Quantum state estimation and large deviations

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Abstract

In this paper we propose a method to estimate the density matrix \( \rho \) of a \( d \)-level quantum system by measurements on the \( N \)-fold system in the joint state \( \rho^\otimes N \). The scheme is based on covariant observables and representation theory of unitary groups and it extends previous results concerning pure states and the estimation of the spectrum of \( \rho \). We show that it is consistent (i.e. the original input state \( \rho \) is recovered with certainty if \( N \to \infty \)), analyze its large deviation behavior, and calculate explicitly the corresponding rate function which describes the exponential decrease of error probabilities in the limit \( N \to \infty \). Finally we discuss the question whether the proposed scheme provides the fastest possible decay of error probabilities.

1 Introduction

The density operator \( \rho \) of a \( d \)-level quantum system (\( d \in \mathbb{N} \)) describes the preparation of the system in all details relevant to statistical experiments, and the task of quantum state estimation is to determine \( \rho \) by measurements on a (possibly large) number \( N \) of systems, which are all prepared according to \( \rho \). In the limit of infinitely many input systems it is of course possible to get exact estimates. If \( N \) remains finite, however, estimation errors are unavoidable. The best we can get (if \( N \) is large enough) is an estimation scheme which produces only small errors or, better to say, which produces large errors only with a small probability.

There are several ways to get “good” estimation schemes. One possibility is to choose an appropriate figure of merit which measures the quality of the estimates (e.g. averaged fidelities with respect to the original density matrix) and to solve the corresponding optimization problem. If we know a priori that the input state \( \rho \) is pure (but otherwise unknown) this approach is very successful and leads to optimal estimators, which can be given in closed form for all finite values of \( N \); cf. e.g. [24, 30, 6, 11, 19, 29, 7]. In the general case, however (i.e. if nothing is known about \( \rho \)) the situation is much more difficult. First of all the result depends much more on the figure of merit chosen than in the pure state case, and even if we have found an appropriate quality criterion it is in

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general very hard to determine the corresponding optimal estimator explicitly for arbitrary \( N \); some results related to this approach can be found in \[36\] \[15\] \[2\].

A way out of this dilemma, is to neglect the quality of the estimates for finite \( N \) and to look for estimation schemes which guarantee at least that error probabilities vanish “as fast as possible” as \( N \) goes to infinity (cf. \[22\] \[24\]; for a collection of recent publications on the subject see also \[18\]). There are two approaches which implement this somewhat vague idea in a mathematically exact way. One possibility is to look at variances (rescaled by \( N \)) in the limit \( N \to \infty \). This is done in several works (cf. e.g. \[17\] \[16\] \[31\] and in particular the papers reprinted in \[18\]) and it leads to quantum analogs of classical Cramer-Rao type bounds. The second idea is to analyze the large deviation behavior of the estimators. To make this more precise let us denote an estimate derived from a measurement on \( N \) systems in the joint state \( \rho^{\otimes N} \) by \( \sigma \). Then we can look at the probability \( P_{N,\varepsilon} \) that the trace-norm distance between \( \rho \) and \( \sigma \) (or any other appropriate distance measure for states) is at least \( \varepsilon \), i.e.

\[
\|\rho - \sigma\|_1 \geq \varepsilon.
\]

Since \( \rho = \sigma \) would be the exact estimate this is clearly an error probability. Now we are interested in those cases where \( P_{N,\varepsilon} \) vanishes exponentially fast in \( N \), i.e.

\[
P_{N,\varepsilon} \approx C_N \exp(-N \inf_{\|\rho - \sigma\|_1 \geq \varepsilon} I(\sigma, \rho)).
\]

Here \( C_N, N \in \mathbb{N} \) is an unknown sequence of positive real numbers, growing at most subexponentially with \( N \) (and which is of no interest for the following), and \( I(\rho, \sigma) \) is a positive function which vanishes iff \( \sigma = \rho \) holds. \( I \) is called the rate function because it describes the exponential rate with which estimation errors vanishes asymptotically. In classical statistics this analysis was initiated by Bahadur \[3\] \[4\] \[5\] and has become in the mean time a classical topic (“Bahadur efficiency”). About the quantum case, however, much less is known, and the results available so far cover three different areas: 1. In \[27\] \[1\] \[21\] an explicit scheme to estimate the spectrum of \( \rho \) is proposed and its rate function is calculated. The latter is shown to be optimal in \[20\]. 2. The rate function of the optimal pure state estimator is calculated in \[19\]. 3. In \[20\] the behavior of quantities like \( \lim_{\varepsilon \to 0} \inf_{\|\rho - \sigma\|_1 \geq \varepsilon} I(\rho, \sigma) \) is analyzed for one-parameter families of states, and the relation to quantum Fisher information is discussed.

The purpose of the present paper is to extend the results about the spectrum in \[27\] and about pure states in \[19\] in two respects. Firstly, we will propose a scheme to estimate the full density matrix which is based on covariant observables \[24\] and which reduces to \[27\] if we look only at the spectrum of \( \rho \). And secondly, we will pose the question whether the proposed scheme is “asymptotically optimal”, i.e. whether its rate function is bigger than the rate function of any other scheme. There is of course no guarantee that a given set of functions admits a maximal element, but in the classical case it is known that such an “optimal rate function” exists (and is given by the classical relative entropy – this is again a consequence of Bahadur’s work \[3\] \[4\] \[5\]). For quantum systems, however, the situation is – not very surprisingly – much more difficult.

The outline of the paper is as follows: In Section 2 we will give a more formal introduction to the questions we are considering and in 3 we will state our main results. The proofs and a more detailed discussion is then distributed among Section 4 (were we will consider U(\( d \))-covariant estimation schemes) and Section 5 (where upper bounds on rate functions will be discussed).
2 Basic definitions

In this section we will present some mathematical preliminaries (in particular basic definitions and terminology) concerning quantum state estimation. A short summary of material from the theory of large deviations used throughout this paper can be found in Appendix A.

2.1 State estimation

Let us consider the $d$-dimensional Hilbert space $\mathcal{H} = \mathbb{C}^d$ and the corresponding set $\mathcal{S}$ of density operators. The task of quantum state estimation is to determine a state $\rho \in \mathcal{S}$ by a measurement on an $N$-fold system, which is prepared in the joint state $\rho \otimes N$. Mathematically this can be described by a normalized POV measure $E_N$ on the state space $\mathcal{S}$ with values in the algebra $\mathcal{B}(\mathcal{H} \otimes N)$ of (bounded) operators on $\mathcal{H} \otimes N$. More precisely, $E_N$ is a (strongly) $\sigma$-additive set function $E_N: \mathcal{B}(\mathcal{S}) \to \mathcal{B}(\mathcal{H} \otimes N)$ with $E_N(\emptyset) \geq 0$, $E_N(\emptyset) = 0$, $E_N(\mathcal{S}) = 1$ I.

Since the number $N$ of systems is arbitrary, we need a whole sequence of observables and we will call each such sequence in the following a full estimation scheme. For a good estimation scheme the quality of the estimates should increase with $N$, i.e. the error probability should decrease and in the limit of infinitely many input systems the estimate should be exact; in other words the sequence of probability measures $(\mu_{N,\rho})_{N \in \mathbb{N}}$ should converge for each $\rho$ weakly to the point measure concentrated at $\rho$. Such an estimation scheme is called consistent.

If we are interested not in the whole state but only in some special properties of $\rho$ (e.g. its von Neumann entropy), described by a function $\mathcal{S} \ni \rho \mapsto p(\rho) \in X$ taking its values in a locally compact, separable metric space $X$ we have to consider more generally POV measures $E_N: \mathfrak{B}(\mathcal{S}) \to \mathcal{B}(\mathcal{H} \otimes N)$ on $\mathcal{S}$ instead of $\mathcal{S}$. As before, $\text{tr}(\rho \otimes N E_N(\Delta))$ is the probability to get an estimate in $\Delta \subset X$. Estimating the spectrum of a density operator is a particular example of this kind. In this case $p$ coincides with

$$s: \mathcal{S} \to \Sigma = \{x \in [0,1]^d | x_1 \geq \cdots \geq x_d \geq 0, \sum_{j=1}^d x_j = 1\}$$

which maps a density operator $\rho$ to its spectrum $s(\rho) \in \Sigma$, i.e. $s_j(\rho) = \langle \chi_j, \rho \chi_j \rangle$ where $\chi_1, \ldots, \chi_d$ denotes an appropriate eigenbasis of $\rho$. We will call $\Sigma$ the set of ordered spectra and $s$ the canonical projection onto $\Sigma$. Let us summarize the discussion up to now in the following definition.

**Definition 2.1** Consider a finite dimensional Hilbert space $\mathcal{H}$, the corresponding set $\mathcal{S}$ of density operators, and a function $p: \mathcal{S} \to X$ taking its values in the locally compact, separable metric space $X$. A sequence $(E_N)_{N \in \mathbb{N}}$ of POV
Equation (3) should satisfy the large deviation principle. A p-estimation scheme is called consistent, if the sequence $(\mu_{N,\rho})_{N \in \mathbb{N}}$ of probability measures defined in (5) converges for each $\rho \in \mathcal{S}$ weakly to a point measure concentrated at $p(\rho) \in X$.

We recover both cases we are mainly interested in if we set $X = \mathcal{S}$ and $p = \text{Id}$ for the full problem and $X = \Sigma$ and $p = s$ for spectral estimation.

Of special importance in this work are estimation scheme with additional symmetry properties: Let us denote the permutation group on $N$ points by $S_N$ and its natural representation on $\mathcal{H}^{\otimes N}$ by $V$, i.e.

$$V_{\sigma} \psi_1 \otimes \cdots \otimes \psi_N = \psi_{\sigma^{-1}(1)} \otimes \cdots \otimes \psi_{\sigma^{-1}(N)}, \quad \sigma \in S_N, \quad \psi_1, \ldots, \psi_N \in \mathcal{H}. \quad (5)$$

An estimation scheme $(E_N)_{N \in \mathbb{N}}$ is called permutation invariant, if

$$V_{\sigma} E_N(\Delta) V_{\sigma}^* = E_N(\Delta) \quad \forall \sigma \in S_N \quad \forall \Delta \in \mathcal{B}(X) \quad (6)$$

holds. Likewise, it is called $U(d)$-covariant (or just covariant) if $U(d)$ acts continuously on $X$ by $U(d) \times X \ni (U, x) \mapsto \alpha_U(x) \in X$ such that the conditions

$$U^{\otimes N} E_N(\Delta) U^{\otimes N} = E_N(\alpha_U(\Delta)) \quad \forall U \in U(d) \quad \forall \Delta \in \mathcal{B}(X) \quad (7)$$

and

$$p(U \rho U^*) = \alpha_U(p(\rho)) \quad \forall U \in U(d) \quad \forall \rho \in \mathcal{S} \quad (8)$$

are satisfied. If the scheme $(E_N)_{N \in \mathbb{N}}$ is consistent, covariance of the projection $p$ is implied by covariance of the measures $E_N$. Furthermore, note that the $U(d)$ operation $\alpha_U$ is uniquely determined (if it exists) due to surjectivity of $p$. For full estimation we have $\alpha_U(\rho) = U \rho U^*$ and for spectral estimation it is the trivial action, i.e. $\alpha_U(x) = x$. Hence, covariant estimation schemes are defined in both cases we are interested in.

### 2.2 Large deviations

Consider now, a Borel set $\Delta \subset X$ and a state $\rho \in \mathcal{S}$ such that $p(\rho) \notin \bar{\Delta}$ (the closure of $\Delta$). The quantity $\mu_{\rho,N}(\Delta)$ is then the probability to get a false estimate in $\Delta$. If the scheme is consistent this probability goes to zero. This is, however, a very weak statement because the convergence can be very slow. As already pointed out in the introduction, we are therefore interested in schemes, where convergence of error probabilities to zero is exponentially fast; in other words for each $\rho \in \mathcal{S}$ the sequence $(\mu_{N,\rho})_{N \in \mathbb{N}}$ of probability measures from Equation (4) should satisfy the large deviation principle\(^1\) with a rate function $I(\rho, \cdot)$. This idea leads to the following definition:

**Definition 2.2** A p-estimation scheme $(E_N)_{N \in \mathbb{N}}$, as described in Definition 2.1 satisfies the large deviation principle (LDP) with rate function $I : \mathcal{S} \times X \to [0, \infty]$ if

1. $I_\rho = I(\rho, \cdot)$ is a rate function (cf. Definition A.1) for each $\rho \in \mathcal{S}$.

2. $I(\rho, x) = 0$ iff $p(\rho) = x$ holds.

\(^1\)A short summary of definitions and theorems from large deviations theory which are relevant for this paper can be found in Appendix A
3. The sequence \((\mu_{N,\rho})_{N \in \mathbb{N}}\) of probability measures \(\mu\) satisfies for each \(\rho \in \mathcal{S}\) the large deviation principle with rate function \(I_{\rho}\).

Note that condition\(\text{[2]}\) guarantees that each scheme which satisfies the LDP is consistent, because the \(\mu_{N,\rho}(\Delta)\) converge to 0, if \(\Delta\) is a closed set which does no contain \(p(\rho)\). Occasionally we will have to refer to the rate function \(I_{\rho}\) of an estimation scheme \((E_N)_{N \in \mathbb{N}}\) without using \((E_N)_{N \in \mathbb{N}}\) directly. In this case we will call \(I_{\rho}\) an admissible rate function.

**Definition 2.3** A function \(I : \mathcal{S} \times X \to [0, \infty]\) which is the rate function of a \(p\)-estimation scheme is called \(p\)-admissible (or just admissible if \(p\) is understood). The set of all \(p\)-admissible rate functions is denoted by \(\mathcal{E}(p)\).

We do not yet know how continuous or discontinuous admissible rate functions can be in their first argument. E.g. an otherwise very bad estimation scheme might provide very fast exponential decay for a particular input state. The discussion in Sections \(\textbf{4.1}\) and \(\textbf{5.4}\) will indicate that discontinuities might occur in particular at the boundary of the state space, while the behavior in the interior of \(\mathcal{S}\) (i.e. at non-degenerate density matrices) seems to be more regular.

To avoid such difficulties let us introduce the following subset of \(\mathcal{E}(p)\):

\[
\mathcal{E}^0(p) = \{ I \in \mathcal{E}(p) \mid I \text{ is lower semi-continuous} \}. \tag{9}
\]

If the map \(p\) we want to estimate is covariant in the sense of Equation \(\textbf{8}\) we can introduce in addition

\[
\mathcal{E}^c(p) = \{ I \in \mathcal{E}(p) \mid I \text{ is covariant} \}, \tag{10}
\]

where we call an admissible rate function covariant, if it is the rate function of a \(U(d)\)-covariant estimation scheme. In contrast to this, any function \(F : \mathcal{S} \times X \to [0, \infty]\) is called \(U(d)\)-invariant if

\[
F(U \rho U^*, \alpha U(x)) = F(\rho, x) \forall U \in U(d) \forall \rho \in \mathcal{S} \forall x \in X \tag{11}
\]

is satisfied. Obviously, each admissible rate function which is covariant is \(U(d)\)-invariant too. It is not clear whether the converse holds as well (i.e. whether \(U(d)\)-invariance of \(I \in \mathcal{E}(p)\) implies covariance). However, problems can occur only on the boundary of \(\mathcal{S}\) (i.e. for degenerate density matrices) and even there only if \(I\) is not lower semicontinuous (cf. Section \(\textbf{1.2}\) for details). Finally note that \(U(d)\)-invariance of \(I \in \mathcal{E}^c(p)\) implies, together with lower semi-continuity of \(I_0(\cdot) = I(\rho, \cdot)\), lower semi-continuity of \(I^c(\cdot) = I(\cdot, x)\) along the orbits of the \(U(d)\) action on \(\mathcal{S}\). The general relation between \(\mathcal{E}^0(p)\) and \(\mathcal{E}^c(p)\) is, however, not clear (i.e. \(I \in \mathcal{E}^c(p)\) can be discontinuous transversal to the orbits).

Ideally, we would like to have estimation schemes \((E_N)_{N \in \mathbb{N}}\) which provide the fastest possible exponential decay of error probabilities. Hence, for a given map \(p : \mathcal{S} \to X\) we are mainly interested in the quantities

\[
\mathcal{I}(p, \sigma) = \sup_{I \in \mathcal{E}(p)} I(\rho, \sigma), \quad \mathcal{I}(p, \sigma) = \sup_{I \in \mathcal{E}(p)} I(\rho, \sigma) \tag{12}
\]

and

\[
\mathcal{I}(p, \sigma) = \sup_{I \in \mathcal{E}(p)} I(\rho, \sigma). \tag{13}
\]
The functions $I_p^\# : S \times X \to [0, \infty]$ thus defined (following the notation introduced above, we will write $I_{1d}^\#$ for full and $I_p^\#$ for spectral estimation), are the least upper bounds on the sets $E^\!(p)$, but they are not necessarily admissible themselves. In slight abuse of language we will call them nevertheless the optimal rate functions. If $I_p$ can be realized as the rate function of a particular estimation scheme $(E_N)_{N \in \mathbb{N}}$, we will call $(E_N)_{N \in \mathbb{N}}$ (strongly) asymptotically optimal.

3 Summary of main results

A particular example for asymptotic optimality arises in classical estimation theory (for finite probability distributions). It is known from Bahadur efficiency that the classical relative entropy is an upper bound for all admissible rate functions; and Sanov’s theorem (cf. eg. [10]) states that this bound can be achieved by the empirical distribution (i.e. relative frequencies in a given sample). The latter provides therefore an asymptotically optimal estimation scheme. For quantum systems the situation is more difficult, and our knowledge is (unfortunately) not yet as complete as for classical estimation. Nevertheless, we have some significant partial results which we want to summarize in this section. The proofs and a more detailed discussion are postponed to Section 4 and 5.

3.1 Estimating the spectrum

The most complete result is available for spectral estimation. To state it let us recall the definition of the scheme presented in [27]. It is based on the decomposition of the representation $U \mapsto U \otimes^N$ of the unitary group $U(d)$ into irreducible components. The latter is given by

$$
\mathcal{H}^\otimes N = \bigoplus_{Y \in \mathcal{Y}_d(N)} \mathcal{H}_Y \otimes K_Y, \quad U^\otimes N = \bigoplus_{Y \in \mathcal{Y}_d(N)} \pi_Y(U) \otimes \mathbb{1},
$$

(14)

where $\mathcal{Y}_d(N)$ denotes the set of Young frames with $d$ rows and $N$ boxes

$$
\mathcal{Y}_d(N) = \{Y \in \mathbb{N}^d | Y_1 \geq \ldots \geq Y_d, \sum_{j=1}^d Y_j = N\},
$$

(15)

$\pi_Y$ denotes the irreducible representation with highest weight $Y$, and $K_Y$ is a multiplicity space which carries an irreducible representation of the symmetric group $S_N$ on $N$ elements:

$$
V_\sigma = \bigoplus_{Y \in \mathcal{Y}_d(N)} \mathbb{1} \otimes \Pi_Y(\sigma), \quad \sigma \in S_N
$$

(16)

where $V_\sigma$ is defined in Equation 5 and $\Pi_Y$ is the irreducible $S_N$ representation defined by the Young frame $Y$.

\footnote{More precisely the $Y_1, \ldots, Y_d$ are the components of the highest weight in a particular basis of the Cartan subalgebra.}
Now we can define a spectral estimation scheme \((\hat{F}_N)_{N \in \mathbb{N}}\) by

\[
\hat{F}_N(\Delta) = \sum_{Y \in \Delta} P_Y,
\]

where \(P_Y\) denotes the projection onto \(\mathcal{H}_Y \otimes K_Y\):

\[
P_Y \in \mathcal{B}(\mathcal{H}_Y^\otimes N), \quad P_Y^2 = P_Y, \quad P_Y^* = P_Y, \quad P_Y \mathcal{H}_Y^\otimes N = \mathcal{H}_Y \otimes K_Y.
\]

In other words \(\hat{F}_N\) is a discrete measure with normalized Young frames \(Y/N\) as possible estimates and the probability to get the outcome \(Y/N\) for input systems in the joint state \(\rho^\otimes N\) is \(\text{tr}(\rho^\otimes N P_Y)\). In [27] it is shown that \(\hat{F}_N\) satisfies the large deviation principle with the classical relative entropy between the probability vectors \(x \in \Sigma\) and \(s(\rho)\) as the rate function \(I(\rho, x)\). As we will see in Subsection 5.2 this is in fact the best that can be achieved (cf. also [20]).

**Theorem 3.1** The spectral estimation scheme \((\hat{F}_N)_{N \in \mathbb{N}}\) defined in [14] is asymptotically optimal; i.e. it satisfies the LDP with the optimal rate function \(\mathcal{I}_s\) defined in Equation (12). In addition \(\mathcal{I}_s = \mathcal{I}_s^0 = \mathcal{I}_s^c\) holds, and \(\mathcal{I}_s\) is given explicitly by

\[
\mathcal{S} \times \Sigma \ni (\rho, x) \mapsto \mathcal{I}_s(\rho, x) = \sum_{j=1}^d x_j \left[\ln(x_j) - \ln(s_j(\rho))\right].
\]

where \(s : \mathcal{S} \to \Sigma\) is the canonical projection from Equation (4).

### 3.2 The full density matrix

For the full problem the best scheme \((\hat{E}_N)_{N \in \mathbb{N}}\) we have found so far is defined by the integral (with an arbitrary continuous function \(f : \mathcal{S} \to \mathbb{R}\))

\[
\int_{\mathcal{S}} f(\rho) \hat{E}_N(d\rho) = \sum_{Y \in \mathcal{Y}_d(N)} \dim \mathcal{H}_Y \int_{U(\mathcal{H}_Y)} f(U \rho_{Y/N} U^*) |\pi_Y(U)\phi_Y\rangle \langle \pi_Y(U)\phi_Y| \otimes 1 \, dU,
\]

where \(\phi_Y \in \mathcal{H}_Y\) is the highest weight vector of the irreducible representation \(\pi_Y\) and \(\rho_x\) denotes for each \(x \in \Sigma\) the diagonal density matrix

\[
\rho_x = \text{diag}(x_1, \ldots, x_d).
\]

The main properties of this scheme are: It projects to the spectral estimation scheme \(\hat{F}_N\) from Subsection 3.1

\[
\hat{E}_N(s^{-1}(\Delta)) = \hat{F}_N(\Delta) \quad \forall \Delta \in \mathcal{B}(\Sigma),
\]

it is covariant (i.e. Equation (17) holds with \(\alpha_U(\rho) = U \rho U^*\)) and permutation invariant (cf. Equation (3)). Measuring \(\hat{E}_N\) can be regarded therefore as a two step process: First measure the observable \(\hat{F}_N\) in terms of the instrument \(T\), which is defined by the family of channels (given in the Schrödinger picture):

\[
T_Y : \mathcal{B}(\mathcal{H}_Y^\otimes N) \ni \omega \mapsto \text{tr}_{K_Y}(P_Y \omega P_Y) \in \mathcal{B}(\mathcal{H}_Y) \quad Y \in \mathcal{Y}_d(N),
\]
where \( \text{tr}_{K_Y} \) denotes the partial trace over \( K_Y \) and the \( P_Y \) are again the projections from \( \mathcal{K} \). If the estimate for the spectrum we get in this way (with probability \( \text{tr}(P_Y \rho \otimes \rho^N) \)) is \( Y/N \), the output of \( T \) is a quantum system (described by the Hilbert space \( \mathcal{H}_Y \) — hence of different type then the input system\(^3\)) in the state \( \text{tr}(P_Y \rho \otimes \rho^N)^{-1} T_Y (\rho \otimes \rho^N) \). On this system we perform a measurement of a covariant observable \( \hat{E}_Y \) with values in \( \mathcal{S}_Y = s^{-1}(Y/N) \) which is defined by the integral

\[
\int_{\mathcal{S}_Y} f(\sigma) E_Y(d\sigma) = \int_{U(d)} f(U \rho_{Y/N} U^*) \langle \pi_Y(U) \phi_Y \rangle \langle \pi_Y(U) \phi_Y \rangle \, dU, \tag{24}
\]

(where \( f \) denotes now a continuous function on \( \mathcal{S}_Y \)) and this gives us an estimate for the eigenvectors of \( \rho \). In the special case of pure states (i.e. if the first measurement gives \( Y/N = (1, 0, 0, \ldots, 0) \)) the observable \( \hat{E}_Y \) is given by

\[
\int_{\mathcal{P}} f(\sigma) \hat{E}_Y(d\sigma) = \int_{\mathcal{P}} f(\sigma) \sigma^{\otimes N}, \quad \text{for} \ Y = (N, 0, \ldots, 0), \tag{25}
\]

where \( \mathcal{P} = s^{-1}(1, 0, \ldots, 0) \) denotes the set of pure states. This observable is known to optimize for each \( N \) global quality criteria like averaged fidelity \([24, 39, 43]\). Hence we can look at \( \hat{E}_N \) as a direct generalization of the best known estimation schemes for the spectrum and for pure states. We discuss this point of view in greater detail in Section 4.4. The large deviation behavior of \( \hat{E}_N \) is described by the following theorem (cf. Section 4.5 for a proof):

**Theorem 3.2** The full estimation scheme \((\hat{E}_N)_{N \in \mathbb{N}}\) defined in Equation \(27\) satisfies the large deviation principle with rate function \( \hat{I} : \mathcal{S} \times \mathcal{S} \to [0, \infty] \)

\[
\hat{I}(\rho, U \rho_x U^*) = \sum_{k=1}^d (x_k \ln(x_k) - (x_k - x_{k+1}) \ln[\text{pm}_k(U^* \rho_U)]) \tag{26}
\]

where \( x = (x_1, \ldots, x_d) \in \Sigma, x_{d+1} = 0, \rho_x \) is the density matrix from Equation \(24\), \( U \in U(d) \), and \( \text{pm}_j(\sigma) \) denotes the principal minor (i.e. the upper left rank \( j \) subdeterminant) of the matrix \( \sigma \).

The best upper bound on the rate function for full estimation schemes we have found so far is derived from quantum hypothesis testing.

**Theorem 3.3** Each admissible rate function \( I : \mathcal{S} \times \mathcal{S} \to [0, \infty] \) is bounded from above by the relative entropy, i.e.

\[
I(\rho, \sigma) \leq S(\rho, \sigma) = \text{tr}(\sigma \ln(\sigma) - \sigma \ln(\rho)) \quad \forall \rho, \sigma \in \mathcal{S}. \tag{27}
\]

The proof will be given in Section 5.2; cf also [20]. It is easy to check numerically that \( \hat{I}(\rho, \sigma) \) and \( S(\rho, \sigma) \) do not coincide in general. If we consider in particular the qubit case \((d = 2)\) and express the density operators \( \rho, \sigma \) in Bloch form, i.e.

\[
\rho = \frac{1}{2} \left[ \mathbb{1} + \vec{x} \cdot \vec{\sigma} \right], \quad \sigma = \frac{1}{2} \left[ \mathbb{1} + \vec{y} \cdot \vec{\sigma} \right] \tag{28}
\]

\(^3\)If \( d = 2 \) holds the situation is special. In this case the output of \( T \) can be regarded as an \( M = Y_1 - Y_2 \) qubit system, and \( T \) itself coincides with the “natural purifier” studied in \([8, 25]\).
(where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices and $\vec{x}, \vec{y} \in \mathbb{R}^3$ with $|\vec{x}|, |\vec{y}| \leq 1$), we get for the rate function $I$ from Equation (26)

$$\hat{I}(\rho, \sigma) = -S(\sigma) - |\vec{y}| \ln \left( \frac{1 + |\vec{x}| \cos \theta}{2} \right) - \frac{1 - |\vec{y}|}{2} \ln \left( \frac{1 - |\vec{x}|^2}{4} \right),$$

(29)

where $\theta$ denotes the angle between $\vec{x}$ and $\vec{y}$ and $S(\sigma)$ is the von Neumann entropy of $\sigma$. The relative entropy of $\sigma$ and $\rho$ becomes

$$S(\rho, \sigma) = -S(\sigma) - \frac{1}{2} \ln (1 + |\vec{x}|^2) - |\vec{y}| \cos(\theta) \ln \left( \frac{1 + |\vec{x}|}{1 - |\vec{x}|^2} \right).$$

(30)

We have plotted both quantities as functions of $\theta$ for two different values of $|\vec{x}| = |\vec{y}|$ in Figure 1, which shows that $I(\rho, \sigma)$ is in general strictly smaller than $S(\rho, \sigma)$.

3.3 Optimal rate functions

Hence, for a general input state $\rho$ we only know for sure that the optimal rate functions defined in Equation (12) and (13) have to satisfy (with $p = \text{Id}$ for full estimation)

$$\hat{I} \leq I^0_{\text{Id}}, I^0_{\text{Id}} \leq I_{\text{Id}} \leq S.$$ 

(31)

This is, however, not as bad as it looks like at a first glance: Since $S(\rho, \sigma)$ and $\hat{I}(\rho, \sigma)$ coincide if $\rho$ and $\sigma$ commute, we get

$$\hat{I}(\rho, \sigma) = I_{\text{Id}}(\rho, \sigma) = S(\rho, \sigma) = \sum_{j=1}^{d} s_j(\sigma) (\ln s_j(\sigma) - \ln s_j(\rho)) \quad \forall \rho, \sigma \in S \text{ with } [\rho, \sigma] = 0.$$ 

(32)

A second partial result arises if the input state is pure. In Proposition 5.5 we will show

$$\hat{I}_{\text{Id}}(\rho, \sigma) = \hat{I}(\rho, \sigma) \quad \forall \rho, \sigma \in S \text{ with } \rho \text{ pure},$$ 

(33)

and in Section 4.4 we will give some heuristic arguments which indicate that $\hat{I}$ and $I^c$ coincide even for general input states. This indicates that $(E_N)_{N \in \mathbb{N}}$ is the best scheme as long as we are insisting on some additional regularity conditions of the rate function – in the case at hand this is covariance. It is not clear, however, whether covariance can be replaced by something more general without breaking the equality with $\hat{I}$. There are at least some indications (cf. Section 5.3) that Equation (33) would still hold if we replace $\hat{I}_{\text{Id}}$ with $I^0_{\text{Id}}$. Note that $\hat{I} \in E^0(p)$ hence (33) already implies $I^0(\rho, \sigma) \geq I^c(\rho, \sigma)$ for pure $\rho$. Our conjecture here is that equality holds for all $\rho$ and $\sigma$.

Another result which can be derived easily from Equation (33) and Proposition 5.4 is $S \not\in E(\text{Id})$, i.e. there is no estimation scheme with relative entropy as its rate function. This follows from the fact that $S$ is lower semicontinuous and $U(d)$-invariant in the sense of Equation (11). Hence $S \in E(\text{Id})$ would imply according to Proposition 5.4 $S \in E^c(\text{Id})$ in contradiction to Equation (33) and the fact that $S(\rho, \sigma) > \hat{I}(\rho, \sigma)$ holds for all pure states $\rho, \sigma$ with $\rho \neq \sigma$ and $\rho \sigma \neq 0$. On the other hand there is strong evidence that $I_{\text{Id}} = S$ holds, i.e. that $S$ is the best upper bound of the set of all admissible rate functions.
Figure 1: Relative entropy and rate function $\hat{I}$ as a function of the angle $\theta$ between the two Bloch vectors $\vec{x}$ and $\vec{y}$. The upper plot corresponds to the case $|\vec{x}| = |\vec{y}| = 0.9$ and the lower to $|\vec{x}| = |\vec{y}| = 0.1$. 
This would imply that we can find for each pair $\rho_0, \sigma_0 \in S$ an $I \in \mathcal{E}(\text{Id})$ such that $I(\rho_0, \sigma_0) = S(\rho_0, \sigma_0)$ holds, but $I$ is much smaller than $S$ (most probably even smaller than $\hat{I}$) almost everywhere else. In Section 5.3 we will discuss these topics in greater detail. For now, let us summarize all our conjectures in the following Equation
\[ \hat{I} = \mathcal{T}_\text{Id}^* = \mathcal{T}_\text{Id}^0 \leq I = S. \] (34)

4 Covariant observables

The aim of this section is to study estimation schemes which are $U(d)$ covariant and permutation invariant, i.e. they do not prefer a special copy of the input state or a particular direction in the Hilbert space $\mathcal{H}$. Among a proof of Theorem 3.2 we will provide several general results, which are useful within the discussion of the questions raised in Section 3.3. Therefore only full estimation schemes are considered in this section (i.e. $p = \text{Id}$), but most of the results in Subsection 4.2 and 4.3 can be generalized quite easily to $p$-estimation schemes, if $p$ is sufficiently covariant.

4.1 Continuity properties

Let us start with some technical results concerning continuity and uniform convergence with respect to the original density matrix $\rho$. They will become crucial within the discussion of group averages in the next section. Some of them, however, are quite interesting in their own right, and it is therefore reasonable to devote a whole subsection for them.

Central subjects of this discussion will be integrals of the form
\[ h_N(\rho, f) = -\frac{1}{N} \ln \int_S e^{-Nf(\sigma)} \text{tr}(\rho^\otimes N E_N(d\sigma)), \] (35)
where $f$ denotes an arbitrary, real valued function on $S$. Quantities of this form usually appear in Varadhan’s Theorem (cf. Theorem A.3), i.e. if the estimation scheme $(E_N)_{N \in \mathbb{N}}$ satisfies the LDP with rate function $I$ we have
\[ \lim_{N \to \infty} h_N(\rho, f) = h(\rho, f) = \inf_{\sigma \in S} (I(\rho, \sigma) + f(\sigma)). \] (36)

If on the other hand $(E_N)_{N \in \mathbb{N}}$ does not necessarily satisfy the LDP but holds for each $f$ and a density matrix $\rho$, the sequence of probability measures $\text{tr}(\rho^\otimes N E_N(\cdot))$ satisfies the Laplace principle (Definition A.4) which is equivalent to the large deviation principle (Theorem A.5). Hence the study of convergence properties of the $h_N(\rho, f)$ is a useful tool to prove that the LDP holds for a given estimation scheme.

In this section we will discuss continuity of $h$ with respect to $\rho$ and uniformity of the convergence $h_N \to h$ (again with respect to $\rho$). The most crucial step in this direction is the following lemma.

**Lemma 4.1** Consider an estimation scheme $(E_N)_{N \in \mathbb{N}}$ satisfying the LDP with rate function $I$, an arbitrary continuous (real valued) function $f$ and the functionals $h_N, h$ defined in Equations (34) and (35).
1. For each non-degenerate density matrix \( \rho \in \mathcal{S} \) and each sequence \( \mathbb{N} \ni N \mapsto \rho_N \in \mathcal{S} \) converging to \( \rho \) we have

\[
\lim_{N \to \infty} h_N(\rho_N, f) = \lim_{N \to \infty} h_N(\rho, f) = h(\rho, f)
\] (37)

2. If \( I \) is lower semicontinuous in both arguments, the lower bound

\[
\liminf_{N \to \infty} h_N(\rho_N, f) \geq h(\rho, f)
\] (38)

holds even for degenerate \( \rho \).

**Proof.** Let us consider part 1 first. In this case the proof mainly depends on the following lemma which allows us to represent one sequence as a convex combination of two others.

**Lemma 4.2** Consider two sequences \( \mathbb{N} \ni N \mapsto \rho_N^{(j)} \in \mathcal{S}, j = 1, 2 \) both converging to the same non-degenerate density matrix \( \rho \in \mathcal{S} \). For each \( \lambda \in \mathbb{R} \) with \( 0 < \lambda < 1 \) there exists an integer \( N_\lambda \in \mathbb{N} \) and a third sequence \( \mathbb{N} \ni N \mapsto \sigma_N \in \mathcal{S} \) such that

\[
\rho_N^{(1)} = \lambda \rho_N^{(2)} + (1 - \lambda) \sigma_N \quad \forall N > N_\lambda
\] (39)

holds.

**Proof.** Let \( \kappa = \inf_{\|\phi\|=1} \langle \phi, \rho \phi \rangle \) and define

\[
\epsilon = \frac{(1 - \lambda)\kappa}{\lambda + 1}.
\] (40)

Since \( \rho \) is non-degenerate, we have \( \kappa > 0 \) and therefore \( \epsilon > 0 \) as well. Hence there is an \( N_\lambda \in \mathbb{N} \) such that (with \( \phi \in \mathcal{H} \) and \( A \in \mathcal{B}(\mathcal{H}) \))

\[
\sup_{\|\phi\|=1} |\langle \phi, (\rho_N^{(j)} - \rho) \phi \rangle| \leq \sup_{\|A\|=1} |\text{tr}((\rho_N^{(j)} - \rho)A)|
\]

\[
= \|\rho_N^{(j)} - \rho\|_1 < \epsilon
\] (42)

holds for all \( N > N_\lambda \) and for \( j = 1, 2 \). In addition we see by the triangle inequality that

\[
\sup_{\|\phi\|=1} |\langle \phi, (\rho_N^{(1)} - \rho_N^{(2)}) \phi \rangle| < 2\epsilon
\]

holds as well for all \( N > N_\lambda \). Now define

\[
\delta = \frac{\kappa}{2\epsilon} - \frac{1}{2} = \frac{\lambda}{1 - \lambda}
\] (44)

(the second equality follows from Equation (40) and)

\[
\sigma_N = -\delta \rho_N^{(2)} + (1 + \delta) \rho_N^{(1)} \quad \text{for } N > N_\lambda
\] (45)

(and \( \sigma_N \in \mathcal{S} \) arbitrary otherwise). Obviously \( \text{tr}(\sigma_N) = 1 \) and

\[
-\frac{\lambda}{1 - \lambda} \rho_N^{(2)} + \frac{1}{1 - \lambda} \rho_N^{(1)} = \sigma_N.
\] (46)
Hence
\[ \rho_N^{(1)} = \lambda \rho_N^{(2)} + (1 - \lambda) \sigma_N \quad \forall N > N_\lambda \] (47)
as stated.

It only remains to show that \( \sigma_N \geq 0 \) (and therefore \( \sigma_N \in S \)) holds for all \( N > N_\lambda \). This follows from
\[
\langle \phi, \sigma_N \phi \rangle = -\delta \langle \phi, \rho_N^{(2)} \phi \rangle + (1 + \delta) \langle \phi, \rho_N^{(1)} \phi \rangle 
\geq -2\delta \epsilon - \delta \langle \phi, \rho_N^{(1)} \phi \rangle + (1 + \delta) \langle \phi, \rho_N^{(1)} \phi \rangle 
\geq -2\delta \epsilon + \langle \phi, \rho_N^{(1)} \phi \rangle 
\geq -2\delta \epsilon + \sigma_N = -\epsilon (2\delta + 1) + \epsilon = 0, 
\] (48)
(49)
(50)
(51)
where we have used Equation (48) in (49), Equation (42) in (50) and the definition of \( \delta \) in (51).

Now let us apply this lemma to \( \rho_N^{(1)} = \rho \) and \( \rho_N^{(2)} = \rho_N \) for all \( N \in \mathbb{N} \). For each \( \lambda \in (0,1) \) we get an \( N_\lambda \in \mathbb{N} \) such that \( h_N(\rho, f) = h_N(\lambda \rho_N + (1 - \lambda) \sigma_N, f) \) holds for all \( N > N_\lambda \). Hence
\[
\lim_{N \to \infty} h_N(\rho, f) = \lim_{N \to \infty} h_N(\lambda \rho_N + (1 - \lambda) \sigma_N, f). 
\] (52)

Using the definition of \( h_N \) in (55) we get:
\[
\begin{align*}
 h_N(\lambda \rho_N + (1 - \lambda) \sigma_N, f) &= \frac{-1}{N} \ln \left( \lambda^N e^{-Nh_N(\rho_N,f)} + \sum_{n=1}^{N} \lambda^{N-n}(1-\lambda)^n \int_S e^{-Nf(\sigma)} \text{tr}(A_N, e^{Nf(\sigma)} \text{tr}(A_N, E_N(\hat{d}))) \right), 
\end{align*}
\] (53)
where \( A_N \) denotes the sum of all tensor products consisting of \( N - n \) factors \( \rho_N \) and \( n \) factors \( \sigma_N \). We can rewrite this expression as
\[
\begin{align*}
 h_N(\lambda \rho_N + (1 - \lambda) \sigma_N, f) &= -\ln \lambda + h_N(\rho_N, f) 
 - \frac{1}{N} \ln \left( 1 + e^{Nh_N(\rho_N,f)} \sum_{n=1}^{N} \left( \frac{1 - \lambda}{\lambda} \right)^n \int_S e^{-Nf(\sigma)} \text{tr}(A_N, E_N(\hat{d}))) \right). 
\end{align*}
\] (54)

Since \( \rho_N \) and \( \sigma_N \) are density matrices, the operators \( A_N \) are positive. Hence, the argument of the last logarithm in Equation (54) is greater than one and the logarithm therefore positive. This implies:
\[
 h_N(\rho_N, f) \geq h_N(\lambda \rho_N + (1 - \lambda) \sigma_N, f) + \ln(\lambda), 
\] (55)
and with Equation (52)
\[
\begin{align*}
 \liminf_{N \to \infty} h_N(\rho_N, f) &\geq \liminf_{N \to \infty} h_N(\lambda \rho_N + (1 - \lambda) \sigma_N, f) + \ln(\lambda) = 
\lim_{N \to \infty} h_N(\rho, f) + \ln(\lambda). 
\end{align*}
\] (56)

Since \( \lambda \in (0,1) \) is arbitrary we get \( \liminf_{N \to \infty} h_N(\rho_N, f) \geq \lim_{N \to \infty} h_N(\rho, f) \).

The other inequality (i.e. \( \limsup_{N \to \infty} h_N(\rho_N, f) \leq \lim_{N \to \infty} h_N(\rho, f) \)) can
be derived with the same argument, if we exchange the role of $\rho$ and $\rho_N$ (i.e. apply Lemma 11.2 to $\rho^{(1)}_N = \rho_N$ and $\rho^{(2)}_N = \rho$ for all $N \in \mathbb{N}$). Hence $\lim_{N \to \infty} h_N(\rho_N, f) = \lim_{N \to \infty} h_N(\rho, f)$ as stated. The equality $\lim_{N \to \infty} h_N(\rho, f) = h(\rho, f)$ follows from Varadhan’s Theorem (Theorem 14.3).

Now consider statement 2. If $\rho$ is degenerate, the method used above can not be applied. However, if the rate function $I$ is sufficiently continuous, we can extend (parts of) the result derived for non-degenerate density matrices to the degenerate case. To this end we need the following lemma:

**Lemma 4.3** Consider a compact metric space $(X, d)$ and a lower semicontinuous function $F : X \times X \to [c, \infty]$, $c \in \mathbb{R}$. The infimum $F(x) = \inf_{y \in X} F(x, y)$ is lower semicontinuous as well.

**Proof.** Due to lower semicontinuity of $F$, we find for each $(x, y) \in X \times X$ and each $\epsilon > 0$ a $\delta_{x,y} > 0$ with

$$d(x, x') < \delta_{x,y}, \quad d(y, y') < \delta_{x,y} \Rightarrow F(x', y') > F(x, y) - \epsilon. \quad (57)$$

Since $X$ is compact, each fixed $x \in X$ admits finitely many points $y_1, \ldots, y_k \in X$ such that the neighborhoods $U_j = \{ y' \in X | d(y', y_j) < \delta_{x,y_j} \}$ overlap $X$. Now define $\delta = \min_j \delta_{x,y_j} > 0$. For each $x'$ satisfying $d(x, x') < \delta$ and each $y' \in X$ there is a $j = 1, \ldots, k$ with $F(x', y') > F(x, y_j) - \epsilon$. Hence $F(x', y') > \inf_y F(x, y) - \epsilon$ and we get

$$d(x, x') < \delta \Rightarrow F(x') = \inf_{y'} F(x', y') > \inf_{y} F(x, y) - \epsilon. \quad (58)$$

Since $\delta > 0$ this shows that $F$ is lower semicontinuous at $x$ and since $x$ is arbitrary the statement follows. \hfill \Box

Let us apply this lemma to $F(\rho, \sigma) = I(\rho, \sigma) + f(\sigma)$. Since $I$ is lower semicontinuous by assumption we get for each $\epsilon > 0$ a $\delta > 0$ such that $\|\rho' - \rho\|_1 < \delta$ implies $h(\rho', f) > h(\rho, f) - \epsilon$. Together with the convexity of the $\delta$-ball around $\rho$ this implies

$$h(\lambda \rho + (1 - \lambda) \rho', f) > h(\rho, f) - \epsilon \quad \forall \lambda \in (0, 1). \quad (59)$$

If $(\rho_N)_{N \in \mathbb{N}}$ is a sequence in $S$ converging to $\rho$, the convex linear combinations $\lambda \rho_N + (1 - \lambda) \rho'$ converges to $\lambda \rho + (1 - \lambda) \rho'$. As in Equation (50) we get

$$\lim_{N \to \infty} h_N(\lambda \rho_N + (1 - \lambda) \rho', f) \leq \liminf_{N \to \infty} h_N(\rho_N, f) - \ln(\lambda). \quad (60)$$

Now assume without loss of generality that $\rho'$ is non-degenerate. Then $\lambda \rho + (1 - \lambda) \rho'$ is non-degenerate as well and we have according to item 1

$$\liminf_{N \to \infty} h_N(\lambda \rho_N + (1 - \lambda) \rho', f) = h(\lambda \rho + (1 - \lambda) \rho', f) > h(\rho, f) - \epsilon. \quad (61)$$

Hence

$$\liminf_{N \to \infty} h_N(\rho_N, f) \geq h(\rho, f) - \epsilon + \ln(\lambda). \quad (62)$$

Since $\epsilon > 0$ and $\lambda \in (0, 1)$ are arbitrary the statement follows. \hfill \Box

According to Proposition 1.2.7 of [13] this lemma implies immediately that the convergence $h_N \to h$ is uniform on each compact set of non-degenerate density matrices.
Proposition 4.4 Consider the same assumptions as in the preceding lemma and a compact set \( K \subset S \) consisting only of non-degenerate density matrices. Then the convergence \( h_N \to h \) is uniform on \( K \), i.e.

\[
\lim_{N \to \infty} \sup_{\rho \in K} |h_N(\rho, f) - h(\rho, f)| = 0
\] (63)

holds.

Another simple consequence of Lemma 4.1 is the continuity of \( h(\cdot, f) \) on the interior of \( S \). The proof is again omitted, since it can be taken without change from [13] (first paragraph of the proof of Proposition 1.2.7).

Proposition 4.5 Consider again the assumptions from Lemma 4.1. The function \( \rho \mapsto h(\rho, f) \in \mathbb{R} \) is continuous at each non-degenerate \( \rho \).

This is a somewhat surprising result, because it is derived without any further assumption on the rate function \( I \). Although it does not imply that \( I(\rho, \sigma) \) is continuous in \( \rho \), it shows at least that the dependence of \( I \) on the original density matrix \( \rho \) is quite regular on the interior of the state space \( S \). On the boundary, however, nothing can be said. The discussion in Sections 5.3 and 5.4 will indicate that this is probably a fundamental aspect of admissible rate functions and not just a problem of the methods used in the proofs.

Let us consider now the natural action of \( U(d) \) on the set \( C(S) \) of continuous functions on \( S \), i.e. for each \( U \in U(d) \) and each \( f \in C(S) \) define \( \alpha_U f \in C(S) \) by

\[
\alpha_U f(\sigma) = f(U\sigma U^*).
\] (64)

Then we can consider for each fixed \( \rho \in S \) and each \( f \) the functions

\[
U(d) \ni U \mapsto h_N(U^* \rho U, \alpha_U f) \in \mathbb{R} \quad \text{and} \quad U(d) \ni U \mapsto h(U^* \rho U, \alpha_U f) \in \mathbb{R},
\] (65)

and pose the same question as above – but now considering the dependency on \( U \) rather than on \( \rho \). The following is the analog of Lemma 4.1.

Lemma 4.6 Consider an estimation scheme \( (E_N)_{N \in \mathbb{N}} \) satisfying the LDP with rate function \( I \), an arbitrary continuous (real valued) function \( f \) and the functionals \( h_N, h \) defined in Equations (35) and (36).

1. For each non-degenerate density matrix \( \rho \in S \) and each sequence \( N \ni N \mapsto U_N \in U(d) \) converging to \( U \in U(d) \) we have

\[
\lim_{N \to \infty} h_N(U_N^* \rho U_N, \alpha_{U_N} f) = \lim_{N \to \infty} h_N(U^* \rho U, \alpha_U f) = h(U^* \rho U, \alpha_U f)
\] (66)

2. If \( I \) is lower semicontinuous in both arguments, the lower bound

\[
\liminf_{N \to \infty} h_N(U_N^* \rho U_N, \alpha_{U_N} f) \geq h(U^* \rho U, \alpha_U f)
\] (67)

holds even for degenerate \( \rho \).

Proof. To prove item 1 let us start with the observation that the function sequence \( (\alpha_{U_M} f)_{M \in \mathbb{N}} \) converges uniformly to \( \alpha_U f \). Due to compactness of \( S \)
the function \( f \) is not just continuous but even uniformly continuous, i.e. for each \( \epsilon > 0 \) there is a \( \delta > 0 \) with

\[
\|\sigma_1 - \sigma_2\|_1 < \delta \Rightarrow |f(\sigma_1) - f(\sigma_2)| < \epsilon.
\]  

(68)

Convergence of \((U_M)_{M \in \mathbb{N}}\) implies the existence of \( M_\epsilon \in \mathbb{N} \) with \( M > M_\epsilon \Rightarrow \|U_M - U\| < \delta/2 \). For each \( \sigma \) and each \( M > M_\epsilon \) we therefore get

\[
\|U_M \sigma U_M^* - U \sigma U^*\|_1 \leq \|U_M \sigma U_M^* - U_M \sigma U^*\|_1 + \|U_M \sigma U^* - U \sigma U^*\|_1
\]  

(69)

\[
\leq \|U_M^* - U^*\| \|\sigma\|_1 + \|U_M - U\| \|U^*\| \|\sigma\|_1 < \delta,
\]  

(70)

which implies together with (68) for an arbitrary \( \sigma \) and \( M > M_\epsilon \)

\[
|h_N(U_M^* \rho U_M, f(\sigma)) - h_N(U \rho U, f(\sigma))| < \epsilon.
\]  

(71)

In other words the convergence \( \alpha_{U_M} f \to \alpha_U f \) is uniform as stated (since \( M_\epsilon \) does not depend on \( \sigma \)).

To proceed, it is necessary to consider the following simple properties of the functionals \( h_N \) and \( h_N \): If \( f, f_1 \) denotes continuous functions on \( S \) and \( \epsilon \in \mathbb{R} \) we have for all \( \rho \)

\[
f(\sigma) \geq f_1(\sigma) \Rightarrow h_N(\rho, f) \geq h_N(\rho, f_1), \text{ and } h_N(\rho, f) + \epsilon = h_N(\rho, f_1) + \epsilon,
\]  

(72)

and from Lemma 4.1 we already know that for all \( \epsilon > 0 \) and all \( f \) there is an \( N[\epsilon, f] \in \mathbb{N} \) with

\[
N > N[\epsilon, f] \Rightarrow |h_N(U_N^* \rho U_N, f) - h(U^* \rho U, f)| < \epsilon.
\]  

(73)

Uniform convergence \( \alpha_{U_M} f \to \alpha_U f \) implies that \( \alpha_U f - \epsilon \leq \alpha_{U_M} f \leq \alpha_U f + \epsilon \) holds for all \( M > M_\epsilon \). Hence for all \( N \in \mathbb{N} \) we have

\[
h_N(U_N^* \rho U_N, \alpha_U f) - \epsilon \leq h_N(U_N^* \rho U_N, \alpha_{U_M} f) \leq h_N(U_N^* \rho U_N, \alpha_U f) + \epsilon
\]  

(74)

according to (72). Together with (73) we get

\[
N > N[\epsilon, \alpha_U f], \quad M > M_\epsilon \Rightarrow |h_N(U_N^* \rho U_N, \alpha_{U_M} f) - h(U^* \rho U, \alpha_U f)| < 2\epsilon,
\]  

(75)

which implies Equation (69).

Statement 2 can be shown in the same way, if we replace Equation (73) by (cf. Lemma 4.1)

\[
N > N[\epsilon, \alpha_U f] \Rightarrow h_N(U_N^* \rho U_N, f) \geq h(U^* \rho U, f) - \epsilon
\]  

(76)

and use only the lower bound of (74). \(\square\)

As in the case of Lemma 4.1 we can now derive continuity and uniformity properties from this result. The following proposition is (again) an immediate consequence of 13 Prop. 1.2.7. The proof is therefore omitted.

**Proposition 4.7** Consider the same assumptions as in Lemma 4.4 and a non-degenerate density matrix \( \rho \).
1. The function

\[ U(d) \ni U \mapsto h(U^* \rho U, \alpha_U f) = \inf_{\sigma \in \mathcal{S}} (I(U^* \rho U, U^* \sigma U) + f(\sigma)) \in \mathbb{R} \]  

is continuous.

2. The convergence of \( h_N(U^* \rho U, \alpha_U f) \) to \( h(U^* \rho U, \alpha_U f) \) is uniform in \( U \), i.e.

\[ \lim_{N \to \infty} \sup_{U \in U(d)} |h_N(U^* \rho U, \alpha_U f) - h(U^* \rho U, \alpha_U f)| = 0 \]  

holds.

4.2 Averaging

Let us consider now the question whether covariance and permutation invariance are “harmful” for the rate function; i.e. can we hope to exhaust the optimal upper bounds from Equation (12) with schemes admitting these symmetry properties? One possible way to answer this question is to start with a general scheme \((E_N)_{N \in \mathbb{N}}\) and to average over the unitary and the permutation group. For the latter this leads to

\[ \mathcal{E}_N(\Delta) = \frac{1}{N!} \sum_{p \in S_N} V_p E_N(\Delta) V_p^*, \]  

and since we have

\[ \text{tr}(\rho^\otimes N V_p E_N(\Delta) V_p^*) = \text{tr}(V_p^* \rho^\otimes N V_p E_N(\Delta)) = \text{tr}(\rho^\otimes N E_N(\Delta)) \]  

for each permutation \( p \in S_N \), we see that the rate function is not changed at all by this procedure. Hence, for the rest of this section we can assume without loss of generality that each scheme is permutation invariant.

This leads us to averages over the unitary group, i.e.

\[ \mathcal{E}_N(\Delta) = \int_{U(d)} U^\otimes N E_N(U^* \Delta U) U^\otimes N^* dU. \]  

Here the situation is (unfortunately) different. The following proposition shows that the convergence behavior of \( \mathcal{E}_N \) is in general worse than that of \( E_N \).

**Proposition 4.8** Consider an estimation scheme \((E_N)_{N \in \mathbb{N}}\) satisfying the LDP with rate function \( I \) and the corresponding averaged scheme \((\mathcal{E}_N)_{N \in \mathbb{N}}\) from Equation (81). For each non-degenerate density matrix \( \rho \) the sequence of probability measures \( \text{tr}(\rho^\otimes N \mathcal{E}_N(\cdot)) \) satisfies the LDP with rate function \( \mathcal{T}_\rho \) given by

\[ \mathcal{T}_\rho(\sigma) = \mathcal{T}(\rho, \sigma) = \inf_{U \in U(d)} I(U^* \rho U, U^* \sigma U). \]  

**Proof.** It is sufficient to show that the measures \( \text{tr}(\rho^\otimes N \mathcal{E}_N(\cdot)) \) satisfy the Laplace principle with the same rate function (cf. Theorem A.3), because the Laplace principle is equivalent to the large deviation principle. Hence we have to show that

\[ \lim_{N \to \infty} \frac{-1}{N} \ln \int_{\mathcal{S}} e^{-N f(\sigma)} \text{tr}(\rho^\otimes N \mathcal{E}_N(d\sigma)) = \inf_{\sigma \in \mathcal{S}} (f(\sigma) + \mathcal{T}(\rho, \sigma)) \]  

(83)
holds for all continuous functions \( f \) on \( S \). Inserting the definition of \( \mathcal{E}_N \) we get

\[
\int_S e^{-N f(\sigma)} \text{tr}(\rho^{\otimes N} \mathcal{E}_N(d\sigma)) = \int_{U(d)} \int_S e^{-N f(U^* \sigma)} \text{tr}((U^* \rho U)^{\otimes N} \mathcal{E}_N(d\sigma)) dU,
\]

or with the notation from Subsection 4.1 (cf. Equations (83) and (84))

\[
\int_S e^{-N f(\sigma)} \text{tr}(\rho^{\otimes N} \mathcal{E}_N(d\sigma)) = \int_{U(d)} e^{-Nh_N(U^* \rho U, \alpha_U f)} dU.
\]

According to Proposition 4.7, the quantity \( h_N(U^* \rho U, \alpha_U f) \) converges uniformly in \( U \) to \( h(U^* \rho U, \alpha_U f) \), i.e. for each \( \epsilon > 0 \) there is an \( N_\epsilon \in \mathbb{N} \) such that

\[
N > N_\epsilon \Rightarrow h(U^* \rho U, \alpha_U f) + \epsilon \geq h_N(U^* \rho U, \alpha_U f) \geq h(U^* \rho U, \alpha_U f) - \epsilon \quad \forall U \in U(d)
\]

holds. Hence, for each \( \epsilon > 0 \) we get

\[
\limsup_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh_N(U^* \rho U, \alpha_U f)} dU \geq \limsup_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh(U^* \rho U, \alpha_U f)} dU.
\]

From Proposition 4.7 we know that \( h(U^* \rho U, \alpha_U f) \) is continuous in \( U \) and we can apply Varadhan’s Theorem (Theorem A.3) to the left hand side of this inequality. Together with

\[
\inf_{U \in U(d)} h(U^* \rho U, \alpha_U f) = \inf_{U \in U(d)} \inf_{\sigma \in S} \{ I(U^* \rho U, \sigma) + f(U^* \sigma) \}
\]

this implies the upper bound

\[
\limsup_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh(U^* \rho U, \alpha_U f)} dU \leq \inf_{\sigma \in S} \{ I(\rho, \sigma) + f(\sigma) \} + \epsilon.
\]

The lower bound

\[
\liminf_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh(U^* \rho U, \alpha_U f)} dU \geq \inf_{\sigma \in S} \{ I(\rho, \sigma) + f(\sigma) \} - \epsilon
\]

can be shown in the same way. Since \( \epsilon > 0 \) was arbitrary, Equation (86) follows from (85), (91) and (92), which concludes the proof.

Hence, the best we can hope is that the averaged scheme satisfies the LDP with rate function \( \mathcal{T} \) which is actually the worst \( U(d) \)-invariant rate function which can be derived from \( I \). Only if \( I \) is \( U(d) \) invariant itself (such that \( \mathcal{T} = I \) holds), the convergence behavior of \( \{ \mathcal{E}_N \}_{N \in \mathbb{N}} \) is as good as that of \( \{ \mathcal{E}_N \}_{N \in \mathbb{N}} \). The following proposition shows that at least in this case the convergence problems on the boundary of \( S \) can be solved.
Proposition 4.9 If \((E_N)_{N \in \mathbb{N}}\) is an estimation scheme satisfying the LDP with a \(U(d)\)-invariant, lower semicontinuous (in both arguments) rate function \(I\), the averaged scheme \((E_N)_{N \in \mathbb{N}}\) defined in Equation (81) satisfies the LDP with the same rate function.

Proof. We will show again the alternative statement that the sequence \(\text{tr}(\rho \otimes N E_N(\cdot))\) satisfies the Laplace principle, i.e. Equation (83) holds for all continuous real-valued functions \(f\) and with \(\tilde{T}\) replaced by \(I\). As in the last proof we can rewrite this in terms of the functionals \(h_N\) and \(h\) defined in Equation (85) and (86), i.e. we have to show that (cf. Equation (85))

\[
\limsup_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh_N(U^* \rho U, f)} dU \leq h(\rho, f) \tag{93}
\]

and

\[
\liminf_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh_N(U^* \rho U, f)} dU \geq h(\rho, f) \tag{94}
\]

hold. But now the convergence of \(h_N(U^* \rho U, f)\) to \(h(\rho, f)\) is only known to be pointwise (and not necessarily uniform) in \(U\). Therefore, we can not proceed as in Proposition 4.8. Instead we will use different strategies for the upper and lower bound.

To get the upper bound note that \(f\) is (as a continuous function on a compact set) bounded from above by a constant \(K > 0\). Therefore the functions \(U \mapsto h_N(U^* \rho U, f)\) are bounded as well (by the same constant) and we get (note that \(h(U^* \rho U, f) = h(\rho, f)\) holds for all \(U\) by assumption)

\[
\lim_{N \to \infty} \int_{U(d)} |h_N(U^* \rho U, f) - h(\rho, f)| dU = 0. \tag{95}
\]

by the dominated convergence theorem. Now let us introduce for each \(\epsilon > 0\) and each \(N \in \mathbb{N}\) the set

\[
\Delta_{N, \epsilon} = \{ U \in U(d) \mid |h_N(U^* \rho U, f) - h(\rho, f)| > \epsilon \}. \tag{96}
\]

From Equation (96) we see that for each \(\delta > 0\) there is an \(N_\delta \in \mathbb{N}\) such that \(N > N_\delta\) implies

\[
|\Delta_{N, \epsilon}| \leq \int_{U(d)} |h_N(U^* \rho U, f) - h(\rho, f)| dU < \epsilon, \tag{97}
\]

where \(|\Delta_{N, \epsilon}|\) denotes the volume of \(\Delta_{N, \epsilon}\) with respect to the Haar measure (note that \(\Delta_{N, \epsilon}\) is due to continuity of \(U \mapsto h_N(U^* \rho U, f)\) open and therefore measurable). Now choose \(\epsilon > 0\) arbitrary and \(\delta = \epsilon/2\) then we have for all \(N > N_\delta\)

\[
\int_{U(d)} e^{-Nh_N(U^* \rho U, f)} dU \geq \int_{U(d) \setminus \Delta_{N, \epsilon}} e^{-Nh_N(U^* \rho U, f)} dU \geq \frac{1}{2} e^{-N(h(\rho, f) + \epsilon)}, \tag{98}
\]

where we have used the fact that \(h_N(U^* \rho U, f) < h(\rho, f) + \epsilon\) holds for all \(U \notin \Delta_{N, \epsilon}\). Taking logarithms and the limit \(N \to \infty\) this implies

\[
\limsup_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh_N(U^* \rho U, f)} dU \leq h(\rho, f) + \epsilon. \tag{99}
\]
Since $\epsilon > 0$ was arbitrary we get the upper bound (93).

To prove the lower bound let us assume first that

$$\liminf_{N \to \infty} \inf_{U \in U(d)} (h_N(U^* \rho_U, \alpha_U f) - h(\rho, f)) \geq 0$$  \hspace{1cm} (100)

does not hold. Then we can find a sequence $(U_N)_{N \in \mathbb{N}}$ of unitaries with

$$\liminf_{N \to \infty} (h_N(U_N^* \rho_{U_N}, \alpha_{U_N} f) - h(\rho, f)) < 0.$$  \hspace{1cm} (101)

But due to compactness of $U(d)$ we can assume without loss of generality that $(U_N)_{N \in \mathbb{N}}$ converges to a unitary $U$. Hence Equation (101) contradicts Statement 2 of Lemma 4.6 (since the rate function $I$ is lower semicontinuous by assumption). Hence Equation (100) is valid and we can find for each $\epsilon > 0$ an $N_\epsilon \in \mathbb{N}$ such that $N > N_\epsilon$ implies

$$h_N(U^* \rho_U, \alpha_U f) > h(\rho, f) - \epsilon \quad \forall U \in U(d).$$  \hspace{1cm} (102)

Hence

$$\liminf_{N \to \infty} -\frac{1}{N} \ln \int_{U(d)} e^{-Nh_N(U^* \rho_U, \alpha_U f)} dU > h(\rho, f) - \epsilon.$$  \hspace{1cm} (103)

Since $\epsilon > 0$ is arbitrary we get the lower bound (94) and the proof is completed.

This result is very useful if we want to check whether a given rate function is admissible or not. Many prominent candidates are $U(d)$-invariant and lower semicontinuous (like relative entropy), and in this case it is according to Proposition 4.9 sufficient to consider only covariant schemes. Important examples of functions which can be tested this way are the optimal rate functions $I_{Id}$ and $I_{0 Id}$ (for $I_{Id}$ this is true at least on the interior of $S$):

**Proposition 4.10** The optimal rate functions $I_{Id}$ and $I_{0 Id}$ are $U(d)$ invariant (i.e. Equation (14) holds with $\alpha_U(\sigma) = U\sigma U^*$).

**Proof.** Since $I_{Id}$ and $I_{0 Id}$ are defined as the upper bounds on $E(\text{Id})$ and $E^0(\text{Id})$ we have to show that these sets are invariant under the operation $I \mapsto I_U$ with $I_U(\rho, \sigma) = I(U\rho U^*, U\sigma U^*)$. Hence consider $I \in E(\text{Id})$. Then there is a full estimation scheme $(E_N)_{N \in \mathbb{N}}$ satisfying LDP with rate function $I$. For each fixed $U \in U(d)$ we can define the translated scheme $(E^U_N(\Delta))_{N \in \mathbb{N}}$ with $E^U_N(\Delta) = U^{\otimes N} \cdot E_N(U \Delta U^*)^{U \otimes N}$. If $\Delta$ is open we get

$$\liminf_{N \to \infty} \frac{1}{N} \ln \text{tr}(\rho^{\otimes N} E^U_N(\Delta)) = \liminf_{N \to \infty} -\frac{1}{N} \ln \text{tr}((U\rho U^*)^{\otimes N} E_N(U \Delta U^*))$$  \hspace{1cm} (104)

$$\leq -\inf_{\sigma \in U \Delta U^*} I(U\rho U^*, \sigma)$$  \hspace{1cm} (105)

$$= -\inf_{\sigma \in \Delta} I(U\rho U^*, U\sigma U^*).$$  \hspace{1cm} (106)

This shows that the large deviation upper bound holds with rate function $I_U$. The lower bound can be shown in the same way. Hence $(E^U_N)_{N \in \mathbb{N}}$ satisfies the LDP with rate function $I_U$, and this implies $I_U \in E(\text{Id})$. Since the operation $I \mapsto I_U$ respects semi-continuity of $I$, invariance of $E^0(\text{Id})$ is trivial and this concludes the proof.
Summarizing the discussion of this subsection we can conclude that averaging is in the context of large deviations not as powerful as it is in other areas like optimal cloning. Nevertheless, it is not completely useless either. In particular the conjecture \( \mathcal{I}^0_{\text{id}} \in \mathcal{E}(\rho) \) is interesting in this regard, because it would imply that \( \mathcal{I}^0_{\text{id}} \) can be derived as the rate function of a covariant scheme. Hence, covariant schemes are an important special case (and therefore worth studying), although they probably can not tell us the whole truth.

4.3 General structure

Now let us have a look at the general structure of covariant and permutation invariant estimation schemes. Our main tool is the following theorem about covariant observables \([24]\).

**Theorem 4.11** Consider a compact group \( G \) which acts transitively on a locally compact, separable metric space \( X \) by \( G \times X \ni (g,x) \mapsto \alpha_g(x) \), and a representation \( \pi \) of \( G \) on a Hilbert space \( \mathcal{H} \). Each POV measure \( E : \mathcal{B}(X) \to \mathcal{B}(\mathcal{H}) \) which is covariant (i.e. \( E(\alpha_g\Delta) = \pi(g)E(\Delta)\pi(g)^* \) for all \( \Delta \in \mathcal{B}(X) \) and all \( g \in G \)) has the form

\[
\int_X f(x)E(dx) = \int_G f(\alpha_g x_0)\pi(g)Q_0\pi(g)^*\mu(dg)
\]

where \( x_0 \in X \) is an (arbitrary) reference point, \( \mu \) is the Haar-measure on \( G \) and \( Q_0 \in \mathcal{B}(\mathcal{H}) \) a positive operator which is uniquely determined by (107) and the choice of \( x_0 \).

Unfortunately this theorem is not applicable to our case, because the action of \( U(d) \) on \( S \) is not transitive. A way out of this dilemma is to look at the fibration \( s : S \to \Sigma \) defined in Equation (4) and to apply the results about transitive group actions to each fiber separately. (For the rest of this section we will use frequently the notations introduced in Section 3.1.)

**Theorem 4.12** Each covariant and permutation invariant observable \( E : \mathcal{B}(S) \to \mathcal{B}(\mathcal{H}^\otimes N) \) has the form (with a continuous function \( f \) on \( S \))

\[
\int_S f(\rho)E(d\rho) = \sum_{Y \in \mathcal{Y}_d(N)} \left[ \int_{U(d)} \pi_Y(U) \left( \int_{\Sigma} f(U\rho_x U^*)q_Y(dx) \right) \pi_Y(U^*)dU \right] \otimes I_Y
\]

with a sequence of (non-normalized) POV measures \( q_Y : \mathcal{B}(\Sigma) \to \mathcal{B}(\mathcal{H}_Y) \), the diagonal matrices \( \rho_x = \text{diag}(x_1,\ldots,x_d) \) from Equation (21) and the unit matrix \( I_Y \in \mathcal{B}(\mathcal{K}_Y) \).

**Proof.** Permutation invariance implies immediately that

\[
E_N(\Delta) = \bigoplus_{Y \in \mathcal{Y}_d(N)} E_{N,Y}(\Delta) \otimes I_Y
\]
holds with $\mathds{1}_Y \in \mathcal{B}(K_Y)$ and a family of POV measures $E_{N,Y} : \mathfrak{B}(S) \to \mathcal{B}(H_Y)$, which are again $U(d)$ covariant:

$$E_{N,Y}(U \Delta U^*) = \pi_Y(U)E_N(\Delta)\pi_Y(U)^* \quad \forall U \in U(d).$$

Hence we only have to look at $E_{N,Y}$ for a fixed $Y \in \mathcal{Y}_d(N)$, Therefore the statement is a consequence of the following lemma.

**Lemma 4.13** Each $U(d)$ covariant observable $E : \mathfrak{B}(S) \to \mathcal{B}(H_Y)$ has the form

$$\int_S f(\rho)E(d\rho) = \int_{U(d)} \pi_Y(U) \left( \int_{\Sigma} f(U\rho x U^*) q(dx) \right) \pi_Y(U^*)dU$$

with an appropriate POV-measure $q : \mathfrak{B}(\Sigma) \to \mathcal{B}(H_Y)$.

**Proof.** To each $\rho \in G$ we can associate the stabilizer subgroup $G_\rho = \{ U \in U(d) \mid U\rho U^* = \rho \}$ of $U(d)$, whose structure is uniquely determined by the degeneracy of the eigenvalues of $\rho$. Hence the set

$$J = \{ G_\rho \mid x \in \Sigma \} \text{ with } \rho_x = \text{diag}(x_1, \ldots, x_d)$$

is finite and for each $\rho$ there is exactly one $G \in J$ such that $G_\rho = UGU^*$ holds with an appropriate unitary $U \in U(d)$. We can decompose $\Sigma$ therefore into a disjoint union $\Sigma = \bigcup_{G \in J} S_G$ of finitely many subsets

$$S_G = \{ \rho \in \Sigma \mid \exists U \in U(d) \text{ with } G_\rho = UGU^* \}.$$  

and similarly we have $\Sigma = \bigcup_{G \in J} \Sigma_G$ with $\Sigma_G = s(S_G)$. By construction each orbit $s^{-1}(x)$, $x \in \Sigma_G$ is naturally homeomorphic to the homogeneous space $X_G = U(d)/G$. Hence, there is a natural homeomorphism $\Phi_G : \Sigma_G \times X_G \to S_G$ which is uniquely determined by

$$\Phi_G(x, [\mathds{1}]) = \rho_x \text{ and } \Phi_G(x, [V]) = V\rho_x V^* \quad \forall x \in \Sigma_G \forall [V] \in X_G.$$  

Note that the crucial property of $\Phi_G$ is to intertwine the group actions $\rho \mapsto U\rho U^*$ and $[V] \mapsto [UV]$ of $U(d)$ on $S_G$ and $X_G$ respectively.

The $S_G$ are in general neither open nor closed, but they are Borel subsets of $\Sigma$ (more precisely differentiable submanifolds with boundary): Since $s$ is continuous, it is obviously sufficient to show that $\Sigma_G \in \mathfrak{B}(\Sigma)$ holds. But this follows from the fact that each $\Sigma_G$ can be expressed as the complement of a Borel set in a finite union of closed sets (this is easy to see but tedious to write down). $S_G \subseteq \mathfrak{B}(S)$ now implies $\mathfrak{B}(S_G) = \{ \Delta \cap S_G \mid \Delta \in \mathfrak{B}(S) \} \subset \mathfrak{B}(S)$ and we can define the POV measures $E_G : \mathfrak{B}(S_G) \to \mathcal{B}(H_Y)$, $E_G(\Delta) = E(\Delta)$. Note that the $E_G$ are not normalized and some of them can vanish completely. Since we can reconstruct $E$ from the $E_G$ by $E(\Delta) = \sum_G E_G(\Delta \cap S_G)$ it is sufficient to prove the statement for each $G$ separately. In addition we can use the homeomorphism $\Phi_G$ from Equation (114) to identify $S_G$ with $\Sigma_G \times X_G$ and $E_G$ with a POVM on $\mathfrak{B}(\Sigma_G \times X_G)$ which is covariant with respect to the group action

$$\Sigma_G \times X_G \ni (x, [V]) \mapsto a^G_U(x, [V]) = (x, [UV]) \in \Sigma_G \times X_G$$

The decomposition of $\Sigma$ into a finite union of fiber bundles we are describing here is a special case of a much more general result (“slice theorem”) about compact $G$-manifolds; cf. [25].
of $U(d)$, i.e.
\[
E_G(\delta_G^\Delta) = \pi_Y(U)E_G(\Delta)\pi_Y(U^*) \quad \forall \Delta \in \mathfrak{B}(\Sigma_G \times X_G) \forall U \in U(d). \tag{116}
\]

This is a direct consequence of the intertwining property of $\Phi_G$ mentioned above.

Now let us consider the Abelian algebras $C(X_G)$ and $C(\Sigma_G)$ of continuous functions on $X_G$ and $\Sigma_G$. Each $h \in C(\Sigma_G)$ defines a positive linear map by
\[
C(X_G) \ni k \mapsto \tilde{E}_{G,h}(k) = \int_{\Sigma_G \times X_G} h(x)k(y)E_G(dx \times dy) \in B(\mathcal{H}_Y). \tag{117}
\]

Positivity and linearity of $\tilde{E}_{G,h}$ imply that it can be expressed as an integral over $X_G$ with respect to a POV measure $E_{G,h}$
\[
\tilde{E}_{G,h}(k) = \int_{X_G} k(y)E_{G,h}(dy) \tag{118}
\]
(this is a general property of positive maps on Abelian algebras; cf. [33]). From (116) it follows immediately that $E_{G,h}$ is covariant and we can apply Theorem 4.11 i.e. there is a positive operator $Q_G(h)$ such that
\[
\tilde{E}_{G,h}(k) = \int_{U(d)} k([U])\pi_Y(U)Q_G(h)\pi_Y(U^*)dU \tag{119}
\]
holds. Note that the distinguished point $x_o$ from Theorem 4.11 is in our case $[I] \in X_G$. Since $Q_Y(h)$ is uniquely defined by this equation (cf. Theorem 4.11) we get another positive linear map $Q_G : C(\Sigma_G) \ni h \mapsto Q(h) \in B(\mathcal{H}_Y)$ which can again be expressed as an integral
\[
Q_G(h) = \int_{\Sigma_G} h(x)q_G(dx), \tag{120}
\]
and we get
\[
\int_{\Sigma_G \times X_G} f(x,y)E_G(dx \times dy) = \\
\int_{U(d)} \pi_Y(U) \left( \int_{\Sigma_G} f([U],x)q_G(dx) \right) \pi_Y(U^*)dU. \tag{121}
\]
for each $f$ of the form $f(x,y) = k(x)h(y)$ with $k \in C(\Sigma_G)$, $h \in C(X_G)$, and by linearity and continuity for each continuous $f$ on $\Sigma_G \times X_G$. Now we can again apply the homeomorphism $\Phi_G$ to map $E_G$ back to a measure on $S_G$. Since $\Phi_G$ intertwines the action of $U(d)$ on $S_G$ and $\Sigma_G \times X_G$ we get from (121)
\[
\int_S f(\rho)E_G(d\rho) = \int_{U(d)} \pi_Y(U) \left( \int_{\Sigma} f(U\rho U^*)q_G(dx) \right) \pi_Y(U^*)dU \tag{122}
\]
Hence the statement of the lemma follows with $q(\Delta) = \sum_G q_G(\Delta \cap \Sigma_G)$. [\hfill \Box]

Together with the decomposition of $E$ from Equation (109), the statement of this lemma concludes the proof of the theorem. [\hfill \Box]
4.4 An explicit scheme

The class of observables described in Theorem 4.12 is still quite big. To reduce the freedom of choice further we can focus our attention to estimation schemes which coincide with $(\hat{F}_N)_{N \in \mathbb{N}}$ from Theorem 3.1, as long as only information about the spectrum of $\rho$ is required. In other words $E_N$ should satisfy for all $N \in \mathbb{N}$

$$E_N(s^{-1}(\Delta)) = \hat{F}_N(\Delta) \quad \forall \Delta \in \mathcal{B}(\Sigma), \quad (123)$$

This leads to the following corollary.

**Corollary 4.14** Each covariant and permutation invariant estimation scheme $(E_N)_{N \in \mathbb{N}}$ which satisfies Equation (123) can be written as

$$\int_S f(\rho)E_N(d\rho) = \sum_{Y \in \mathcal{Y}_d(N)} \int_{U(d)} f(U\rho_{Y/N}U^*) U^{\otimes N} (Q_Y \otimes \mathbb{1}) U^{\otimes N^*} dU, \quad (124)$$

with a family of operators $Q_Y \in \mathcal{B}(H_Y)$.

**Proof.** Equation (123) implies immediately that the POV measures $q_Y$ from Proposition 4.12 are discrete, i.e.

$$q_Y = \sum_{Z \in \mathcal{Y}_d(N)} q_{YZ} \delta_{Z/N} \quad (125)$$

where $\delta_{Z/N}$ denotes the Dirac measure at $Z/N \in \Sigma$ and $q_{YZ} \in \mathcal{B}(H_Y)$. Hence $E_N$ becomes

$$\int_S f(\rho)E_N(d\rho) = \sum_{Y \in \mathcal{Y}_d(N)} \int_{U(d)} f(U\rho_{Y/N}U^*) U^{\otimes N} \hat{Q}_Y U^{\otimes N^*} dU, \quad (126)$$

with

$$\hat{Q}_Y = \sum_{Z \in \mathcal{Y}_d(N)} q_{YZ} \otimes \mathbb{1}. \quad (127)$$

Using the definition of $\hat{F}_N$ in Equation (17) and again Equation (123) we get

$$P_Y = \hat{F}_N(\{Y/N\}) = E_N(s^{-1}(Y/N)) = \int_{U(d)} U^{\otimes N} \hat{Q}_Y U^{\otimes N^*} dU, \quad (128)$$

but this implies that $\hat{Q}_Y$ must be of the form $\hat{q}_Y \otimes \mathbb{1}$ with $q_Y \in \mathcal{B}(H_Y)$. Hence (127) implies $q_{ZY} = 0$ for $Y \neq Z$, which proves the corollary. \(\square\)

Since the estimation scheme $(\hat{F}_N)_{N \in \mathbb{N}}$ is asymptotically optimal, condition (123) looks at a first glance very natural. In contrast to permutation invariance and covariance, however, we have no proof that it does not “harm” the rate function. In other words the crucial question is: Given a covariant and permutation invariant estimation scheme $(E_N)_{N \in \mathbb{N}}$ satisfying LDP with rate function $I$, does there exist a scheme $(\tilde{E}_N)_{N \in \mathbb{N}}$ which satisfies Equation (123) and the LDP with a rate function $\tilde{I}$ such that $I \leq \tilde{I}$ holds? A possible strategy towards a proof might be to define $\tilde{E}_N$ by Equation (124) with $Q_Y = \int q_Y(dx)$ and the POV measures $q_Y$ which define $E_N$ according to Theorem 4.12. The hard part
(which we haven’t solved up to now) is of course to show that the rate function
\( \hat{I} \) of such a scheme is at least as good as \( I \).

If we accept condition \( \text{(123)} \) nevertheless, the estimation scheme \( (\hat{E}_N)_{N \in \mathbb{N}} \) arises from Corollary \( \text{(14)} \) if we choose
\[
Q_Y = \dim \mathcal{H}_Y |\phi_Y\rangle \langle \phi_Y|,
\]
where \( \phi_Y \) denotes the highest weight vector of the irreducible representation \( \pi_Y \). To see (heuristically) why this should be a good choice for the \( Q_Y \), consider a nonsingular, diagonal density matrix \( \rho = e^H \) with \( h = \text{diag}(h_1, \ldots, h_d) \) and \( h_1 \geq \cdots \geq h_d \). Since \( E_N \) projects to \( F_N \) we know already that we get an exact estimate for the spectrum of \( \rho \) in the limit \( N \to \infty \). To get a consistent scheme we need operators \( Q_Y \) such that the quantities
\[
\text{tr}(\pi_Y(\rho^*U)Q_Y) \dim K_Y = \text{tr}((\rho^*U)^{\otimes N}(Q_Y \otimes \mathbb{1}))
\]
(regarded as densities along the orbits \( S_Y = s^{-1}(Y/N) \)) are more and more concentrated on the density operators with the correct eigenvectors, i.e. to \( \rho_{Y/N} \).

Since \( Y \in \mathcal{Y}_d(N) \) is the highest weight of the irreducible representation \( \pi_Y \) and \( \phi_Y \) its highest weight vector, the highest eigenvalue of \( \pi_Y(\rho) \) is given by \( \exp(\sum_j Y_j h_j) \) and \( \phi_Y \in \mathcal{H}_Y \) is the corresponding eigenvector. All other eigenvalues grow with a lower exponential rate (or decay faster, depending on the chosen normalization). The matrix element \( \langle \phi_Y, \pi_Y(\rho)\phi_Y \rangle \) dominates therefore all other eigenvalues in the limit \( N \to \infty \). Hence the density \( \text{(130)} \) has the desired behavior if we choose \( Q_Y = |\phi_Y\rangle \langle \phi_Y| \). Note that the reasoning just sketched indicate that for any consistent scheme of the form \( \text{(124)} \) the overlap of the \( Q_Y \) with \( |\phi_Y\rangle \langle \phi_Y| \) should not decay too fast (at most polynomial). In the case of pure input state we will make this reasoning more precise; cf. Section \( \text{5.3} \).

### 4.5 Proof of Theorem \( \text{3.2} \)

Our next task is to prove Theorem \( \text{3.2} \) i.e. we have to show that the estimation scheme \( \hat{E}_N \) defined in Equation \( \text{(20)} \) satisfies the LDP with rate function \( \hat{I} \) given in \( \text{(20)} \). The first step is to check that \( \hat{I} \) is well defined.

**Lemma 4.15** There is a (unique) function \( \hat{I} \) on \( S \times S \) which satisfies
\[
\hat{I}(\rho, \rho_x U^*) = \sum_{j=1}^d x_j \ln(x_j) - I_1(\rho, U, x)
\]
and
\[
I_1(\rho, U, x) = \sum_{j=1}^d (x_j - x_{j+1}) \ln[\rho_m(U^* \rho U)]
\]
where we have set \( x_{d+1} = 0 \). \( \hat{I} \) is positive and \( \hat{I}(\rho, \sigma) = 0 \) implies \( \sigma = \rho \).

**Proof.** To prove that \( \hat{I} \) is well defined we have to show that \( U_1 \rho_x U_1^* = U_2 \rho_x U_2^* \implies I_1(\rho, U_1, x) = I_1(\rho, U_2, x) \). This is equivalent to \([U, \rho_x] = 0 \implies I_1(\rho, U, x) = I_1(\rho, U, x) \). To exploit the relation \([U, \rho_x] = 0 \) let us introduce \( k \leq d \) integers \( 1 = j_0 < j_1 < \cdots < j_k = d + 1 \) such that \( x_{j_\alpha} > x_{j_{\alpha+1}} \) and \( x_j = x_{j_\alpha} > 0 \) holds for \( j_\alpha \leq j < j_{\alpha+1} \) and \( \alpha < k \). Then we have
\[
I_1(\rho, U, x) = \sum_{\alpha=1}^k (x_{j_{\alpha-1}} - x_{j_\alpha}) \ln[\rho_m(U^* \rho U)]
\]

\[25\]
On the other hand \([U, \rho_x] = 0\) implies that \(U\) is block diagonal

\[
U = \text{diag}(U_0, \ldots, U_{k-1}) \text{ with } U_\alpha \in U(d_\alpha), \ d_\alpha = j_{\alpha+1} - j_\alpha.
\] (133)

Hence we have \(\text{pm}_j,_{\alpha-1}(U^*\rho U) = \text{pm}_j,_{\alpha-1}(\rho)\) for all such \(U\) and all \(\rho\) with \(1 \leq \alpha \leq k\). Together with Equation (132) this shows that \(\hat{I}\) is well defined.

To prove positivity we have to show that \(\inf U \hat{I}(\rho, U\rho_x U^*) \geq 0\) holds for each \(\rho\) and \(x\). Hence we have to minimize \(\hat{I}\) (for fixed \(x\) and \(\rho\)) and since \(x_j \geq x_{j+1}\) this implies that we have to maximize the minors of \(U^*\rho U\). To this end let us denote the eigenvalues of \(\rho\) and the upper left \(j \times j\) submatrix of \(U^*\rho U\) by \(\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d\) respectively \(\lambda_1^{(j)} \geq \lambda_2^{(j)} \geq \cdots \geq \lambda_j^{(j)}\). The minors of \(U^*\rho U\) then become \(\text{pm}_j(U^*\rho U) = \lambda_1^{(j)} \cdots \lambda_j^{(j)}\). According to [23 Thm 4.3.15] the \(\lambda_j^{(j)}\) satisfy the constraint \(\lambda_k \geq \lambda_k^{(j)}\) for all \(k = 1, \ldots, j\), and this bound is (obviously) saturated if \(U^*\rho U\) is diagonal in the preferred basis. Hence we get \(\text{pm}_j(U^*\rho U) \leq \lambda_1 \cdots \lambda_j\) and therefore

\[
\hat{I}(\rho, U\rho_x U^*) \geq \sum_{j=1}^d x_j \ln(x_j) - \sum_{j=1}^d (x_j - x_{j+1}) \ln(\lambda_1 \cdots \lambda_j).
\] (134)

Expanding the logarithms and reshuffling the second sum leads to

\[
\hat{I}(\rho, U\rho_x U^*) \geq \sum_{j=1}^d x_j (\ln(x_j) - \ln(\lambda_j)),
\] (135)

and equality holds iff \(\rho\) and \(\sigma = U\rho_x U^*\) are simultaneously diagonalizable. Since the left hand side of this inequality is a relative entropy of classical probability distributions, we see that \(\hat{I}\) is positive and \(\hat{I}(\sigma) = 0\) holds iff \(\sigma = \rho\). \(\square\)

Now let us show that \((\hat{E}_N)_{N \in \mathbb{N}}\) satisfies the LDP with rate function \(\hat{I}\). As in the proof of Proposition [12] we will do this by proving the equivalent statement that \((\hat{E}_N)_{N \in \mathbb{N}}\) satisfies the Laplace principle with the same rate function, i.e.

\[
\lim_{N \to \infty} \frac{-1}{N} \ln \int_S e^{-Nf(\sigma)} \text{tr}(\rho \otimes N \hat{E}_N(\text{d}\sigma)) = \inf_{\sigma \in S} \left( f(\sigma) + \hat{I}(\rho, \sigma) \right)
\] (136)

should hold for all continuous functions \(f\) on \(S\). If we insert the definition of \(\hat{E}_N\), the integral on the left hand side becomes

\[
\int_S e^{-Nf(\sigma)} \text{tr}(\rho \otimes N \hat{E}_N(\text{d}\sigma)) = \sum_{Y \in \mathcal{Y}_d(N)} \dim \mathcal{H}_Y \int_{U(d)} e^{-Nf(U^*\rho U)} \text{tr}((U^*\rho U) \otimes N |\phi_Y\rangle \langle \phi_Y| \otimes Y) \text{d}U,
\] (137)

where \(Y\) denotes the unit operator on \(K_Y\). Now assume that \(\rho\) is non-degenerate (i.e. \(\rho \in \text{GL}(d, \mathbb{C})\)) then we can rewrite the density in this integral to

\[
\text{tr}((U^*\rho U) \otimes N |\phi_Y\rangle \langle \phi_Y| \otimes Y) = \text{tr}(P_Y(U^*\rho U) \otimes N P_Y |\phi_Y\rangle \langle \phi_Y| \otimes Y)
\] = \(\dim K_Y \text{tr}(\pi_Y(U^*\rho U) |\phi_Y\rangle \langle \phi_Y|)
\] = \(\dim K_Y \langle \phi_Y, \pi_Y(U^*\rho U)\phi_Y \rangle
\] (138) (139) (140)
where we have used in the second equation that $P_Y(U^*\rho U)^{\otimes N}Y_Y = \pi_Y(U^*\rho U)^{\otimes N}$ holds. The matrix elements of $\pi_Y(U^*\rho U)$ with respect to the highest weight vector can be expressed as ([33] § 49 or [34] Sect. IX.8)

$$
\langle \phi_Y, \pi_Y(U^*\rho U)\phi_Y \rangle = \prod_{k=1}^d p_{m_k}(U^*\rho U)^{Y_k-Y_{k+1}},
$$

(141)

where we have set $Y_{d+1} = 0$. The right hand side of this equation makes sense even if the exponents are not integer valued. We can rewrite therefore Equation (137) with the probability measure

$$
\int_{\Sigma} h(x)\nu_N(dx) = \frac{1}{d^N} \sum_{Y \in \mathcal{Y}_d(N)} h(\frac{Y}{N}) \dim(H_Y) \dim(K_Y)
$$

(142)

to get

$$
\int_{\mathcal{S}} e^{-Nf(\sigma)} \mathrm{tr}(\rho^{\otimes N} \hat{E}_N(d\sigma))
$$

(143)

$$
= \int_{\mathcal{S}} \int_{U(d)} d^N e^{-Nf(U\rho U^*)} \prod_{k=1}^d p_{m_k}(U^*\rho U)^{N(x_k-x_{k+1})} dU\nu_N(dx)
$$

(144)

$$
= \int_{\mathcal{S}} \int_{U(d)} \exp\left(-N\left[f(U\rho U^*) - \ln(d) - I_1(U,\rho,x)\right]\right) dU\nu_N(dx)
$$

(145)

where

$$
I_1(\rho, U, x) = \sum_{k=1}^d (x_k - x_{k+1}) \ln\left[p_{m_k}(U^*\rho U)\right]
$$

(146)

is the function from Equation (131). Now we need the following Lemma

**Lemma 4.16** The probability measures $\nu_N$ defined in Equation (142) satisfy the large deviation principle with rate function

$$
I_0(x) = \ln(d) + \sum_{j=1}^d x_j \ln(x_j).
$$

(147)

**Proof.** This follows immediately from Theorem 3.1 with $\rho = \frac{1}{d}$ (cf. also [12]). □

Obviously the product measure $\nu_N(dx) \times dU$ satisfies the LDP with the same rate function. Moreover, the function in the argument of the exponential in Equation (143) is continuous in $x$ and $U$. Hence we can apply Varadhan’s theorem to Equation (145) and get

$$
\lim_{N \to \infty} -\frac{1}{N} \ln \int_{\mathcal{S}} e^{-Nf(\sigma)} \mathrm{tr}(\rho^{\otimes N} \hat{E}_N(d\sigma))
$$

(148)

$$
= \inf_{x, U} \left(f(U\rho U^*) - \ln(d) - I_1(U, \rho, x) + I_0(x)\right)
$$

(149)

$$
= -\inf_{x, U} \left(f(U\rho U^*) + \sum_{j=1}^d x_j \ln(x_j) - I_1(U, \rho, x)\right),
$$

(150)
which proves Theorem 3.2 for non-degenerate density matrices.

Now assume that \( \rho \) is degenerate and has rank \( r < d \). By continuity in \( \rho \), Equations (140) and (141) imply that

\[
\text{tr} \left( (U^* \rho U) \otimes \mathbb{1}_Y \right) = \dim K_Y \prod_{k=1}^d \text{pm}_k(U^* \rho U)^{Y_k - Y_{k+1}}
\]

holds as in the non-degenerate case. The only difference is that the right hand side can vanish now, and it vanishes in particular for all \( Y \) with \( Y_k > 0 \) for \( k > r \) (because all minors with \( k > r \) vanish for any \( U \)). Instead of (144) we therefore get

\[
\int_S e^{-N f(\sigma)} \text{tr}(\rho \otimes N \tilde{E}_N(d\sigma)) \]

\[
= \int_{\Sigma_r} \int_{U(d)} r^N e^{-N f(U \rho U^*)} \prod_{k=1}^r \text{pm}_k(U^* \rho U)^{N(x_k - x_{k+1})} dU \nu_{N,r}(dx)
\]

with

\[
\Sigma_r = \{ x \in \Sigma \mid x_k = 0 \ \forall k > r \}
\]

and

\[
\int_{\Sigma_r} h(x) \nu_{N,r}(dx) = \frac{1}{d^N} \sum_{Y \in \mathcal{Y}_r(N)} h \left( \frac{Y}{N} \right) \dim(H_Y) \dim(K_Y).
\]

Note that the difference between \( \nu_N \) and \( \nu_{N,r} \) is just the summation over all Young frames with \( r \) rows instead of \( d \) rows. The right hand side of Equation (151) can still vanish because the unitary matrix \( U \) is a \( d \times d \) matrix. Hence we can exclude

\[
\mathcal{M} = \{ U \in U(d) \mid \text{pm}_r(U^* \rho U) = 0 \}
\]

from the domain of integration without changing the value of the integral in (152). Hence we get

\[
\int_S e^{-N f(\sigma)} \text{tr}(\rho \otimes N \tilde{E}_N(d\sigma))
\]

\[
= \int_{\Sigma_r} \int_{U(d) \setminus \mathcal{M}} \exp \left( -N \left[ f(U \rho_x U^*) - \ln(r) - I_1(U, \rho, x) \right] \right) dU \nu_{N,r}(dx).
\]

The domain \( \Sigma_r \times (U(d) \setminus \mathcal{M}) \) is open in \( \Sigma_r \times U(d) \) and \( I_1 \) is continuous on it. Hence we can apply Varadhan’s Theorem and proceed as in the non-degenerate case.

### 5 Upper bounds

In this section we will provide a detailed discussion of general upper bounds on admissible rate functions. This includes in particular the proofs of Theorems 3.1 and 3.3.
5.1 Hypothesis testing

Let us start with a very brief review of some material from quantum hypothesis testing (for a detailed discussion cf. [22, 24, 18]), because it can be used to derive related results for estimation schemes. As in state estimation the task of hypothesis testing is to determine a state from measurements on N systems. In hypothesis testing, however, we know a priori that only a finite number of different states can occur. For our purposes it is sufficient to distinguish only between two states $\rho_0, \rho_1 \in S$. This can be done by an observable of the N-fold system with values in the set $\{0, 1\}$, where we conclude from the outcome $j \in \{0, 1\}$ that the initial preparation was done according to $\rho_j$. Mathematically such an observable is given by a positive operator $A_N \in \mathcal{B}(\mathcal{H}^\otimes N)$ with $A_N \leq I$ and $\text{tr}(\rho_j^\otimes N A_N)$ is the probability to get the result 0 during a measurement on N systems in the joint state $\rho_j^\otimes N$. Hence the two quantities

$$\alpha_N(A_N) = \text{tr}(\rho_0^\otimes N (I - A_N)), \quad \beta_N(A_N) = \text{tr}(\rho_1^\otimes N A_N)$$ (157)

are error probabilities. More precisely $\alpha_N(A_N)$ is the probability to detect $\rho_1$ although the initial preparation was given by $\rho_0^\otimes N$ (error of the first kind) and $\beta_N(A_N)$ is the probability for the converse situation (error of the second kind). Ideally we would like to have a test which minimizes $\alpha_N$ and $\beta_N$. This is however impossible because we can always reduce one quantity at the expense of the other. A possible solution of this problem is to make $\beta_N(A_N)$ as small as possible under the constraint that $\alpha_N(A_N)$ remains bounded by some $\epsilon > 0$. The corresponding minimal (second kind) error probability is therefore

$$\beta_N^*(\epsilon) = \inf \{ \beta_N(A_N) \mid A_N \in \mathcal{B}(\mathcal{H}^\otimes N), \ 0 \leq A_N \leq I, \ \alpha_N(A_N) \leq \epsilon \}. \quad (158)$$

Stein’s Lemma describes the behavior of $\beta_N^*(\epsilon)$ in the limit $N \to \infty$; the quantum version is shown in [23, 32].

**Theorem 5.1 (Quantum Stein’s Lemma)** For any $0 < \epsilon < 1$ the equality

$$\lim_{N \to \infty} \frac{1}{N} \ln \beta_N^*(\epsilon) = -S(\rho_1, \rho_0)$$ (159)

holds.

5.2 State estimation

Let us consider now a (full) estimation scheme $(E_N)_{N \in \mathbb{N}}$. One possibility to distinguish between two states $\rho$ and $\sigma$ is to choose a neighborhood $\Delta \in \mathcal{B}(S)$ of $\sigma$ with $\rho \not\in \Delta$ and to use the tests $A_N = E_N(\Delta)$. If $(E_N)_{N \in \mathbb{N}}$ is consistent, the corresponding first kind error probability $\alpha_N(A_N)$ vanishes in the limit $N \to \infty$ and we can apply Stein’s Lemma to get a bound on $\beta_N(A_N) = \text{tr}(\rho^\otimes N E_N(\Delta))$. Exploiting this idea more carefully leads to the following theorem.

**Theorem 5.2** Consider a continuous map $p : S \to X$ onto a locally compact, separable metric space $X$. The optimal rate function $\mathcal{I}_p$ defined in Equation (12) satisfies the inequality

$$\mathcal{I}_p(\rho, x) \leq \inf_{\sigma \in p^{-1}(x)} S(\rho, \sigma) \quad \forall \rho \in S \ \forall x \in X,$$ (160)

where $S$ denotes the quantum relative entropy.
Proof. For each pair $\rho_0, \rho_1$ of density operators with $p(\rho_0) \neq p(\rho_1)$ we can find a sequence of tests $(A_N)_{N \in \mathbb{N}}$ by $A_N = E_N(\Delta)$ with an appropriate Borel set $\Delta \subset X$. If $\Delta \in \mathfrak{B}(X)$ is a neighborhood of $p(\rho_0)$, consistency of $(E_N)_{N \in \mathbb{N}}$ implies that for all $\epsilon > 0$ there is an $N_\epsilon \in \mathbb{N}$ such that

$$a_N(A_N) = 1 - \text{tr}(E_N(\Delta)\rho_0^N) < \epsilon$$ (161)

holds for all $N > N_\epsilon$. Hence Stein’s Lemma implies

$$\limsup_{N \to \infty} -\frac{1}{N} \ln b_N(A_N) = \limsup_{N \to \infty} -\frac{1}{N} \ln \text{tr}(\rho_1^N E_N(\Delta)) \leq S(\rho_1, \rho_0).$$ (162)

Now assume that the rate function $I$ satisfies $I(p_1, x_0) > S(\rho_1, \rho_0)$ for some $\rho_0, \rho_1$ with $p(\rho_0) = x_0$ and $p(\rho_1) \neq x_0$. Since $I(p_1, \cdot)$ is lower semi-continuous we find a closed neighborhood $\Delta$ of $x_0$ such that

$$I(p_1, x) \geq S(p_1, \rho_0) + \delta \quad \forall x \in \Delta$$ (163)

holds for an appropriate $\delta > 0$. Hence the large deviation upper bound (164) implies

$$\limsup_{N \to \infty} \frac{1}{N} \ln \text{tr}(\rho_1^N E_N(\Delta)) \leq -\inf_{x \in \Delta} I(p_1, x)$$ (164)

$$\liminf_{N \to \infty} \frac{1}{N} \ln \text{tr}(\rho_1^N E_N(\Delta)) \geq \inf_{x \in \Delta} I(p_1, x) \geq S(p_1, \rho_0) + \delta.$$ (165)

in contradiction to Equation (162). Hence $I(p_1, x_0) \leq S(\rho_0, \rho_1)$ for all $\rho_0$ with $p(\rho_0) = x_0$, which concludes the proof. □

Proof of Theorem 3.3. If we apply this theorem to full estimation schemes (i.e. $X = S$ and $p = \text{Id}$) we get $I(\rho, \sigma) \leq S(\rho, \sigma) \quad \forall \rho, \sigma \in S$ and Theorem 3.2 follows as a simple corollary. □

Proof of Theorem 3.1. For a spectral estimation schemes with rate function $I$ Theorem 3.2 implies that $I(\rho, x) \leq \inf_{s(\sigma) = x} S(\rho, \sigma)$ holds. But the infimum on the right hand side is achieved if $\sigma$ and $\rho$ commute and the eigenvalues in a joint eigenbasis are given in the same order. In this case we have

$$S(\rho, \sigma) = \sum_{j=1}^d x_j (\ln x_j - \ln r_j) = S(x, r)$$ (166)

where $s(\sigma) = x = (x_1, \ldots, x_d)$ and $s(\rho) = r = (r_1, \ldots, r_d)$ denote the ordered spectra of $\sigma$ and $\rho$ and $S(r, x)$ is the classical relative entropy of the probability vectors $r$ and $x$. Hence for spectral estimation the upper bound (164) becomes

$$I(\rho, x) \leq S(s(\rho), x) \quad \forall \rho \in S \forall x \in \Sigma.$$ (167)

But from 27 we know already that the scheme $(\hat{F}_N)_{N \in \mathbb{N}}$ defined in 17 saturates this bound; hence $(\hat{F}_N)_{N \in \mathbb{N}}$ is asymptotically optimal as stated in Theorem 3.1. □

If we are looking in particular at full estimation, the method used in the proof of Theorem 3.2 can be improved significantly. The following lemma, which expresses the rate function explicitly as a limit over a sequence of operators, is of great use in the next subsection.
Lemma 5.3 Consider a full estimation scheme \((E_N)_{N \in \mathbb{N}}\) satisfying the LDP with rate function \(I : S \times S \to [0, \infty]\) and two states \(\rho, \sigma \in S\). There is a sequence \((\Delta_N)_{N \in \mathbb{N}}\) of Borel sets \(\Delta_N \subset S\) satisfying

\[
\lim_{N \to \infty} \text{tr}(\sigma^N E_N(\Delta_N)) = 1 \tag{168}
\]

\[
\lim_{N \to \infty} -\frac{1}{N} \ln \text{tr}(\rho^N E_N(\Delta_N)) = I(\rho, \sigma) \tag{169}
\]

and

\[
U \Delta_N U^* = \Delta_N \quad \forall U \in U(d) \quad \text{with} \quad [U, \sigma] = 0 \tag{170}
\]

Proof. For each \(k \in \mathbb{N}\) consider the set

\[
\tilde{\Delta}_k = \{ \omega \in S \mid \|\sigma - \omega\|_1 \leq k^{-1} \} \subset S, \tag{171}
\]

which obviously has the symmetry property \(170\). Since the scheme \((E_N)_{N \in \mathbb{N}}\) is consistent (since \((E_N)_{N \in \mathbb{N}}\) satisfies the LDP this follows directly from Definition 2.2) we have for each \(k \in \mathbb{N}\) an index \(N'_k \in \mathbb{N}\) such that

\[
\text{tr}(\sigma^N E_N(\tilde{\Delta}_k)) \geq 1 - \frac{1}{k} \geq 1 - \frac{1}{k} \tag{172}
\]

holds for all \(N \geq N'_k\). In addition we get for each \(k \in \mathbb{N}\)

\[
\lim_{N \to \infty} -\frac{1}{N} \ln \text{tr}(\rho^N E_N(\tilde{\Delta}_k)) = \inf_{\omega \in \tilde{\Delta}_k} I(\rho, \omega) \tag{173}
\]

by combining the large deviation upper and lower bounds. Hence for each \(k \in \mathbb{N}\) there is an \(N''_k \in \mathbb{N}\) with

\[
\left| \frac{-1}{N} \ln \text{tr}(\rho^N E_N(\tilde{\Delta}_k)) - \inf_{\omega \in \tilde{\Delta}_k} I(\rho, \omega) \right| < \frac{1}{k} \tag{174}
\]

for all \(N \geq N''_k\). Now let us recursively define a strictly increasing sequence \((N_k)_{k \in \mathbb{N}}\) of integers by \(N_1 = 1\) and \(N_k = \max\{N'_k, N''_k, N_{k-1} + 1\}\), and set

\[
\Delta_N = \tilde{\Delta}_k \quad \text{for} \quad N_k \leq N < N_{k+1}. \tag{175}
\]

For each \(N \geq N_k\) we therefore have an integer \(l \geq k\) with \(N_l \leq N < N_{l+1}\) and \(\Delta_N = \tilde{\Delta}_l\). Since \(N_l \leq N\) implies in particular \(N \geq N'_l\) we have due to \(172\)

\[
\text{tr}(\sigma^N E_N(\Delta_N)) = \text{tr}(\sigma^N E_N(\tilde{\Delta}_l)) \geq 1 - \frac{1}{l} \geq 1 - \frac{1}{k}, \tag{176}
\]

and this implies Equation \(168\). Similarly we have \(N_l \geq N''_l\) and therefore with \(174\)

\[
\left| \frac{-1}{N} \ln \text{tr}(\rho^N E_N(\Delta_N)) - \inf_{\omega \in \Delta_N} I(\rho, \omega) \right| =
\left| \frac{-1}{N} \ln \text{tr}(\rho^N E_N(\tilde{\Delta}_l)) - \inf_{\omega \in \tilde{\Delta}_l} I(\rho, \omega) \right| < \frac{1}{l} \leq \frac{1}{k}. \tag{177}
\]
Now note that the sequence \((\Delta_N)_{N \in \mathbb{N}}\) forms a neighborhood base at \(\sigma \in \mathcal{S}\), more precisely
\[
\Delta_{N+1} \subset \Delta_N \quad \forall N \in \mathbb{N} \quad \text{and} \quad \bigcap_{N=1}^{\infty} \Delta_N = \{\sigma\}.
\] (178)

Lower semi-continuity of \(I_\rho(\cdot) = I(\rho, \cdot)\) implies in addition that
\[
U_k = I_\rho^{-1}([I_\rho(\sigma) - k^{-1}, \infty])
\] (179)
is for each \(k \in \mathbb{N}\) an open neighborhood of \(\sigma\). Hence we have a \(M_k \in \mathbb{N}\) such that \(M \geq M_k\) implies \(\Delta_M \subset U_k\) and therefore
\[
I(\rho, \sigma) \geq \inf_{\omega \in \Delta_M} I(\rho, \omega) \geq I(\rho, \sigma) - \frac{1}{k} \quad \forall M \geq M_k.
\] (180)

Now assume that \(N \geq \max\{N_k, M_k\}\) then we get with Equation (177)
\[
\left| \frac{-1}{N} \ln \text{tr}(\rho \otimes^N E_N(\Delta_N)) - I(\rho, \sigma) \right| \leq \left| \frac{-1}{N} \ln \text{tr}(\rho \otimes^N E_N(\Delta_N)) - \inf_{\omega \in \Delta_N} I(\rho, \omega) \right| + \left| \inf_{\omega \in \Delta_N} I(\rho, \omega) - I(\rho, \sigma) \right| \leq \frac{2}{k}
\] (181)
and this implies Equation (169), which concludes the proof. \(\square\)

## 5.3 Pure states

The main purpose of this section is to provide a proof of Equation (33), where we have claimed that \(\hat{I}\) and \(I_c^{\text{Id}}\) coincide for pure input states. This is basically quite simple. We will take, however, a small detour which allows us to have a closer look beyond the covariant case (Subsection 5.4).

Let us consider first a pure state \(\rho\) and a mixed state \(\sigma\). From Equation (26) we see immediately that this implies \(\hat{I}(\rho, \sigma) = \infty\). Since \(\hat{I}\) is a lower bound on all \(I_{\text{Id}}^\#\) we get
\[
I_{\text{Id}}(\rho, \sigma) = I_{\text{Id}}^0(\rho, \sigma) = I_{\text{Id}}^{\text{cov}}(\rho, \sigma) = \hat{I}(\rho, \sigma) = \infty \quad \forall \rho \text{ pure} \quad \sigma \text{ mixed}.
\] (182)

Hence only the case where \(\rho\) and \(\sigma\) are both pure needs to be discussed. For the rest of this section we will assume (unless something different is explicitly stated) therefore that
\[
\rho = |\phi\rangle\langle\phi|, \quad \sigma = |\psi\rangle\langle\psi| \quad \text{with} \quad \phi, \psi \in \mathcal{H}, \quad \|\phi\| = \|\psi\| = 1
\] (183)
holds. The rate function \(\hat{I}\) then has the following simple structure:
\[
\hat{I}(\rho, \sigma) = -\ln \text{tr}(\rho \sigma) = -\ln \left(\langle\phi, \psi\rangle^2\right).
\] (184)

Now we need the following lemma which shows that we can assume without loss of generality that the operators \(E_N(\Delta_N)\) from Lemma 5.3 are rank one projectors.
Lemma 5.4 Consider an admissible rate function $I \in \mathcal{E}(\text{Id})$ and two pure states $\rho = |\phi\rangle \langle \phi|$, $\sigma = |\psi\rangle \langle \psi|$. There is a sequence $(\Psi_N)_{N \in \mathbb{N}}$ of normalized vectors $\Psi_N \in \mathcal{H}_+^{\otimes N}$ (the symmetric subspace of $\mathcal{H}^{\otimes N}$) such that

$$\liminf_{N \to \infty} \frac{-1}{N} \ln \langle \phi^{\otimes N}, \Psi_N \rangle \geq I(\rho, \sigma)$$

(185)

and

$$\lim_{N \to \infty} \langle \Psi_N, \psi^{\otimes N} \rangle^2 = 1$$

(186)

holds. If $I$ is covariant we can choose $\Psi_N = \psi^{\otimes N}$.

Proof. Consider a full estimation scheme $(E_N)_{N \in \mathbb{N}}$ satisfying the LDP with rate function $I$ and the sequence $(\Delta_N)_{N \in \mathbb{N}}$ of Borel sets $\Delta_N \subset S$ from Lemma 5.3. Since only the overlap of $E_N(\Delta_N)$ with $\phi^{\otimes N}$ and $\psi^{\otimes N}$ are of interest, we can assume without loss of generality that $E_N(\Delta_N)$ is supported by the symmetric tensor product $\mathcal{H}_+^{\otimes N}$. Now choose a $0 < \lambda < 1$ and denote the spectral projector of $E_N(\Delta_N)$ belonging to the interval $[1 - \lambda, 1]$ by $P_{N,\lambda}$. Obviously we have due to Equation (187)

$$\langle \psi^{\otimes N}, E_N(\Delta_N) \phi^{\otimes N} \rangle \leq \langle \psi^{\otimes N}, P_{N,\lambda} \phi^{\otimes N} \rangle$$

(187)

and

$$= (1 - \lambda) + \lambda \langle \psi^{\otimes N}, P_{N,\lambda} \phi^{\otimes N} \rangle.$$

(188)

Equation (187) therefore implies

$$\lim_{N \to \infty} \langle \psi^{\otimes N}, P_{N,\lambda} \phi^{\otimes N} \rangle = 1$$

(189)

Hence for each $0 < \delta < 1$ there is an $N_\delta \in \mathbb{N}$ such that

$$\langle \psi^{\otimes N}, P_{N,\lambda} \phi^{\otimes N} \rangle \geq 1 - \delta$$

(190)

holds for all $N \geq N_\delta$. Now we define for $N$ with $P_{N,\lambda} \phi^{\otimes N} \neq 0$ (which due to Equation (190) is true if $N$ is large enough)

$$\Psi_N = \frac{P_{N,\lambda} \phi^{\otimes N}}{\|P_{N,\lambda} \phi^{\otimes N}\|}$$

(191)

and $\Psi_N$ arbitrary for all other $N$. Equation (191) implies immediately (186). The bound (185) follows from

$$\langle \phi^{\otimes N}, E_N(\Delta_N) \phi^{\otimes N} \rangle \geq (1 - \lambda) \langle \phi^{\otimes N}, P_{N,\lambda} \phi^{\otimes N} \rangle,$$

(192)

which in turn implies

$$I(\rho, \sigma) = \lim_{N \to \infty} \frac{-1}{N} \ln \langle \phi^{\otimes N}, E_N(\Delta_N) \phi^{\otimes N} \rangle$$

(193)

$$\leq \liminf_{N \to \infty} \frac{-1}{N} \ln \langle \phi^{\otimes N}, (1 - \lambda) P_{N,\lambda} \phi^{\otimes N} \rangle$$

(194)

$$= \liminf_{N \to \infty} \frac{-1}{N} \ln \langle \phi^{\otimes N}, P_{N,\lambda} \phi^{\otimes N} \rangle$$

(195)

$$\leq \liminf_{N \to \infty} \frac{-1}{N} \ln \langle \phi^{\otimes N}, \Psi_N \rangle^2$$

(196)
where we have used in the last equation that \( P_{N,\lambda} \Psi_N = \Psi_N \) and therefore \( P_{N,\lambda} \geq |\Psi_N\rangle \langle \Psi_N| \) holds if \( N \) is large enough.

Now assume that \( I \) is covariant. This implies by definition that we can choose \((E_N)_{N \in \mathbb{N}}\) to be covariant as well and we get according to Equation (170)

\[
U^\otimes N \Delta_N U^\otimes N^* = E_N(\Delta_N) \quad \forall U \in \mathcal{U}(d) \text{ with } [U, \sigma] = 0.
\]

(197)

Since \( P_{N,\lambda} \) is a spectral projector of \( E_N(\Delta_N) \) we get

\[
U^\otimes N P_{N,\lambda} U^\otimes N^* = P_{N,\lambda}
\]

for the same set of \( U \) and since \( \sigma = |\psi\rangle \langle \psi| \) this implies

\[
U^\otimes N \Psi_N = \Psi_N
\]

(198)

for all \( U \) with \( U \psi = \psi \) and all \( \Psi_N \) from Equation (191). It is easy to see that \( \Psi_N = \psi^\otimes N \) is the only vector in \( \mathcal{H}^\otimes N \) with this property. ✷

With this lemma it is now very easy to determine \( I^c_{\text{id}}(\rho, \cdot) \) for pure input states \( \rho \). As already stated in Section 3.3 we get (cf. in this context the analysis of covariant pure state estimation in [19])

**Proposition 5.5** For each pure state \( \rho \) and all \( \sigma \in \mathcal{S} \) the equality

\[
I^c_{\text{id}}(\rho, \sigma) = \hat{I}(\rho, \sigma) = \begin{cases} \infty & \text{if } \sigma \text{ is mixed} \\ - \ln \text{tr}(\rho \sigma) & \text{if } \sigma \text{ is pure} \end{cases}
\]

holds.

Proof. Since \( \hat{I} \) is covariant we have \( I^c_{\text{id}}(\rho, \sigma) \geq \hat{I}(\rho, \sigma) \) for all \( \rho, \sigma \in \mathcal{S} \). If \( \rho \) is pure and \( \sigma \) is mixed we have \( \hat{I}(\rho, \sigma) = \infty \) and therefore \( I^c(\rho, \sigma) = \hat{I}(\rho, \sigma) \). If both states are pure we get from Lemma 5.4

\[
I^c(\rho, \sigma) \leq \lim_{N \to \infty} - \frac{1}{N} \ln |\langle \phi^\otimes N, \psi^\otimes N \rangle|^2 = - \ln \text{tr}(\rho \sigma) = \hat{I}(\rho, \sigma)
\]

which concludes the proof. ✷

Together with the arguments from Section 4.3 this result supports our conjecture from Section 3.3 that \( I^c_{\text{id}} \) and \( \hat{I} \) coincide also for mixed input states.

### 5.4 Beyond covariance

If we look at Equation (186) and compare it with the reasoning in the last proof we might think that covariance is not really needed here, because \( \Psi_N \) converges to \( \psi^\otimes N \) in the limit \( N \to \infty \) even without further assumptions on \( I \). This impression, however, is wrong, because the vectors \( \psi^\otimes N \) and \( \phi^\otimes N \) become more and more orthogonal as \( N \) increases and therefore the part of \( \Psi_N \) which is orthogonal to \( \psi^\otimes N \) can play a crucial role (although it vanishes in the limit \( N \to \infty \)). The relation of the optimal rate functions \( I_{\text{id}} \) and \( I^0_{\text{id}} \) to \( \hat{I} \) and relative entropy \( S \) needs therefore more discussion. Although we are not yet able to give complete results we will collect in the following some (informal) arguments which supports the two conjectures \( I_{\text{id}} = S \) and \( I^0_{\text{id}} = \hat{I} \) from the end of Section 3.3.

As in the last section we will consider only pure states, i.e. we will evaluate a rate function \( \hat{I}(\rho, \sigma) \) only for \( \rho = |\phi\rangle \langle \phi| \) and \( \sigma = |\psi\rangle \langle \psi| \). In addition we will
assume that \( \mathcal{H} \) is two-dimensional (this can be done without loss of generality, because we just have to replace \( \mathcal{H} \) with the subspace generated by \( \psi \) and \( \phi \)). Hence we can set

\[
\psi = |0\rangle \quad \text{and} \quad \phi = \phi_{p,\alpha} = \sqrt{p} |0\rangle + e^{i\alpha} \sqrt{1-p} |1\rangle
\]  \hspace{1cm} (201)

with \( 0 \leq p \leq 1 \), \( \alpha \in (-\pi, \pi] \) and an arbitrary but fixed basis \( |0\rangle, |1\rangle \) of \( \mathcal{H} \). In the number basis \( |k; N\rangle \in \mathcal{H}_+^\otimes N \), \( k = 0, \ldots, N \)

\[
|k; N\rangle = \left( \begin{array}{c} N \end{array} \right)^{-1/2} S_N |0\rangle^\otimes (N-k) \otimes |1\rangle^\otimes k
\]  \hspace{1cm} (202)

(where \( S_N \) is the projector to \( \mathcal{H}_+^\otimes N \)) the vectors \( \Psi_N \in \mathcal{H}_+^\otimes N \) from Lemma 5.4 can then be written as

\[
\Psi_N = \sum_{k=0}^{N} f_{N,k} |k; N\rangle
\]  \hspace{1cm} (203)

and \( \phi^\otimes N \) becomes

\[
\phi^\otimes N = \phi_{p,\alpha}^\otimes N = \sum_{k=0}^{N} \left( \begin{array}{c} N \end{array} \right) 1/2 \sqrt{p}^{N-k} \sqrt{1-p}^k e^{ik\alpha} |k; N\rangle.
\]  \hspace{1cm} (204)

Let us consider the conjecture \( I_{Id} = S \) first. In the case of pure states this would imply that we can find for each pair of pure states \( \sigma \neq \rho_0 \) an admissible rate function \( I \) with \( I(\rho_0, \sigma) = \infty \). A possible way to prove this could consist of two steps:

- **Step 1.** Find a sequence \( (A_N)_{N \in \mathbb{N}} \) of operators such that

\[
\lim_{N \to \infty} -\frac{1}{N} \ln \text{tr}(\rho_0^\otimes N A_N) = \infty, \quad \lim_{N \to \infty} \text{tr}(\sigma^\otimes N A_N) = 1
\]  \hspace{1cm} (205)

and

\[
\lim_{N \to \infty} -\frac{1}{N} \ln \text{tr}(\rho^\otimes N A_N) = I^* (\rho) > 0 \quad \forall \rho \neq \sigma
\]  \hspace{1cm} (206)

holds.

- **Step 2.** Find a full estimation scheme \( (E_N)_{N \in \mathbb{N}} \) and a sequence \( (\Delta_N)_{N \in \mathbb{N}} \) of Borel sets \( \Delta_N \subset S \) shrinking to \( \sigma \) such that \( E_N(\Delta_N) = A_N \) holds for all \( N \in \mathbb{N} \).

To implement the second step we would need a converse of Lemma 5.3 and such a result is (unfortunately) not yet available. The problem here is not to construct some POV measures with \( E_N(\Delta_N) = A_N \), but to construct them such that the resulting scheme satisfies the LDP (which includes in particular consistency). It seems, however, that this is more a technical then a fundamental problem.

The first step is much easier to perform\(^5\). Assume that \( \rho_0 = |\phi_{q,\beta}\rangle \langle \phi_{q,\beta}| \) holds with \( \phi_{q,\beta} \) from (201). Then we set \( A_N = |\Psi_N\rangle \langle \Psi_N| \) and define \( \Psi_N \) according to (203) by

\[
f_{N,0} = -N_N \sqrt{N} \sqrt{1-q} e^{i\beta}, \quad f_{N,1} = N_N \sqrt{q}
\]  \hspace{1cm} (207)

\(^5\)However, it is not sufficient to find a sequence of tests which saturates the bound from Stein’s lemma, because Equation 206 would not necessarily hold in this case.
with the normalization
\[ N_N = \left( N(1 - q) + q \right)^{-1/2} \]  
and \( f_{N,k} = 0 \) for all \( k > 1 \). Obviously we have
\[ \langle \Psi_N, \phi_{q,d}^{\otimes N} \rangle = 0 \text{ and } \lim_{N \to \infty} f_{N,0} = 1 \]  
which implies Equations (205). On the other hand we get \( I^\sigma(\rho) = -\ln \text{tr}(\rho \sigma) \) for each pure \( \rho \neq \rho_0 \) and therefore Equation (206) holds as well. Hence there is strong evidence behind the conjecture \( \mathcal{I}_{\text{id}} = S \) from Section 3.3 (at least for pure input states).

The method used in the last paragraph can be easily generalized to construct a sequence of operators \((\mathcal{A}_N)_{N \in \mathbb{N}}\) such that the function \( I^\sigma \) from (206) becomes infinite at finitely many points or even on a countable dense subset of the space \( \mathcal{P} \) of pure states. This is, however, not sufficient to disprove the conjecture \( \mathcal{I}_{\text{id}} = S \) from Section 3.3 (at least for pure input states).

To this end consider \( A_N = |\Psi_N\rangle \langle \Psi_N| \) with \( \Psi_N \) from Lemma 5.4 and a fixed \( 0 < p < 1 \) such that
\[ \lim_{N \to \infty} -\frac{1}{N} \ln \left( |\langle \Psi_N, \phi_{p,\alpha}^{\otimes N} \rangle|^2 \right) = -\ln p \]  
holds for all \( \alpha \) with \(-\pi < \alpha_- < \alpha < \alpha_+ < \pi\) for some bounds \( \alpha_-, \alpha_+ \). To rewrite this in a more convenient way let us identify the interval \((-\pi, \pi] \) with the unit circle \( S^1 \) and consider the sequence \((F_N)_{N \in \mathbb{N}}\), \( F_N \in L^2(S^1) \) with
\[ F_N = \| F_N \|^{-1} \tilde{F}_N, \quad \tilde{F}_N(\alpha) = \langle \Psi_N, \phi_{p,\alpha}^{\otimes N} \rangle. \]  
In the orthonormal basis \((e_k)_{k \in \mathbb{Z}}, e_k \in L^2(S^1), e_k(\alpha) = (2\pi)^{-1/2} \exp(ik\alpha)\) these vectors become
\[ \tilde{F}_N(\alpha) = \sum_{k=0}^{N} \sqrt{\frac{(N-k)!}{k!}} \sqrt{p}^{N-k} \sqrt{1-p^k} e^{ik\alpha}, \]  
and hence all \( F_N \) are elements of the positive frequency subspace
\[ \mathbb{H}^2(S^1) = \text{span}\{e_k \mid k \geq 0\} \subset L^2(S^1). \]  
In addition we can conclude immediately from Equation (186) and \( |0, N\rangle = \psi^{\otimes N} \) the inequality
\[ \lim_{N \to \infty} -\frac{1}{N} \ln \left( \| \tilde{F}_N \|^2 \right) = -\ln p. \]  
Hence to get (210) the functions \( F_N \) have to converge pointwise and exponentially fast to 0 on the interval \((\alpha_-, \alpha_+)\). To find such a sequence is difficult due to the following lemma.

**Lemma 5.6** A function \( F \in \mathbb{H}^2(S^1) \) which vanishes on a non-empty subinterval \((\alpha_-, \alpha_+)\) of \( S^1 \) vanishes completely.
The proof of this lemma uses the fact that each smooth element of $H^2(S^1)$ is the boundary value of an analytic function on the unit disc (cf. [37] for details). For us it shows that the $F_N$ can not vanish on $(\alpha_-, \alpha_+)$ because $\|F_N\| = 1$ by construction. It is even impossible that the sequence $(F_N)_{N \in \mathbb{N}}$ converges (in norm) to a function $F \in L^2(S^1)$, because this $F$ would satisfy again $\|F\| = 1$, $F \in H^2(S^1)$ and $F(\alpha) = 0$ for all $\alpha \in (\alpha_-, \alpha_+)$. The only way out is to find a sequence which does not converge for all $\alpha$. Such a series can be constructed if we allow infinitely fast oscillations in the limit $N \to \infty$ (start with a sequence which converges in $L^2(S^1)$ and shift its elements to the positive frequency space). However, even then there are two additional requirements: 1. The vectors $\Psi_N$ (and therefore the coefficients $f_{N,k}$) have to satisfy the constraints $\|\Psi_N\| = 1$ and $\lim_{N \to \infty} \|f_{N,0}\| = 1$ and 2. $\lim_{N \to \infty} F_N(\alpha) = 0$ must hold not only for all $\alpha \in (\alpha_-, \alpha_+)$, but also for all $p \in (p_-, p_+)$ for some $0 < p_- < p_+ < 1$. We have not yet succeeded to construct a sequence $(\Psi_N)_{N \in \mathbb{N}}$ which satisfies all these condition, but what we can say already at this point is the following: If there is a rate function $I \in \mathcal{E}^0(\text{Id})$ with $I(\rho, \sigma) > \hat{I}(\rho, \sigma)$ for some $\rho, \sigma$, then the corresponding estimation scheme must develop very irregular behavior with respect to relative phases and this indicates that a more detailed analysis of phase estimation might solve our problem.

A Some material from large deviations theory

The purpose of this appendix is to collect some material about large deviation theory which is used throughout this paper. For a more detailed presentation we refer the reader to monographs like [14, 13, 10].

**Definition A.1** A function $I : X \to [0, \infty]$ on a locally compact, separable, metric space $X$ is called a rate function if

1. $I \neq \infty$
2. $I$ is lower semi-continuous.
3. $I$ has compact level sets, i.e. $I^{-1}([-\infty, c])$ is compact for all $c \in \mathbb{R}$.

**Definition A.2** Let $(\mu_N)_{N \in \mathbb{N}}, N \in \mathbb{N}$ be a sequence of probability measures on the Borel subsets of a locally compact, separable metric space $X$ and $I : X \to [0, 1]$ a rate function in the sense of Definition A.1. We say that $(\mu_N)_{N \in \mathbb{N}}$ satisfies the large deviation principle with rate function $I : X \to [0, \infty]$ if the following conditions hold:

1. For each closed subset $\Delta \subset \Sigma$ we have

$$\limsup_{N \to \infty} \frac{1}{N} \ln \mu_N(\Delta) \leq -\inf_{x \in \Delta} I(x) \quad (215)$$

2. For each open subset $\Delta \subset \Sigma$ we have

$$\liminf_{N \to \infty} \frac{1}{N} \ln \mu_N(\Delta) \geq -\inf_{x \in \Delta} I(x) \quad (216)$$
The most relevant consequence of this definition is the following theorem of Varadhan \cite{35}, which describes the behavior of some expectation values in the limit $N \to \infty$:

**Theorem A.3 (Varadhan)** Consider a sequence $(\mu_N)_{N \in \mathbb{N}}$, $N \in \mathbb{N}$ of probability measures on $X$ satisfying the large deviation principle with rate function $I : X \to [0, \infty]$ and a continuous function $f : X \to \mathbb{R}$ which is bounded from below. Then the following equality holds:

$$
\lim_{N \to \infty} \frac{1}{N} \ln \int_E e^{-Nf(x)} \mu_N(dx) = - \inf_{x \in E} \{f(x) + I(x)\}.
$$

(217)

Varadhan’s theorem has a converse: If we know that a sequence of measures $\mu_N$ satisfies Equation (217) for all bounded continuous functions it can be shown that the $\mu_N$ satisfy the large deviation principle as well. Following \cite{13} we have:

**Definition A.4** Let $(\mu_N)_{N \in \mathbb{N}}$ be a sequence of measures on a locally compact, separable metric space $X$ and $I : X \to [0, \infty]$ a rate function. We say that $(\mu_N)_{N \in \mathbb{N}}$ satisfy the Laplace principle with rate function $I$, if we have

$$
\lim_{N \to \infty} \frac{1}{N} \ln \int_E e^{-Nf(x)} \mu_N(dx) = - \inf_{x \in E} \{f(x) + I(x)\}.
$$

(218)

for all bounded continuous functions $f : E \to \mathbb{R}$.

**Theorem A.5** The Laplace principle implies the large deviation principle with the same rate function.

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