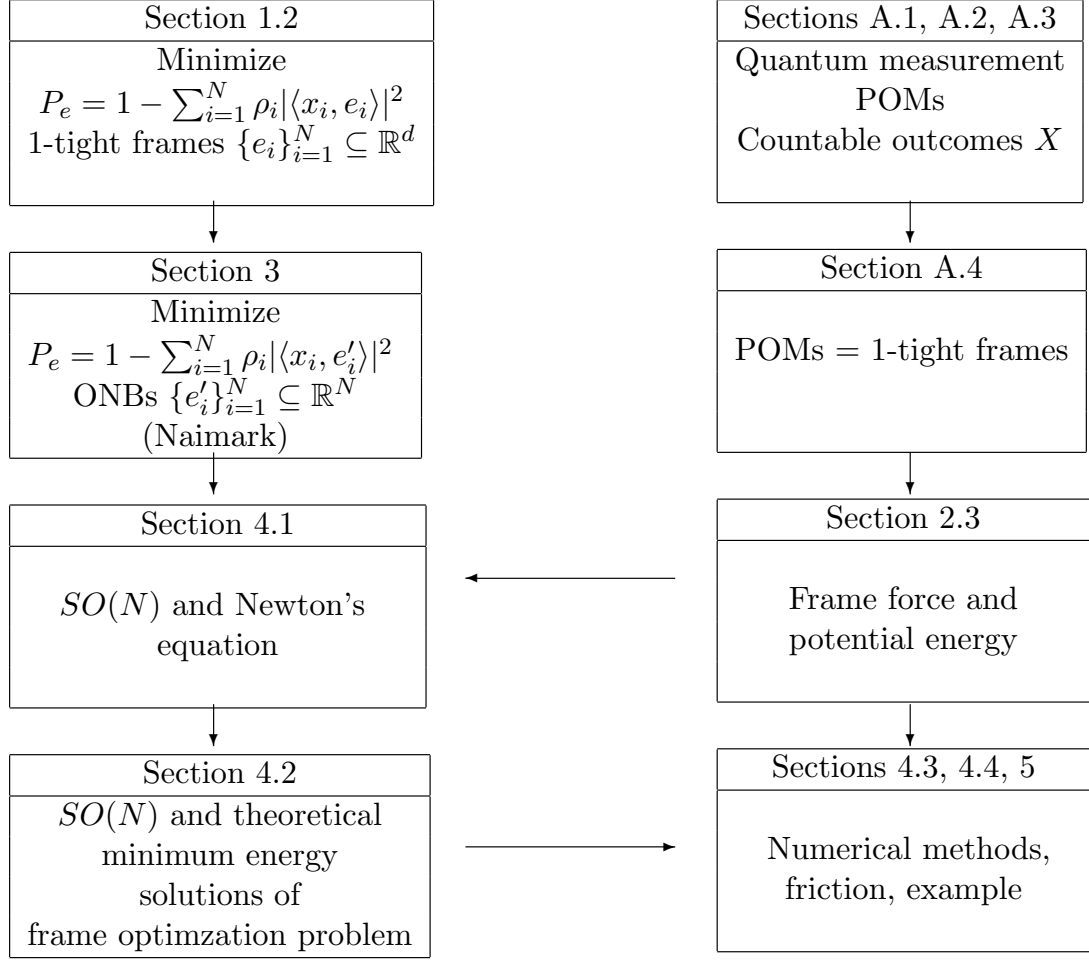


FIGURE 1. Outline of the solution.

the 1-tight frames that minimize the error term P_e . With this perspective, we comment on how different numerical methods can be used to approximate the 1-tight frames that solve the frame optimization problem.

Finally, in Section 5, we give an example of computing a solution to the frame optimization problem for the case $N = 2$. The purpose of Section 5 is to serve as an introduction to the ongoing numerical work found in [41].

2. PRELIMINARIES

2.1. Newtonian mechanics of 1 particle. Suppose $x : \mathbb{R} \rightarrow \mathbb{R}^d$ is twice differentiable. For $t \in \mathbb{R}$, we denote the derivative of x at t as $\dot{x}(t)$ and the second derivative as $\ddot{x}(t)$. $x(t)$ is interpreted as the position of a particle in \mathbb{R}^d at time $t \in \mathbb{R}$. A force acting on x is a vector field $F : \mathbb{R}^d \rightarrow \mathbb{R}^d$, and it determines the dynamics of x by *Newton's equation*

$$\ddot{x}(t) = F(x(t)). \quad (2.1)$$

The force F is a *conservative force* if there exists a differentiable function $V : \mathbb{R}^d \rightarrow \mathbb{R}$ such that

$$F = -\nabla V,$$

where ∇ is the d -dimensional gradient. V is called the *potential* of the force F . The following elementary theorem [46] shows that energy is conserved under a conservative force.

Theorem 2.1. *If $x : \mathbb{R} \rightarrow \mathbb{R}^d$ is a solution of Newton's equation (2.1) and the force is conservative, then the total energy, defined by*

$$E(t) = \frac{1}{2}[\dot{x}(t)]^2 + V(x(t)), \quad t \in \mathbb{R},$$

is constant with respect to the variable t .

2.2. Central force. Suppose we have an ensemble of particles in \mathbb{R}^d that interact with one another by a conservative force $F : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$. Given two particles $a, b \in \mathbb{R}^d$, a "feels" the force from b given by $F(a, b)$, i.e., as functions of time $\ddot{a}(t) = F(a(t), b(t))$. This action defines the dynamics on the entire ensemble. If the force is conservative, then there exists a potential function $V : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ such that

$$F(a, b) = -\nabla_{a-b} V(a, b),$$

where ∇_{a-b} is the gradient taken by keeping b fixed and differentiating with respect to a . The force F is a *central force* if its magnitude depends only on the distance $\|a - b\|$, that is, if there exists a function $f : \mathbb{R}^+ \rightarrow \mathbb{R}$ such that

$$\forall a, b \in \mathbb{R}^d, \quad F(a, b) = f(\|a - b\|)[a - b].$$

($\mathbb{R}^+ = (0, \infty)$.) In this case, the same can be said of the potential, that is, if the force is conservative and central, then there is a function $v : \mathbb{R}^+ \rightarrow \mathbb{R}$ such that

$$\forall a, b \in \mathbb{R}^d, \quad V(a, b) = v(\|a - b\|). \quad (2.2)$$

Computing the potential corresponding to a conservative central force is not difficult. In fact, for any $a, b \in \mathbb{R}^d$, the condition,

$$F(a, b) = -\nabla_{(a-b)} V(a, b),$$

implies that

$$\forall r \in \mathbb{R}^+, \quad v'(r) = -rf(r), \quad (2.3)$$

which, in turn, allows us to compute V because of (2.2). To verify (2.3), first note that

$$\forall x = (x_1, \dots, x_d) \in \mathbb{R}^d, \quad \nabla \|x\| = \begin{bmatrix} \frac{x_1}{\sqrt{x_1^2 + \dots + x_d^2}} \\ \vdots \\ \frac{x_d}{\sqrt{x_1^2 + \dots + x_d^2}} \end{bmatrix} = \frac{x}{\|x\|}.$$

Thus, writing $x = a - b \in \mathbb{R}^d$, we compute

$$-\nabla V(a, b) = -\nabla v(\|x\|)\|x\| = -v'(\|x\|)\nabla\|x\| = -v'(\|x\|)\frac{x}{\|x\|};$$

and, setting the right side equal to $F(a, b) = f(\|x\|)x$, we obtain

$$v'(\|x\|) = -\|x\|f(\|x\|),$$

which is (2.3).

2.3. Frame force. Two electrons with charge e and positions given by $x, y \in \mathbb{R}^3$ "feel" a repulsive force given by Coulomb's law. Particle x "feels" the force $F(x, y)$, exerted on it by particle y , given by the formula,

$$F(x, y) = K \frac{e^2}{\|x - y\|^3} (x - y),$$

where K is Coulomb's constant. Suppose we have a metallic sphere where a number of electrons move freely and interact with each other by the Coulomb force. An unresolved problem in physics is to determine the equilibrium positions of the electrons, that is, to specify an arrangement of the electrons where all of the interaction Coulomb forces cancel so that there is no motion [4, 3]. This phenomena corresponds to the minimization of the Coulomb potential.

In [5], Fickus and one of the authors used this idea to characterize all finite unit normed tight frames, see Theorems 2.2 and 2.3. The goal was to find a force, which they called *frame force*, such that the equilibrium positions on the sphere would correspond to finite unit normed tight frames. Given two points $x, y \in \mathbb{R}^d$. By definition, the particle x "feels" the frame force $FF(x, y)$, exerted on it by particle y , given by the formula,

$$FF(x, y) = \langle x, y \rangle (x - y). \quad (2.4)$$

It can be shown that $FF(x, y)$ is a central force with the *frame potential* FP given by

$$FP(x, y) = \frac{1}{2} |\langle x, y \rangle|^2.$$

Let $\{x_i\}_{i=1}^N \subseteq \mathbb{R}^d$ be a unit normed set, i.e., $\{x_i\}_{i=1}^N \subseteq S^{d-1}$, the unit sphere in \mathbb{R}^d . The *total frame potential* is

$$TFP(\{x_i\}_{i=1}^N) = \sum_{m=1}^N \sum_{n=1}^N |\langle x_m, x_n \rangle|^2.$$

The equilibrium points of the frame force on S^{d-1} produce all finite unit normed tight frames in the following way.

Theorem 2.2. *Let $N \leq d$. The minimum value of the total frame potential, for the frame force (2.4) and N variables, is N ; and the minimizers are precisely all of the orthonormal sets of N elements in \mathbb{R}^d .*

Theorem 2.3. *Let $N \geq d$. The minimum value of the total frame potential, for the frame force (2.4) and N variables, is N^2/d ; and the minimizers are precisely all of the finite unit normed tight frames of N elements for \mathbb{R}^d .*

3. A CLASSICAL MECHANICAL INTERPRETATION OF THE FRAME OPTIMIZATION PROBLEM

In this section we shall use the concept of frame force defined by (2.4) to give the frame optimization problem an interpretation in terms of classical mechanics, even though it is essentially equivalent to a quantum detection problem from quantum mechanics. To this end we first reformulate Problem 1.2 in terms of orthonormal bases instead of 1-tight frames. This can be done by means of Naimark's theorem [19, 25]. In fact, each tight frame can be considered as a projection of an equal normed orthogonal basis, where the orthogonal basis exists in a larger ambient Hilbert space. The following is a precise statement of Naimark's theorem, see [16], and see [19, 47] for full generality.

Theorem 3.1. *(Naimark) Let H be a d -dimensional Hilbert space and let $\{e_i\}_{i=1}^N$ be an A -tight frame for H . There exists an orthogonal basis $\{e'_i\}_{i=1}^N \subseteq H'$ for H' , where H' is an N -dimensional Hilbert space such that H is a linear subspace of H' , where each $\|e'_i\| = A$, and for which*

$$\forall i = 1, \dots, N, \quad P_H e'_i = e_i,$$

where P_H is the orthogonal projection of H' onto H .

We now prove the converse of Naimark's theorem, that is, we prove the assertion that the projection of an orthonormal basis gives rise to a 1-tight frame.

Proposition 3.2. *Let H' be an N -dimensional Hilbert space and let $\{e'_i\}_{i=1}^N$ be an orthonormal basis for H' . For any linear subspace $U \subseteq H'$, $\{P_U e'_i\}_{i=1}^N$ is a 1-tight frame for U , where P_U denotes the orthogonal projection of H' onto U .*

Proof. For any $x \in U$, note that $P_U x = x$. Since $\{e'_i\}_{i=1}^N$ is an orthonormal basis for H' we can write

$$\|x\|^2 = \sum_{i=1}^N |\langle e'_i, x \rangle|^2 = \sum_{i=1}^N |\langle e'_i, P_U x \rangle|^2 = \sum_{i=1}^N |\langle P_U e'_i, x \rangle|^2.$$

Since this is true for all $x \in U$, it follows that $\{P_U e'_i\}_{i=1}^N$ is a 1-tight frame for U . \square

Theorem 3.3. *Let H be a d -dimensional Hilbert space, and let $\{x_i\}_{i=1}^N \subseteq H$ be a sequence of unit normed vectors with a sequence $\{\rho_i\}_{i=1}^N \subseteq \mathbb{R}$ of positive weights that sums to 1. Let H' be an N -dimensional Hilbert space such that H is a linear subspace of H' , and let $\{e_i\}_{i=1}^N$ be a 1-tight frame for H that minimizes P_e over all N element 1-tight frames for H , i.e.,*

$$P_e(\{e_i\}_{i=1}^N) = \inf \{P_e(\{y_i\}_{i=1}^N) : \{y_i\}_{i=1}^N \text{ a 1-tight frame for } H\}.$$

(A minimizer exists by Theorem A.7.) Assume $\{e'_i\}_{i=1}^N$ is an orthonormal basis for H' that minimizes P_e over all orthonormal bases for H' , i.e.,

$$P_e(\{e'_i\}_{i=1}^N) = \inf \{P_e(\{y_i\}_{i=1}^N) : \{y_i\}_{i=1}^N \text{ an orthonormal basis in } H'\}.$$

Then

$$P_e(\{e_i\}_{i=1}^N) = P_e(\{e'_i\}_{i=1}^N) = P_e(\{P_H e'_i\}_{i=1}^N),$$

where P_H is the orthogonal projection onto H .

Proof. Since each $x_i \in H$, note that $P_H x_i = x_i$; and so, using the fact that P_H is self-adjoint, we have

$$\begin{aligned} P_e(\{e'_i\}_{i=1}^N) &= 1 - \sum_{i=1}^N \rho_i |\langle x_i, e'_i \rangle|^2 = 1 - \sum_{i=1}^N \rho_i |\langle P_H x_i, e'_i \rangle|^2 \\ &= 1 - \sum_{i=1}^N \rho_i |\langle x_i, P_H e'_i \rangle|^2 = P_e(\{P_H e'_i\}_{i=1}^N). \end{aligned}$$

It remains to show that $P_e(\{e_i\}_{i=1}^N) = P_e(\{e'_i\}_{i=1}^N)$. By Proposition 3.2, $\{P_H e'_i\}_{i=1}^N$ is a 1-tight frame for H . Thus, by the definition of the set $\{e_i\}_{i=1}^N \subseteq H$, it follows that

$$P_e(\{e'_i\}_{i=1}^N) = P_e(\{P_H e'_i\}_{i=1}^N) \geq P_e(\{e_i\}_{i=1}^N).$$

Now, by Naimark's theorem, there exists an orthonormal basis $\{y_i\}_{i=1}^N \subseteq H'$ such that

$$\{P_H y_i\}_{i=1}^N = \{e_i\}_{i=1}^N.$$

Hence, we have

$$\begin{aligned} P_e(\{e_i\}_{i=1}^N) &= 1 - \sum_{i=1}^N \rho_i |\langle x_i, e_i \rangle|^2 = 1 - \sum_{i=1}^N \rho_i |\langle x_i, P_H y_i \rangle|^2 \\ &= 1 - \sum_{i=1}^N \rho_i |\langle P_H x_i, y_i \rangle|^2 = 1 - \sum_{i=1}^N \rho_i |\langle x_i, y_i \rangle|^2 \\ &= P_e(\{y_i\}_{i=1}^N) \geq P_e(\{e'_i\}_{i=1}^N), \end{aligned}$$

where the last inequality follows from the definition of the set $\{e'_i\}_{i=1}^N \subseteq H'$. The result follows. \square

We conclude that finding an N element 1-tight frame $\{e_i\}_{i=1}^N$ for H that minimizes P_e over all N element 1-tight frames is equivalent to finding an orthonormal basis $\{e'_i\}_{i=1}^N$ for H' that minimizes P_e over all orthonormal bases for H' . Once we find $\{e'_i\}_{i=1}^N \subseteq H'$ that minimizes P_e , we project back onto H , and $\{P_H e'_i\}_{i=1}^N$ is a 1-tight frame for H that minimizes P_e over all N element 1-tight frames.

Consequently, the frame optimization problem can be stated in the following way.

Problem 3.4. Let H be a d -dimensional Hilbert space, and let $\{x_i\}_{i=1}^N \subseteq H$ be a sequence of unit norm vectors with a sequence $\{\rho_i\}_{i=1}^N \subseteq \mathbb{R}$ of positive weights that sums to 1. Assume $N \geq d$. Let H' be an N -dimensional Hilbert space such that H is a linear subspace of H' . The frame optimization problem is to find an orthonormal basis $\{e'_i\}_{i=1}^N \subseteq H'$ that minimizes P_e over all N element orthonormal sets in H' .

Using the definition of the frame force in Section 2.3, the frame optimization problem can now be given a classical mechanical interpretation in the case where $H = \mathbb{R}^d$. This interpretation motivates our approach in Section 4. Let $H \subseteq H' = \mathbb{R}^N$. We want to find an orthonormal basis $\{e'_i\}_{i=1}^N \subseteq H'$ that minimizes P_e over all orthonormal bases in H' . We consider the quantity P_e as a potential

$$V = P_e = \sum_{i=1}^N \rho_i (1 - |\langle x_i, e'_i \rangle|^2) = \sum_{i=1}^N V_i,$$

where each

$$V_i = \rho_i (1 - \langle x_i, e'_i \rangle^2) = \rho_i \left(1 - \left(1 - \frac{1}{2} \|x_i - e'_i\|^2 \right)^2 \right),$$

and where we have used the fact that $\|x_i\| = \|e'_i\| = 1$ as well as the relation

$$\|x_i - e'_i\|^2 = \langle x_i - e'_i, x_i - e'_i \rangle = \|x_i\|^2 - 2\langle x_i, e'_i \rangle + \|e'_i\|^2 = 2 - 2\langle x_i, e'_i \rangle.$$

Since each V_i is a function of the distance $\|x_i - e'_i\|$, V_i corresponds to a conservative central force between the points x_i and e'_i given by $F_i = -\nabla_i V_i$, where ∇_i is an N -dimensional gradient taken by keeping x_i fixed and differentiating with respect to the variable e'_i . Setting $x = \|x_i - e'_i\|$, we can write

$$V_i(x_i, e'_i) = v_i(\|x_i - e'_i\|) = \rho_i \left[1 - \left(1 - \frac{1}{2} x^2 \right)^2 \right].$$

Taking the derivative with respect to x gives

$$v'_i(x) = -2\rho_i \left(1 - \frac{1}{2} x^2 \right) (-x) = 2\rho_i \left(1 - \frac{1}{2} x^2 \right) x = -x f_i(x),$$

so that

$$f_i(x) = -2\rho_i \left(1 - \frac{1}{2}x^2\right).$$

Therefore, the corresponding central force can be written as

$$F_i(x_i, e'_i) = f_i(\|x_i - e'_i\|)(x_i - e'_i) = -2\rho_i \left(1 - \frac{1}{2}\|x_i - e'_i\|^2\right) (x_i - e'_i) = -2\rho_i \langle x_i, e'_i \rangle (x_i - e'_i).$$

F_i is frame force!

Thus, the setup for the frame optimization problem can be viewed as a physical system, where the given vectors $\{x_i\}_{i=1}^N$ are fixed points on the unit sphere in H' ; and we have a "rigid" orthonormal basis $\{e'_i\}_{i=1}^N$ which moves according to the frame force F_i between each e'_i and x_i . The problem is to find the equilibrium set $\{\bar{e}'_i\}_{i=1}^N$. These are the points where all the forces F_i balance and produce no net motion. In this situation, the potential V obtains an extreme value, and, in particular, we shall consider the case in which V is minimized.

4. SOLUTION OF FRAME OPTIMIZATION PROBLEM

4.1. Differential equations on $O(N)$. Using Newton's equation and the orthogonal group $O(N)$, we produce a system of differential equations associated with the setup of Section 3.

Let $\{b_i\}_{i=1}^N$ be a fixed orthonormal basis for H' . Since $O(N)$ is a smooth compact $N(N-1)/2$ -dimensional manifold [51], there exists a finite number of open sets U_k , $k = 1, \dots, M$, in $\mathbb{R}^{N(N-1)/2}$ and smooth mappings $\Theta_k : U_k \rightarrow O(N)$, $k = 1, \dots, M$, such that

$$\bigcup_{k=1}^M \Theta_k(U_k) = O(N).$$

Since any two orthonormal bases are related by an orthogonal transformation, then, for each $k = 1, \dots, M$, we can smoothly parameterize the orthonormal basis $\{b_i\}_{i=1}^N$ in terms of $N(N-1)/2$ real variables $(q_1, \dots, q_{N(N-1)/2}) \in U_k$ by the rule

$$\{e'_i(q_1, \dots, q_{N(N-1)/2})\}_{i=1}^N = \{\Theta_k(q_1, \dots, q_{N(N-1)/2})b_i\}_{i=1}^N,$$

which defines a family of orthonormal bases $\{e'_i\}_{i=1}^N$ for H' . As k goes from 1 to M , we obtain all possible orthonormal bases in H' . We now use Newton's equation to convert the frame forces F_i , $i = 1, \dots, N$, acting on an orthonormal basis $\{e'_j\}_{j=1}^N$ for H' into a set of differential equations that determines the dynamics of coordinate functions $q(t) = (q_1(t), \dots, q_{N(N-1)/2}(t)) \in [C^2(\mathbb{R})]^{N(N-1)/2}$.

We treat P_e as a potential and use Newton's equation to obtain

$$\ddot{q}(t) = -\nabla V = -\nabla P_e(q(t)) \Rightarrow \begin{pmatrix} \ddot{q}_1(t) \\ \vdots \\ \ddot{q}_{N(N-1)/2}(t) \end{pmatrix} = - \begin{pmatrix} \frac{\partial P_e}{\partial q_1}(q(t)) \\ \vdots \\ \frac{\partial P_e}{\partial q_{N(N-1)/2}}(q(t)) \end{pmatrix},$$

where $V = P_e$. Note that

$$\begin{aligned} -\frac{\partial V}{\partial q_j} &= -\frac{\partial}{\partial q_j} \sum_{i=1}^N V_i \\ &= -\sum_{i=1}^N \nabla V_i \cdot \frac{\partial e'_i}{\partial q_j} = 2 \sum_{i=1}^N \rho_i \langle x_i, e'_i \rangle (e'_i - x_i) \cdot \frac{\partial e'_i}{\partial q_j} \\ &= 2 \sum_{i=1}^N \rho_i \langle x_i, e'_i \rangle \left\langle e'_i, \frac{\partial e'_i}{\partial q_j} \right\rangle - 2 \sum_{i=1}^N \rho_i \langle x_i, e'_i \rangle \left\langle x_i, \frac{\partial e'_i}{\partial q_j} \right\rangle. \end{aligned}$$

Using the fact that $\langle e'_i, e'_i \rangle = 1$ and taking the derivative of this expression with respect to q_j give

$$\left\langle \frac{\partial}{\partial q_j} e'_i, e'_i \right\rangle + \left\langle e'_i, \frac{\partial}{\partial q_j} e'_i \right\rangle = 0.$$

Consequently,

$$\left\langle \frac{\partial}{\partial q_j} e'_i, e'_i \right\rangle = 0,$$

and we have

$$\frac{\partial V}{\partial q_j} = -2 \sum_{i=1}^N \rho_i \langle x_i, e'_i \rangle \left\langle x_i, \frac{\partial e'_i}{\partial q_j} \right\rangle.$$

Therefore, Newton's equation of motion becomes the $N(N-1)/2$ equations,

$$\ddot{q}_j(t) = -2 \sum_{i=1}^N \rho_i \langle x_i, e'_i \rangle \left\langle x_i, \frac{\partial e'_i}{\partial q_j} \right\rangle, \quad j = 1, \dots, N(N-1)/2. \quad (4.1)$$

By Theorem 2.1, it can be shown that if $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is a solution to (4.1), then the *energy*,

$$E(t) = \frac{1}{2} \sum_{i=1}^{N(N-1)/2} |\dot{q}_i(t)|^2 + P_e(q_1(t), \dots, q_{N(N-1)/2}(t)),$$

is a constant in time t .

We summarize the relationship between the parameterized orthogonal group and the solutions of Newton's equation in Figure 2. The analytic assertions of this relationship are the content of Theorems 4.1 and 4.2.

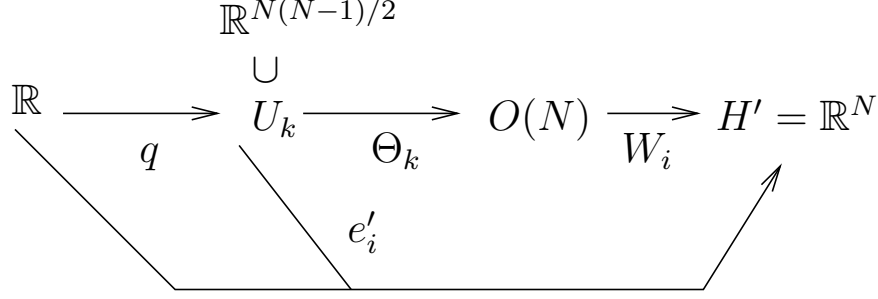


FIGURE 2. Relation between the orthogonal group and the solutions of Newton's equation of motion. W_i is defined for all $\theta \in O(N)$ by $W_i(\theta) = \theta b_i \in \mathbb{R}^N$.

Theorem 4.1. *Let H be a d -dimensional Hilbert space, and let $\{x_i\}_{i=1}^N \subseteq H$ be a sequence of unit norm vectors with a sequence $\{\rho_i\}_{i=1}^N \subseteq \mathbb{R}$ of positive weights that sums to 1. Assume $\{\bar{e}'_i\}_{i=1}^N$ is an orthonormal basis that minimizes P_e . Let $\Theta_k(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}) \in O(N)$ have the property that*

$$\forall i = 1, \dots, N, \quad e'_i(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}) = \bar{e}'_i.$$

Then the constant function,

$$(q_1(t), \dots, q_{N(N-1)/2}(t)) = (\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}), \quad (4.2)$$

is a solution of Newton's equation of motion in $O(N)$ that minimizes the energy E , and

$$\forall j = 1, \dots, N(N-1)/2, \quad \sum_{i=1}^N \rho_i \langle x_i, e'_i(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}) \rangle \left\langle x_i, \frac{\partial e'_i}{\partial q_j}(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}) \right\rangle = 0. \quad (4.3)$$

Proof. First, since $\{e'_i\}_{i=1}^N$ minimizes P_e at the point $(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2})$, we must have

$$\forall j = 1, \dots, N(N-1)/2, \quad \frac{\partial P_e}{\partial q_j}(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}) = 0.$$

Since

$$\frac{\partial P_e}{\partial q_j} = \sum_{i=1}^N \rho_i \langle x_i, e'_i \rangle \left\langle x_i, \frac{\partial e'_i}{\partial q_j} \right\rangle$$

we have (4.3).

Second, we show that (4.2) is a solution of Newton's equation. Because $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is constant with respect to t , we have

$$\begin{aligned} \ddot{q}_i(t) &= 0 = -2 \frac{\partial P_e}{\partial q_j}(q_1, \dots, q_{N(N-1)/2}) \\ &= -2 \sum_{i=1}^N \rho_i \langle x_i, e'_i(q_1(t), \dots, q_{N(N-1)/2}(t)) \rangle \left\langle x_i, \frac{\partial e'_i}{\partial q_j}(q_1(t), \dots, q_{N(N-1)/2}(t)) \right\rangle. \end{aligned}$$

Therefore, $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is a solution of Newton's equation.

Finally, for each $i = 1, \dots, N(N-1)/2$, we have $\dot{q}_i(t) = 0$, and so the energy E satisfies

$$E = P_e.$$

Since $e'_i(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2})$ minimizes P_e , it follows that the energy is minimized. \square

The following theorem relates the solutions of Newton's equation with the frame optimization problem.

Theorem 4.2. *Given the hypotheses of Theorem 4.1. Let $(q_1(t), \dots, q_{N(N-1)/2}(t))$ be a solution of Newton's equation of motion that minimizes the energy E . Then $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is a constant solution, i.e.,*

$$\forall i = 1, \dots, N(N-1)/2, \quad \frac{dq_i}{dt}(t) = 0,$$

and

$$\{P_H e'_i(q_1(t), \dots, q_{N(N-1)/2}(t))\}_{i=1}^N \subseteq H$$

is a 1-tight frame for H that minimizes P_e .

Proof. Suppose $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is a solution of Newton's equations of motion that minimizes the energy E . Assume that $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is not a constant solution. Denote by $(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2})$ a point from Theorem 4.1 such that

$$\{e'_i(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2})\}_{i=1}^N$$

is an orthonormal basis that minimizes P_e . Since $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is not a constant solution, there exists a $t_0 \in \mathbb{R}$ such that the kinetic energy

$$T = \frac{1}{2} \sum_{i=1}^{N(N-1)/2} |\dot{q}_i(t_0)|^2 \neq 0,$$

and, by Theorem 2.1, the energy is constant. Thus, for all t , we have

$$\begin{aligned} E(q_1(t), \dots, q_{N(N-1)/2}(t)) &= T(q_1(t_0), \dots, q_{N(N-1)/2}(t_0)) + P_e(q_1(t_0), \dots, q_{N(N-1)/2}(t_0)) \\ &> P_e(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}) = E(\tilde{q}_1, \dots, \tilde{q}_{N(N-1)/2}), \end{aligned}$$

which contradicts the assumption that $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is a solution that minimizes the energy E . It follows that $(q_1(t), \dots, q_{N(N-1)/2}(t))$

must be a constant solution. Hence, $T = 0$, and so $(q_1(t), \dots, q_{N(N-1)/2}(t))$ minimizes $E = P_e$. By Theorem 3.3 it follows that

$$\{P_H e'_i(q_1(t), \dots, q_{N(N-1)/2}(t))\}_{i=1}^N \subseteq H$$

is a 1-tight frame for H that minimizes P_e . \square

4.2. Parameterization on $SO(N)$. Let $\{b_i\}_{i=1}^N$ be a fixed orthonormal basis for H' . We can locally parameterize the elements in $O(N)$ by $N(N-1)/2$ variables so that $\theta(q_1, \dots, q_{N(N-1)/2}) \in O(N)$. We obtain a smooth parameterization of $\{b_i\}_{i=1}^N$ by setting

$$\forall i = 1, \dots, N, \quad e'_i(q_1, \dots, q_{N(N-1)/2}) = \theta(q_1, \dots, q_{N(N-1)/2})b_i. \quad (4.4)$$

$O(N)$ has two connected components, $SO(N)$ and $G(N) = O(N) \setminus SO(N)$. The parameterization (4.4) depends on the choice of which component, $SO(N)$ or $G(N)$, we find or choose $\theta(q_1, \dots, q_{N(N-1)/2})$.

Lemma 4.3. *Let $\{b_i\}_{i=1}^N$ be a fixed orthonormal basis for an N -dimensional Hilbert space H' , and let $\xi : H' \rightarrow H'$ denote the linear transformation defined by*

$$\xi(b_i) = \begin{cases} -b_i, & \text{if } i = 1 \\ b_i, & \text{if } N > i > 1. \end{cases}$$

Define the function $g : SO(N) \rightarrow G(N)$ by

$$\forall \theta \in SO(N), \quad g(\theta) = \theta \cdot \xi.$$

Then g is a bijection.

Proof. For all $\theta \in SO(N)$, it is clear that $g(\theta) \in G(N)$ since

$$\det(\theta) = 1 \Rightarrow \det(g(\theta)) = \det(\theta \cdot \xi) = \det(\theta) \cdot \det(\xi) = -1 \Rightarrow g(\theta) \in G(N).$$

With respect to the basis $\{b_i\}_{i=1}^N$, we can write ξ as

$$\xi = \begin{bmatrix} -1 & 0 & & & \\ 0 & 1 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}.$$

Thus, ξ is invertible, and hence injective. The surjectivity is elementary to check, and so g is a bijection. \square

Theorem 4.4. *Let $\{b_i\}_{i=1}^N$ be a fixed orthonormal basis for the real N -dimensional Hilbert space H' , and let $\{x_i\}_{i=1}^N \subseteq H'$ be a sequence of unit normed vectors with a sequence $\{\rho_i\}_{i=1}^N \subseteq \mathbb{R}$ of positive weights that sums to 1. Consider the error function $P_e : O(N) \rightarrow \mathbb{R}$ defined by*

$$\forall \theta \in O(N), \quad P(\theta) = 1 - \sum_{i=1}^N \rho_i |\langle x_i, \theta b_i \rangle|^2.$$

Since $SO(N)$ is compact and P is continuous on $O(N)$, there exists $\theta' \in SO(N)$ such that

$$\forall \theta \in SO(N), \quad P(\theta') \leq P(\theta).$$

Similarly, since $G(N)$ is compact, there exists $\theta'' \in G(N)$ such that

$$\forall \theta \in G(N), \quad P(\theta'') \leq P(\theta).$$

Then,

$$P(\theta') = P(\theta'').$$

Proof. First, note that, for any $\theta \in SO(N)$,

$$\begin{aligned} P(g(\theta)) &= 1 - \sum_{i=1}^N \rho_i |\langle x_i, g(\theta)b_i \rangle|^2 \\ &= 1 - \sum_{i=1}^N \rho_i |\langle x_i, \theta \cdot \xi b_i \rangle|^2 \\ &= 1 - \rho_1 |\langle x_1, \theta(-b_1) \rangle|^2 - \sum_{i=2}^N \rho_i |\langle x_i, \theta b_i \rangle|^2 \\ &= 1 - \rho_1 |\langle x_1, \theta(b_1) \rangle|^2 - \sum_{i=2}^N \rho_i |\langle x_i, \theta b_i \rangle|^2 \\ &= P(\theta). \end{aligned}$$

We complete the proof by contradiction. Suppose that $P(\theta') \neq P(\theta'')$. Consider the case that $P(\theta'') > P(\theta')$. Then $g(\theta') \in G(N)$ has the property that $P(\theta'') > P(\theta') = P(g(\theta'))$ which contradicts the definition of $\theta'' \in G(N)$. A similar argument works for the case with $P(\theta'') < P(\theta')$ by considering the function $g^{-1} : G(N) \rightarrow SO(N)$. \square

By the above theorem, it suffices to do the parameterization in our analysis over $SO(N)$.

4.3. Friction. Since our force is conservative, the energy $E(t)$ for the solutions of Newton's equation is a constant function. If these solutions are not minimum energy solutions, it is possible that if we add a friction term to the original equations, then the new set of solutions may converge to a minimum energy solution. These modified equations of motion with friction are

$$\forall j = 1, \dots, N(N-1)/2, \quad \ddot{q}_j + \frac{\partial P_\epsilon}{\partial q_j} = -\dot{q}_j. \quad (4.5)$$

Theorem 4.5. *Assume that $(q_1(t), \dots, q_{N(N-1)/2}(t))$ is a solution to the modified equations of motion (4.5). The energy E satisfies*

$$\frac{d}{dt} E(t) = - \sum_{i=1}^{N(N-1)/2} \dot{q}_i(t)^2. \quad (4.6)$$

Proof. Multiplying the modified equations of motion (4.5) by \dot{q}_j and summing over j give

$$\sum_{j=1}^{N(N-1)/2} \left[\ddot{q}_j + \frac{\partial P_e}{\partial q_j} \right] \dot{q}_j = - \sum_{j=1}^{N(N-1)/2} \dot{q}_j^2.$$

The first term on the left side is

$$\sum_{j=1}^{N(N-1)/2} \ddot{q}_j \dot{q}_j = \frac{d}{dt} \frac{1}{2} \sum_{j=1}^{N(N-1)/2} [\dot{q}_j]^2,$$

and the second term on the left side is

$$\sum_{j=1}^{N(N-1)/2} \frac{\partial P_e}{\partial q_j} \dot{q}_j = \frac{dP_e}{dt}.$$

Therefore, we have

$$\frac{d}{dt} E(t) = \frac{d}{dt} \left(\frac{1}{2} \sum_{j=1}^{N(N-1)/2} [\dot{q}_j(t)]^2 + P_e(q(t)) \right) = - \sum_{j=1}^{N(N-1)/2} \dot{q}_j(t)^2,$$

and this is (4.6). \square

4.4. Numerical considerations. Recall that Theorem 4.1 states that the minimum energy solutions satisfy

$$\sum_{i=1}^N \rho_i \langle x_i, e_i(q(t)) \rangle \left\langle x_i, \frac{\partial e_i}{\partial q_j}(q(t)) \right\rangle = 0. \quad (4.7)$$

This opens the problem to numerical approximations. For example a multi-dimensional Newton iteration can be used to approximate these $(q_1, \dots, q_{N(N-1)/2})$ that satisfy (4.7). Furthermore, the error P_e can now be considered as a smooth function of the variables $q = (q_1, \dots, q_{N(N-1)/2})$, i.e.,

$$P_e(q) = 1 - \sum_{i=1}^N \rho_i |\langle x_i, e_i(q) \rangle|^2. \quad (4.8)$$

As such, other numerical methods become available. For example, the conjugate gradient method can be used to approximate a 1-tight frame that minimizes P_e as written in (4.8), see [41] for this and for the implementation of multidimensional Newton iteration.

The modified equations with friction, viz., (4.5), give a method of taking a tight frame with a particular detection error and constructing another tight frame with a smaller detection error. Let $\{b_i\}_{i=1}^N$ be a fixed orthonormal basis for an N -dimensional Hilbert space H' . Suppose we have a 1-tight frame $\{e_i\}_{i=1}^N$ for the d -dimensional Hilbert space H with a given error, and we want to find another 1-tight frame with a smaller error. Let $\{e'_i\}_{i=1}^N$ be

the orthonormal basis for H' obtained from $\{e_i\}_{i=1}^N$ by Naimark's theorem, and let $\Theta(q_1, \dots, q_{N(N-1)/2})$ be a local parameterization of $SO(N)$ such that

$$\{\Theta(0, \dots, 0)b_i\}_{i=1}^N = \{e'_i\}_{i=1}^N.$$

Assume $q(t)$ is a solution of the modified equations of motion with friction, viz., (4.5), with initial conditions

$$q(0) = \dot{q}(0) = 0.$$

If q is not a constant solution then, by Theorem 4.5, for all $t > 0$ where the solution is defined, we obtain that

$$\{P_H \Theta(q(t))b_i\}_{i=1}^N$$

is a 1-tight frame with a smaller detection error than that associated with $\{e'_i\}_{i=1}^N$. In this case, there are numerical methods available for approximating the solution q , and, hence, leading to the construction of 1-tight frame minimizers. For example, one can use a Runge-Kutta method, see [41].

It is possible that the parametrized error $P_e(q)$ has many local minima. Conjugate gradient methods applied to the original equations (4.1) (as previously mentioned) and solutions to the modified equations of motion (4.5) can be used to determine these minima. It seems natural that simulated annealing global minimization algorithms [42] can be used to refine our local minimization technique.

It should be pointed out that numerical methods have been developed, using semidefinite programming [26], to approximate tight frames that solve a *modified* quantum detection problem. As far as the actual quantum detection problem, a matricial iterative scheme has been developed [21], which can be considered as an alternative to our approach. Our analysis, using concepts inspired by geometry and classical physics, can be generalized to approximate tight frames that minimize other types of error terms, see [41]. There has been analogous work using ideas from classical mechanics to develop numerical methods that approximate solutions for a variety of other mathematical problems, e.g., see [34, 35, 48, 36].

5. EXAMPLE FOR $N = 2$

Consider the case where we are given $\{x_i\}_{i=1}^2 \subseteq H = \mathbb{R}^2$ with a sequence $\{\rho_i\}_{i=1}^2$ of positive weights that sum to 1.

We want to find an orthonormal system $\{e'_i\}_{i=1}^2$ that minimizes P_e . $SO(2)$ is a 1-dimensional manifold. A parameterization of $SO(2)$ can be given for all $q \in [0, 2\pi)$:

$$\Theta(q) = \begin{pmatrix} \cos(q) & -\sin(q) \\ \sin(q) & \cos(q) \end{pmatrix}.$$

Let $\{b_i\}_{i=1}^2$ be the standard orthonormal basis for $H = \mathbb{R}^2$. We construct the parameterized orthonormal set by defining

$$e'_1(q) = \Theta(q)b_1 = \begin{pmatrix} \cos(q) \\ \sin(q) \end{pmatrix}, \quad e'_2(q) = \Theta(q)b_2 = \begin{pmatrix} -\sin(q) \\ \cos(q) \end{pmatrix}.$$

Now, assume q is a function of time. We have

$$\frac{d}{dq} e'_1(q(t)) = \frac{d}{dq} \begin{pmatrix} \cos(q(t)) \\ \sin(q(t)) \end{pmatrix} = \begin{pmatrix} -\sin(q(t)) \\ \cos(q(t)) \end{pmatrix} = e'_2(q(t)),$$

and

$$\frac{d}{dq} e'_2(q(t)) = \frac{d}{dq} \begin{pmatrix} -\sin(q(t)) \\ \cos(q(t)) \end{pmatrix} = \begin{pmatrix} -\cos(q(t)) \\ -\sin(q(t)) \end{pmatrix} = -e'_1(q(t)).$$

Substituting these derivatives of e'_i into Newton's equation of motion (4.1) give

$$\ddot{q}(t) = 2[\rho_2 \langle x_2, e'_2(q(t)) \rangle \langle x_2, e'_1(q(t)) \rangle - \rho_1 \langle x_1, e'_1(q(t)) \rangle \langle x_1, e'_2(q(t)) \rangle],$$

which is a second-order ordinary differential equation.

In \mathbb{R}^2 , the minimizer can be explicitly found. To this end and to simplify the notation, we begin by writing

$$e'_i = e'_i(q(t)) \text{ and } q = q(t).$$

Next, denote the given vectors by

$$x_1 = \begin{pmatrix} a \\ b \end{pmatrix} \text{ and } x_2 = \begin{pmatrix} c \\ d \end{pmatrix}.$$

As such, we obtain

$$\begin{aligned} \sum_{i=1}^2 \rho_i \langle e'_i, x_i \rangle^2 &= \rho_1 (a \cos(q) + b \sin(q))^2 + \rho_2 (-c \sin(q) + d \cos(q))^2 \\ &= (\rho_1 a^2 + \rho_2 d^2) \cos^2(q) + 2(\rho_1 ab - \rho_2 cd) \cos(q) \sin(q) + (\rho_1 b^2 + \rho_2 c^2) \sin^2(q) \\ &= (\rho_1 a^2 + \rho_2 d^2 - \rho_1 b^2 - \rho_2 c^2) \cos^2(q) + 2(\rho_1 ab - \rho_2 cd) \cos(q) \sin(q) + (\rho_1 b^2 + \rho_2 c^2) \\ &= \alpha \cos^2(q) + \beta \cos(q) \sin(q) + \gamma, \end{aligned}$$

where

$$\begin{aligned} \alpha &= (\rho_1 a^2 + \rho_2 d^2 - \rho_1 b^2 - \rho_2 c^2) \\ \beta &= 2(\rho_1 ab - \rho_2 cd) \\ \gamma &= (\rho_1 b^2 + \rho_2 c^2). \end{aligned}$$

Hence, we have

$$\begin{aligned} \sum_{i=1}^2 \rho_i \langle e'_i, x_i \rangle^2 &= \cos(q) [\alpha \cos(q) + \beta \sin(q)] + \gamma \\ &= \sqrt{\alpha^2 + \beta^2} \cos(q) [\cos(\xi) \cos(q) + \sin(\xi) \sin(q)] + \gamma, \end{aligned}$$

where $\xi \in [0, 2\pi)$ has the property that

$$\cos(\xi) = \frac{\alpha}{\sqrt{\alpha^2 + \beta^2}}, \quad \sin(\xi) = \frac{\beta}{\sqrt{\alpha^2 + \beta^2}}.$$

Using the relation $\cos(A)\cos(A+B) = \frac{1}{2}[\cos(2A+B) + \cos(B)]$, we compute

$$\begin{aligned} \sum_{i=1}^2 \rho_i \langle e'_i, x_i \rangle^2 &= \sqrt{\alpha^2 + \beta^2} \cos(q) [\cos(\xi) \cos(q) + \sin(\xi) \sin(q)] + \gamma \\ &= \sqrt{\alpha^2 + \beta^2} \cos(q) [\cos(q - \xi)] + \gamma \\ &= \frac{\sqrt{\alpha^2 + \beta^2}}{2} [\cos(2q - \xi) + \cos(\xi)] + \gamma. \end{aligned}$$

Therefore, to minimize the error P_e , we want to maximize $\sum_{i=1}^2 \rho_i \langle x_i, e'_i \rangle^2$, and this occurs exactly when $q = \xi/2 + \pi n$ for some integer n . Consequently, we can write our solution as

$$q = \frac{1}{2} \tan^{-1} \left(\frac{2(\rho_1 ab - \rho_2 cd)}{(\rho_1 a^2 + \rho_2 d^2 - \rho_1 b^2 - \rho_2 c^2)} \right) + \pi n$$

for some $n \in \mathbb{N}$.

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APPENDIX A. APPENDIX

A.1. Quantum measurement theory. Quantum theory gives the probability that a measured outcome lies in a specified region [38, 58, 11], see Definition A.4. These probabilities are defined in terms of positive operator-valued measures.

Definition A.1. Let \mathcal{B} be a σ -algebra of sets of X , and let H be a separable Hilbert space. A *positive operator-valued measure* (POM) is a function $\Pi : \mathcal{B} \rightarrow \mathcal{L}(H)$ such that:

1. $\forall U \in \mathcal{B}$, $\Pi(U)$ is a positive self-adjoint operator $H \rightarrow H$,
2. $\Pi(\emptyset) = 0$ (zero operator),
3. \forall disjoint $\{U_i\}_{i=1}^{\infty} \subseteq \mathcal{B}$, $x, y \in H \Rightarrow \left\langle \Pi \left(\bigcup_{i=1}^{\infty} U_i \right) x, y \right\rangle = \sum_{i=1}^{\infty} \langle \Pi(U_i) x, y \rangle$,
4. $\Pi(X) = I$ (identity operator).

Every dynamical quantity in quantum mechanics, e.g., the energy or momentum of a particle, corresponds to a space of outcomes X and a POM Π . We think of X as the space of all possible values the dynamical quantity can attain. X could be countable or uncountable.

- Example A.2.** (1) Suppose we wanted to measure the energy of a hydrogen atom. The energy levels of a hydrogen atom are discrete, and X consists of all the possible discrete energy levels. Hence, X is countable. In this case, $H = L^2(\mathbb{R}^3)$ and \mathcal{B} is the power set of X .
- (2) On the other hand, if we were measuring the position of an electron orbiting its nucleus, then X is the space of all possible spatial locations of the electron, i.e., $X = \mathbb{R}^3$ which is uncountable. In this case, $H = L^2(\mathbb{R}^3)$ and \mathcal{B} is the Borel algebra of \mathbb{R}^3 .

See [33, 58] for discussions of the notion of the state of a system and the model of physical systems in terms of Hilbert spaces.

Definition A.3. Given a separable Hilbert space H , a measurable space (\mathcal{B}, X) , and a POM Π . If the state of the system is given by $x \in H$ with $\|x\| = 1$, then the *probability that the measured outcome lies in a region* $U \in \mathcal{B}$ is defined by

$$P_{\Pi}(U) = \langle x, \Pi(U)x \rangle.$$

This definition can be viewed as that of a *POM measurement*, cf., [27] for an alternative definition.

Typically in quantum mechanics, measurements are modeled using resolutions of the identity [52, 33, 22]. Using POMs in the theory of quantum measurement instead of traditional resolutions of the identity have some advantages. For example, in some situations, using a POM measurement decreases the likelihood of making a measurement error [50]. Also, the foundation of quantum encryption, where messages cannot be intercepted by an eavesdropper, is based on the theory of POM measurements [10]. Physical realizations of POM measurements can be found in [13, 12].

A.2. Quantum mechanical quantum detection. We define the quantum detection problem as given in [25, 24].

Suppose we have a separable Hilbert space H corresponding to a physical system, but that we cannot determine beforehand the state of the physical system. However, suppose we do know that the state of the system must be in one of a countable set $\{x_i\}_{i \in K} \subseteq H$ (where $K \subseteq \mathbb{Z}$) of possible unit normed states with corresponding sequence $\{\rho_i\}_{i \in K}$ of probabilities that sum to 1. By this we mean that ρ_i is the probability that the system is in the state x_i . The *problem* is to determine the state of the system, and the only way to do this is to perform a measurement. Consequently, the problem is to construct a POM Π with outcomes $X = K$ with the property that if the state of the system is x_i for some $i \in K$, then the measurement asserts that the system is in the i th state with high probability

$$P(j) = \langle x_i, \Pi(j)x_i \rangle \approx \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$

If the state of the system is x_i , then $\langle x_i, \Pi(j)x_i \rangle$ is the probability that the measuring device outputs j . Thus, $\langle x_i, \Pi(i)x_i \rangle$ is the probability of a

correct measurement. Since each x_j occurs with probability ρ_j , the average probability of a correct measurement is

$$\mathcal{E}(\text{correct}) = \mathcal{E}(\{\langle x_i, \Pi(i)x_i \rangle\}_{i \in K}) = \sum_{i \in K} \rho_i \langle x_i, \Pi(i)x_i \rangle.$$

Quite naturally, the *probability of a detection error*, i.e., the average probability that the measurement is incorrect, is given by

$$P_e = 1 - \sum_{i \in K} \rho_i \langle x_i, \Pi(i)x_i \rangle. \quad (\text{A.1})$$

Hence, we want to construct a POM Π that minimizes P_e , and this is the quantum mechanical *quantum detection problem* corresponding to Problems 1.2 and 3.4.

A.3. A closer look at the quantum detection error. We shall verify our assertion in Section A.2 that P_e , defined by (A.1), is the average of the probabilities of incorrect measurements. If the state of the system is x_i for some $i \in K$ and if $i \neq j$, then $\langle x_i, \Pi(j)x_i \rangle$ is the probability that we incorrectly measure the system to be x_j , an incorrect measurement. Thus, the average probability of an incorrect measurement is given by

$$\mathcal{E}(\text{incorrect}) = \mathcal{E}(\{\langle x_i, \Pi(j)x_i \rangle\}_{i \neq j}) = \sum_{i \neq j} \rho_i \langle x_i, \Pi(j)x_i \rangle.$$

We want to show that $P_e = \mathcal{E}(\text{incorrect})$. To verify this, note that

$$\begin{aligned} \sum_{i \neq j} \rho_i \langle x_i, \Pi(j)x_i \rangle + \sum_{i \in K} \rho_i \langle x_i, \Pi(i)x_i \rangle &= \sum_{i, j \in K} \rho_i \langle x_i, \Pi(j)x_i \rangle = \sum_{i \in K} \rho_i \left\langle x_i, \sum_{j \in K} \Pi(j)x_i \right\rangle \\ &= \sum_{i \in K} \rho_i \langle x_i, Ix_i \rangle = \sum_{i \in K} \rho_i = 1. \end{aligned}$$

Therefore,

$$P_e = 1 - \sum_{i \in K} \rho_i \langle x_i, \Pi(i)x_i \rangle = \sum_{i \neq j} \rho_i \langle x_i, \Pi(j)x_i \rangle = \mathcal{E}(\text{incorrect}).$$

A.4. Using tight frames to construct POMs. The theory of tight frames can be used to construct POMs. Let H be a separable Hilbert space and let $K \subseteq \mathbb{Z}$. Assume $\{e_i\}_{i \in K} \subseteq H$ is a 1-tight frame for H . Define a family $\{\Pi(w)\}_{w \subseteq K}$ of self-adjoint positive operators on H by the formula,

$$\forall x \in H, \quad \Pi(w)x = \sum_{i \in w} \langle x, e_i \rangle e_i.$$

It is clear that this family of operators satisfies conditions 1-3 of the definition of a POM. Since $\{e_i\}_{i \in K}$ is a 1-tight frame, we also have

$$\forall x \in H, \quad \Pi(K)x = \sum_{i \in K} \langle x, e_i \rangle e_i = x,$$

and so condition 4 is satisfied, where $X = K$. Thus, Π , constructed in this manner, is a POM.

Remark A.4. In this case, the detection error P_e becomes

$$\begin{aligned} P_e &= 1 - \sum_{i \in K} \rho_i \langle x_i, \Pi(i)x_i \rangle \\ &= 1 - \sum_{i \in K} \rho_i \langle x_i, \langle e_i, x_i \rangle e_i \rangle \\ &= 1 - \sum_{i \in K} \rho_i |\langle x_i, e_i \rangle|^2. \end{aligned} \tag{A.2}$$

Thus the quantum mechanical quantum detection problem reduces to finding a 1-tight frame that minimizes the right side of (A.2); and this right side is the basic error term (1.1) of the frame optimization problem.

The following result is a converse of our construction of a POM (for the σ -algebra of all subsets of \mathbb{Z}) for a given 1-tight frame for H .

Theorem A.5. *Let H be a d -dimensional Hilbert space. Given a POM Π with a countable set X . There exists a subset $K \subseteq \mathbb{Z}$, a 1-tight frame $\{e_i\}_{i \in K}$ for H , and a disjoint partition $\{B_i\}_{i \in X} \subseteq \mathcal{B}$ of K such that*

$$\forall i \in X \text{ and } \forall x \in H, \quad \Pi(i)x = \sum_{j \in B_i} \langle x, e_j \rangle e_j.$$

Proof. For each $i \in X$, $\Pi(i)$ is self-adjoint and positive by definition (noting positive implies self-adjoint in the complex case). Thus, by the spectral theorem, for each $i \in X$, there exists an orthonormal set $\{v_j\}_{j \in B_i} \subseteq H$ and positive numbers $\{\lambda_j\}_{j \in B_i}$ such that

$$\forall x \in H, \quad \Pi(i)x = \sum_{j \in B_i} \lambda_j \langle x, v_j \rangle v_j = \sum_{j \in B_i} \langle x, e_j \rangle e_j,$$

where

$$\forall j \in B_i, \quad e_j = \sqrt{\lambda_j} v_j.$$

Since $\Pi(X) = I$ we have that

$$\forall x \in H, \quad x = \Pi(X)x = \sum_{j \in \cup_i B_i} \langle x, e_j \rangle e_j.$$

It follows that $\{e_j\}_{j \in K}$ is a 1-tight frame for H . \square

Consequently, if the Hilbert space H is finite-dimensional, analyzing quantum measurements with a discrete set X of outcomes reduces to analyzing tight frames.

Keeping in mind that we want to *construct* and *compute* solutions to the frame optimization problem, we now prove that solutions do in fact *exist*. The proof uses a compactness argument. We start with a lemma.

Lemma A.6. *Assume that $\{e_i\}_{i=1}^N$ is an A -tight frame for a d -dimensional Hilbert space H . Then,*

$$\forall i = 1, \dots, N, \quad \|e_i\| \leq \sqrt{A}.$$

Proof. Note that for any $1 \leq k \leq N$ we have

$$\begin{aligned} A\|e_k\|^2 &= \sum_{i=1}^N |\langle e_k, e_i \rangle|^2 \\ &= \|e_k\|^4 + \sum_{i \neq k} |\langle e_k, e_i \rangle|^2. \end{aligned}$$

Hence,

$$\|e_k\|^4 - A\|e_k\|^2 = - \sum_{i \neq k} |\langle e_k, e_i \rangle|^2 \leq 0,$$

and so

$$\|e_k\|^2 - A \leq 0. \quad \square$$

Theorem A.7. *Suppose H is a d -dimensional Hilbert space, and let $\{x_i\}_{i=1}^N \subseteq H$ be a sequence of vectors with a sequence $\{\rho_i\}_{i=1}^N \subseteq \mathbb{R}$ of positive numbers that sums to 1. There exists a 1-tight frame $\{e_i\}_{i=1}^N \subseteq H$ for H that minimizes the error*

$$P_e = 1 - \sum_{i=1}^N \rho_i |\langle x_i, e_i \rangle|^2,$$

where the minimization is taken over all 1-tight frames for H of N elements.

Proof. Let F be the set of all N element 1-tight frames. We can write this set as

$$F = \left\{ \{v_i\}_{i=1}^N \subseteq H : \sum_{i=1}^N v_i v_i^* = I \right\},$$

where $v^* : H \rightarrow \mathbb{K}$, $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$, is defined by

$$\forall x \in H, \quad v^* x = \langle x, v \rangle.$$

Also, for any set $\{u_i\}_{i=1}^N \subseteq H$, define the norm,

$$\|\{u_i\}_{i=1}^N\| = \sum_{i=1}^N \|u_i\|_H,$$

where $\|\cdot\|_H$ is the norm on H ; and define the operator norm for any $d \times d$ matrix M as

$$\|M\| = \sup_{\|v\|_H=1} \|Mv\|_H.$$

(We are using $\|\cdot\|_H$ to distinguish between other norms in this proof.)

We shall first verify that F is closed in H . Suppose we have a sequence $\{\{u_i^k\}_{i=1}^N\}_{k=1}^\infty \subseteq F$ such that

$$\lim_{k \rightarrow \infty} \|\{u_i^k\}_{i=1}^N - \{u_i\}_{i=1}^N\| = 0$$

for some set $\{u_i\}_{i=1}^N \subseteq H$. Then, given any $\epsilon > 0$, there exists a $k > 0$ such that $\|\{u_i^k\}_{i=1}^N - \{u_i\}_{i=1}^N\| < \epsilon$. To show $\{u_i\}_{i=1}^N \in F$ we begin with the estimate,

$$\begin{aligned}
\left\| \sum_{i=1}^N u_i u_i^* - I \right\| &= \left\| \sum_{i=1}^N u_i u_i^* - \sum_{i=1}^N u_i^k (u_i^k)^* \right\| + \left\| \sum_{i=1}^N u_i^k (u_i^k)^* - I \right\| \\
&= \left\| \sum_{i=1}^N u_i u_i^* - \sum_{i=1}^N u_i^k (u_i^k)^* \right\| \\
&= \sup_{\|v\|_H=1} \left\| \sum_{i=1}^N \langle v, u_i^k \rangle u_i^k - \langle v, u_i \rangle u_i \right\|_H \\
&\leq \sup_{\|v\|_H=1} \sum_{i=1}^N \|\langle v, u_i^k \rangle u_i^k - \langle v, u_i \rangle u_i\|_H \\
&\leq \sup_{\|v\|_H=1} \sum_{i=1}^N \left(\|\langle v, u_i^k \rangle u_i^k - \langle v, u_i^k \rangle u_i\|_H + \|\langle v, u_i^k \rangle u_i - \langle v, u_i \rangle u_i\|_H \right) \\
&= \sup_{\|v\|_H=1} \sum_{i=1}^N \left(|\langle v, u_i^k \rangle| \|u_i^k - u_i\|_H + |\langle v, u_i^k - u_i \rangle| \|u_i\|_H \right) \\
&\leq \sup_{\|v\|_H=1} \left(\|\{u_i^k\}_{i=1}^N - \{u_i\}_{i=1}^N\| \max_{1 \leq i \leq N} \|u_i^k\|_H + \|\{u_i^k\}_{i=1}^N - \{u_i\}_{i=1}^N\| \max_{1 \leq i \leq N} \|u_i^k\|_H \right) \\
&\leq 2\epsilon \max_{1 \leq i \leq N} \|u_i^k\|_H \leq 2\epsilon,
\end{aligned}$$

where in the last inequality, we used Lemma A.6 with $A = 1$. Since $\epsilon > 0$ is arbitrary, it follows that

$$\sum_{i=1}^N u_i u_i^* = I,$$

and hence $\{u_i\}_{i=1}^N \in F$. Thus, F is closed.

F is also bounded since, given any $\{u_i\}_{i=1}^N \in F$, we know by Lemma A.6 that

$$\|\{u_i\}_{i=1}^N\| = \sum_{i=1}^N \|u_i\|_H \leq N.$$

Let $\{x_i\}_{i=1}^N \subseteq H$ be the fixed sequence as given in the hypothesis, and define the function $f : F \rightarrow \mathbb{R}$, which depends on $\{x_i\}_{i=1}^N$, by

$$\forall \{e_i\}_{i=1}^N \in F, \quad f(\{e_i\}_{i=1}^N) = 1 - \sum_{i=1}^N \rho_i |\langle x_i, e_i \rangle|^2.$$

Given any $\{u_i\}_{i=1}^N, \{v_i\}_{i=1}^N \in F$, we have

$$\begin{aligned}
|f(\{v_i\}_{i=1}^N) - f(\{u_i\}_{i=1}^N)| &= \left| \sum_{i=1}^N \rho_i |\langle x_i, u_i \rangle|^2 - \sum_{i=1}^N \rho_i |\langle x_i, v_i \rangle|^2 \right| \\
&\leq \sum_{i=1}^N \rho_i \left| |\langle x_i, u_i \rangle|^2 - |\langle x_i, v_i \rangle|^2 \right| \\
&= \sum_{i=1}^N \rho_i (|\langle x_i, u_i \rangle| - |\langle x_i, v_i \rangle|)(|\langle x_i, u_i \rangle| + |\langle x_i, v_i \rangle|) \\
&\leq C \sum_{i=1}^N |\langle x_i, u_i \rangle - \langle x_i, v_i \rangle| \\
&= C \sum_{i=1}^N |\langle x_i, u_i - v_i \rangle| \\
&\leq C \sum_{i=1}^N \|x_i\|_H \|u_i - v_i\|_H \\
&\leq C \max_{1 \leq i \leq N} \|x_i\|_H \|\{u_i\}_{i=1}^N - \{v_i\}_{i=1}^N\|,
\end{aligned}$$

where, by Lemma A.6,

$$C = \max_{1 \leq i \leq N} \|x_i\|_H (\|u_i\|_H + \|v_i\|_H) \leq 2 \max_{1 \leq i \leq N} \|x_i\|_H.$$

Therefore, f is continuous on F . Since F is compact, it follows that there exists $\{e_i\}_{i=1}^N \in F$ that minimizes f . \square

A.5. MSE criterion. As mentioned earlier, some authors have solved a frame optimization problem using the MSE error. MSE error coincides with the quantum detection error P_e when the weights are all equal and the given vectors have an additional structure known as geometrical uniformity, see [23, 57, 29].

Definition A.8. Let $\mathcal{Q} = \{U_i\}_{i=1}^N$ be a finite Abelian group of N unitary linear operators on a Hilbert space H . A set $\{x_i\}_{i=1}^N \subseteq H$ is *geometrically uniform* if there exists an $x \in H$ such that

$$\{x_i\}_{i=1}^N = \{U_i x\}_{i=1}^N.$$

Definition A.9. Let H be a separable Hilbert space, let $K \subseteq \mathbb{Z}$, and let $\{x_i\}_{i \in K}$ be a frame for H . The associated *frame operator* is the mapping $S : H \rightarrow H$ defined by

$$\forall y \in H, \quad S(y) = \sum_{i \in K} \langle y, x_i \rangle x_i.$$

Problem A.10. Given a unit normed set $\{x_i\}_{i=1}^N \subseteq H$, where H is d -dimensional, and a sequence $\{\rho_i\}_{i=1}^N \subseteq \mathbb{R}$ of positive weights that sums to 1. The *weighted MSE problem* is to construct a 1-tight frame $\{e_i\}_{i=1}^N$ that minimizes

$$E = \sum_{i=1}^N \rho_i \|x_i - e_i\|^2,$$

taken over all N -element 1-tight frames for H .

A unique solution of the weighted MSE problem can be constructed if all of the weights are equal and if $\{x_i\}_{i=1}^N$ is a frame for H [15, 23, 25, 24, 27, 21, 53].

Theorem A.11. Let $\{x_i\}_{i=1}^N$ be a frame for H with frame operator S . $\{S^{-1/2}x_i\}_{i=1}^N$ is the unique 1-tight frame such that

$$\sum_{i=1}^N \|x_i - S^{-1/2}x_i\|^2 = \inf \left\{ \sum_{i=1}^N \|x_i - e_i\|^2 : \{e_i\}_{i=1}^N \text{ 1-tight frame for } H \right\},$$

and, with S having eigenvalues $\{\lambda_j\}_{j=1}^d$, we have

$$\sum_{i=1}^N \|x_i - S^{-1/2}x_i\|^2 = \sum_{j=1}^d (\lambda_j - 2\sqrt{\lambda_j} + 1).$$

Further, if $\{x_i\}_{i=1}^N$ is geometrically uniform then $\{S^{-1/2}x_i\}_{i=1}^N$ minimizes the detection error P_e if all of the weights are equal, and $\{S^{-1/2}x_i\}_{i=1}^N$ is a geometrically uniform set under the same Abelian group \mathcal{Q} associated with $\{x_i\}_{i=1}^N$.

Remark A.12. According to Theorem A.11, $\{S^{-1/2}x_i\}_{i=1}^N$ is the unique 1-tight frame that minimizes the MSE. However, it is not the unique minimizer of P_e . For example, the set $\{(-1)^j S^{-1/2}x_i\}_{j=1}^N$ is also a minimizer of P_e .

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