Jonckheere-Terpstra test for nonclassical error versus log-sensitivity relationship of quantum spin network controllers

E. Jonckheere, S. G. Schirmer, and F. C. Langbein

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Abstract

Selective information transfer in spin ring networks by landscape shaping control has the property that the error $1 - \mathrm{prob}$, where prob is the transfer success probability, and the sensitivity of the probability to spin coupling errors are "positively correlated," meaning that both are statistically increasing across a family of controllers of increasing error. Here, we examine the rank correlation between the error and another measure of performance—the logarithmic sensitivity—used in robust control to formulate the fundamental limitations. Contrary to error versus sensitivity, the error versus logarithmic sensitivity correlation is less obvious, because its weaker trend is made difficult to detect by the noisy behavior of the logarithmic sensitivity across controllers of increasing error numerically optimized in a challenging landscape. This results in the Kendall τ test for rank correlation between the error and the log sensitivity to be pessimistic with poor confidence. Here it is shown that the Jonckheere-Terpstra test, because it tests the Alternative Hypothesis of an ordering of the medians of some groups of log sensitivity data, alleviates this problem and hence singles out cases of anti-classical behavior of "positive correlation" between the error and the logarithmic sensitivity.

1 Introduction

One of the tenets of classical linear Single Degree of Freedom (SDoF) multivariable control [24] is that the two fundamental figures of merit—tracking error and logarithmic sensitivity to model uncertainty—are in conflict. The former is quantified by the sensitivity matrix $S = (I + L)^{-1}$ and the latter by the complementary sensitivity $T = L(I + L)^{-1}$, where $L(s)$ is the input loop matrix. Specifically,

$$e_{\text{track}}(s) = S(s)r(s),$$

where $r(s)$ is an extraneous reference and $e_{\text{track}}(s)$ is the tracking error, as shown in Fig. 1. $T(s)$ appears in the logarithmic sensitivity of $S(s)$ as $S^{-1}(dS) = (dL)L^{-1}T$. The conflict is obvious from $S + T = I$. The SDoF limitation can be overcome by a 2-Degree of Freedom (2DoF) configuration, as already pointed out by Horowitz [8, Chap. Six] and recently made explicit in [3, 32].

The present paper reformulates the quantum spin excitation transport in the context of SDoF control by formulating the fidelity of the transport in terms of a "tracking error." Reasoning classically, the "tracking error" would be the difference between the wave function $|\Psi(t)\rangle$

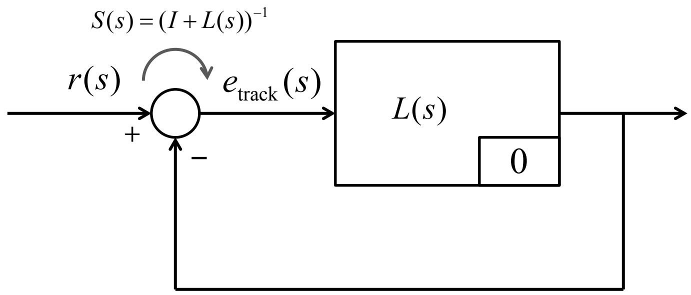

Figure 1: Classical error e_{track}.

and the target quantum spin excitation state. The fundamental issue is that the quantum mechanical wave function is defined up to a global phase factor that should not affect the tracking performance if it reflects the fidelity of the transport. This requires *projectivization of the tracking error* to make it relevant to quantum transport. This raises the issue as to whether the *projectivization of the tracking error* is enough of a departure from classical control to warrant a challenge to the classical limitations. The approach developed here is statistical. From a great many case-studies involving numerical optimization of transport controllers between various pairs of spins in rings of a various number of spins [20], it is shown that, depending on how far the excitation is transported, classical limitations need not hold.

The transport controller can be optimized in two different ways. Either the fidelity is maximized at a precise time, or it is maximized over a finite time window. Here we consider the latter case and relegate the former to a companion paper.

The emphasis on spin *rings* is motivated by their structure as prototype of quantum routers [15] and by the ring structure of the LH2 light harvesting complex [33, Fig. 3], [34, Fig. 1].

The present paper follows in the footsteps of a series of papers on quantum networks [11, 12, 13, 14, 15, 19, 25] by the authors, primarily motivated by quantum communications mediated by spin XX or Heisenberg coupling.

1.1 Paper outline

The paper is organized as follows: In Section 2, we define the quantum excitation transport in rings as the problem of moving an initial state to a target state and contrast it with classical tracking control. In particular, we show that the quantum transport problem has an unconventional sensitivity matrix relating the target state to the projective tracking error; we further argue that this sensitivity matrix does not easily lend itself to an analytical formulation of the limitations on achievable performance. In Section 3, we develop a statistical rank correlation rather than analytical approach to the problem: given many controllers achieving various levels of accuracy, two rank correlation tests—Kendall τ and Jonckheere-Terpstra—are proposed to investigate whether the error and the logarithmic sensitivity are inversely correlated, as classical control would predict. The results are expanded upon in Section 4, showing that in many cases the Null Hypothesis of no rank correlation is rejected in favor of the Alternate Hypothesis of a positive rank correlation, in contradiction with classical control. Finally, in Section 5, we argue that in excitation transport between nearby spins, classical limitations are overcome, while they tend to survive in case of transport between nearly diametrically opposed spins in rings.

2 Tracking error formulation of quantum spin excitation transport

2.1 Excitation transport in networks of spins

Single excitation transport [15] in a N_s-spin ring of single excitation $N_s \times N_s$ Hamiltonian

$$H = \begin{pmatrix} 0 & J_{1,2} & 0 & \dots & 0 & J_{1,N_s} \\ J_{1,2} & 0 & J_{2,3} & & 0 & 0 \\ 0 & J_{2,3} & 0 & & 0 & 0 \\ \vdots & & \ddots & \ddots & \ddots & \\ 0 & 0 & 0 & & 0 & J_{N_s-1,N_s} \\ J_{1,N_s} & 0 & 0 & \dots & J_{N_s-1,N_s} & 0 \end{pmatrix} \tag{1}$$

endeavors to force the solution to Schrödinger's equation

$$|\dot{\Psi}(t)\rangle = -iH|\Psi(t)\rangle + u(t), \quad \Psi(0) = |\mathrm{IN}\rangle, \tag{2}$$

to move from an initial single excitation state $|\mathrm{IN}\rangle$ to some terminal single excitation state $|\mathrm{OUT}\rangle$ by means of some control $u(\cdot)$.

The concept of single excitation refers to some subspace invariant under the total dynamics of XX (Heisenberg) Hamiltonian

$$\sum_{k=1}^{N_s} J_{k,k+1}(X_k X_{k+1} + Y_k Y_{k+1}(+Z_k Z_{k+1})),$$

where X_k, Y_k, Z_k are the Pauli x, y, z operators, respectively, of the spin k in the ring, $\{X,Y,Z\}_{N_s+1} = \{X,Y,Z\}_1$, and $J_{k,k+1} = J_{k+1,k}$ is the coupling strength between spins k and $k+1$ with $J_{N_s,N_s+1} = J_{N_s,1}$. The operator $Z = \sum_{k=1}^{N_s}(I + Z_k)$ counts the number of spins that are in the excited state and the number of such spins remains invariant under the total motion. By definition, in the single excitation subspace, the number of spins in the excited state remains exactly one. In particular, $|\mathrm{IN}\rangle = e_m$ and $|\mathrm{OUT}\rangle = e_n$, where $\{e_k : k = 1, ..., N_s\}$ is the natural basis of $\mathbb{C}^{N_s}$ and $1 \leq m, n \leq N_s$. In the single excitation subspace, the dynamics reduces to (2).

The excitation transport problem can, in some sense, be viewed as the problem of having $|\Psi(t)\rangle$ track $|\mathrm{OUT}\rangle$. However, there are significant discrepancies between classical and quantum tracking control. First of all, the fundamental quantum figure of merit is not some error but the probability of successful transport of the excitation, or squared fidelity, $|\langle \mathrm{OUT}|\Psi(t_f)\rangle|^2$, where t_f is the time at which the excitation is read out. To simplify the exposition, assume that the probability achieves its maximum, $|\langle \mathrm{OUT}|\Psi(t_f)\rangle|^2 = 1$, in which case it is easily seen that $|\Psi(t_f)\rangle = e^{-i\phi(t_f)}|\mathrm{OUT}\rangle$, or equivalently $|\Psi(t_f)\rangle - e^{-i\phi(t_f)}|\mathrm{OUT}\rangle = 0$ for some global phase factor $\phi(t_f)$. More generally, it is not difficult to show that

$$\left\| |\mathrm{OUT}\rangle - e^{i\phi(t_f)}|\Psi(t_f)\rangle \right\|^2 = 2\underbrace{(1 - |\langle \mathrm{OUT}|\Psi(t_f)\rangle|)}_{\mathrm{err}^2(t_f)}, \tag{3}$$

for

$$\phi(t_f) = -\angle\langle \text{OUT}|\Psi(t_f)\rangle.$$

It thus appears that the quantum transport problem of maximizing $|\langle \text{OUT}|\Psi(t_f)\rangle|$ or its "windowed" version $\frac{1}{\delta t}\int_{t_f-\delta t/2}^{t_f+\delta t/2} |\langle \text{OUT}|\Psi(t)\rangle| dt$ is equivalent to minimizing some "tracking error" with the discrepancy that it is not required that the difference between the current state and the target state be small in the ordinary sense, but small in the sense of $\min_\phi \||\text{OUT}\rangle - e^{i\phi}\Psi(t_f)\|$. The latter is related to the Fubini-Study metric [6, p. 31] on the complex projective space $\mathbb{CP}^{N_s-1}$.

We will refer to the left-hand side of (3) as the *projective tracking error.*

2.2 Classical-quantum controller structure discrepancies

The controller in (2) is taken as a perturbation of the Hamiltonian (1),

$$u(t) = -iD|\Psi(t)\rangle, \tag{4}$$

where D is a time-invariant diagonal matrix of spatialy distributed biases that are shaping the energy landscape. The time-invariance of D makes the controller linear, as opposed to bilinear if D were time-dependent [5, 22]. Even though the controller is linear, it departs from classical control in the sense that the controller is *selective,* that is, D depends on both $|\text{IN}\rangle$ and $|\text{OUT}\rangle$. $|\text{IN}\rangle$ is the initial condition and, more importantly, $|\text{OUT}\rangle$ is to be interpreted as the reference. The controller is not driven by the tracking error, but depends on *both* the current state and the target state; from this point of view, the controller is of the 2DoF configuration. Note however that D depends on $|\text{OUT}\rangle$ in some combinatorial fashion as there are only N_s possible $|\text{OUT}\rangle$'s.

Last but not least, the unitary evolution has the property that the controller is not asymptotically stable. Indeed, let D be a controller that achieves $\||\text{OUT}\rangle - e^{-i(H+D)t}|\text{IN}\rangle\| \leq \epsilon$. Take an initial state $|\text{IN}\rangle'$ nearby $|\text{IN}\rangle$, that is, $\||\text{IN}\rangle - |\text{IN}\rangle'\| = \eta$. Using the unitary property of the evolution and the triangle inequality, we derive

$$\begin{aligned}
\eta &= \|e^{-i(H+D)t}(|\text{IN}\rangle - |\text{IN}\rangle')\| \\
&= \|(e^{-i(H+D)t}|\text{IN}\rangle - |\text{OUT}\rangle) + (|\text{OUT}\rangle - e^{-i(H+D)t}|\text{IN}\rangle')\| \\
&\leq \epsilon + \||\text{OUT}\rangle - e^{-i(H+D)t}|\text{IN}\rangle'\|,
\end{aligned}$$

which yields

$$\||\text{OUT}\rangle - e^{-i(H+D)t}|\text{IN}\rangle'\| \geq \eta - \epsilon.$$

Thus for an infinitesimally accurate controller ($\epsilon \downarrow 0$), the perturbed state will remain away from the target $|\text{OUT}\rangle$. The latter has the consequence that the controller is not a classical asymptotically stabilizing controller; it is only Lyapunov stable and for certain cases the controller can achieve *Anderson localization* [2, 9, 18].

With these significant departures from classicality, one wonders whether the fundamental error versus log sensitivity limitation is still in force. The problem is that the phase factor appearing in the quantum tracking error does not lead to a classical sensitivity function. In [25], a sensitivity matrix $\mathscr{S}(s)$ was defined via the Laplace transform $\hat{\mathscr{L}}$ of the projective tracking error as

$$\hat{\mathscr{L}}(|\text{OUT}\rangle 1(t) - e^{i\phi(t)}\Psi(t)) = \mathscr{S}(s)|\text{OUT}\rangle \tag{5}$$

for $\phi(t)$ achieving the minimum of $\||\text{OUT}\rangle - e^{i\phi(t)}\Psi(t)\|$. However, this sensitivity function involves complex domain convolution and a clear relationship between $\mathscr{S}(s)$ and its sensitivity to parameters J (a generic notation for $J_{k,k+1}$) in H cannot be expected. For this reason, we propose a statistical approach based on a great many numerical optimization experiments.

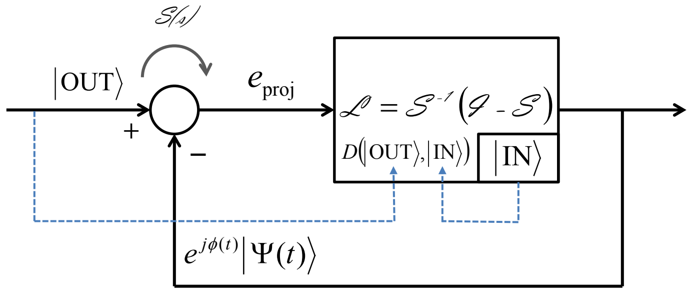

Figure 2: Projective error $|\mathrm{OUT}\rangle - e^{j\phi(t)}|\Psi(t)\rangle$. Note that, contrary to the classical case of Fig. 1, the sensitivity matrix $\mathscr{S}$ is first defined, from which the fictitious loop function $\mathscr{L}$ is defined. The loop matrix is initialized with $|\mathrm{IN}\rangle$. The dotted paths are nonclassical and indicate that the gain D depends on both $|\mathrm{IN}\rangle$ and $|\mathrm{OUT}\rangle$.

Note that, here, we define a sensitivity matrix without proceeding from a loop matrix as done classically. However, a fictitious loop matrix can be defined as

$$\mathscr{L} = \mathscr{S}^{-1}(I - \mathscr{S})$$

and plugged in the feedback diagram of Fig. 2. Clearly, the conventional architecture is recovered, but for a very special loop matrix that embodies the projectivization of the error.

From (5), it is clear that the sensitivity of the sensitivity $\mathscr{S}$ relative to J amounts to sensitivity of err as defined by (3). From the classical control viewpoint, the log-sensitivity is

$$\frac{d\mathrm{err}}{dJ}\frac{1}{\mathrm{err}} = -\frac{1}{4}\frac{1}{\sqrt{\mathrm{prob}}}\frac{d\mathrm{prob}}{dJ}\frac{1}{1-\sqrt{\mathrm{prob}}}.$$

The right-hand side is easily derived from the definition of err taken from (3). If prob ≈ 1, as the data base retains only those controllers with an error not exceeding 0.1, then there is concordance between the left-hand side and the way the log-sensitivity is computed, viz., $\frac{d\mathrm{prob}}{dJ}\frac{1}{1-\mathrm{prob}} = \frac{d\mathrm{prob}}{dJ}\frac{1}{(1-\sqrt{\mathrm{prob}})(1+\sqrt{\mathrm{prob}})} \approx \frac{1}{2}\frac{d\mathrm{prob}}{dJ}\frac{1}{(1-\sqrt{\mathrm{prob}})}$.

3 Methods

3.1 Overview

Here, as a first step towards an understanding of the error versus sensitivity issue, we proceed numerically by comparing the error $1-|\langle \mathrm{OUT}|\Psi(t)\rangle|^2$ and its (logarithmic) sensitivity to modeling uncertainties in H across a variety of controllers with error not exceeding 0.1 (see [20] for the data). Precisely, we considered *all* rings from $N_s = 3$ to $N_s = 20$ spins together with *all* transfers between any two spins. This amounts, up to symmetry, to a total of 108 case-studies. For every $N_s \in [2, 3, \ldots, 19, 20]$ and every ($|\mathrm{IN}\rangle = 1, |\mathrm{OUT}\rangle \leq \lceil N_s/2 \rceil$) pair, controllers D were computed by numerical optimization runs of $1 - |\langle \mathrm{OUT}|e^{-i(H+D)t_f}|\mathrm{IN}\rangle|^2$ relative to D, t_f, either at the precise time t_f or over a window around t_f, and controllers were ordered by increasing error, as explained in [19, 25] and as illustrated in Fig. 3. Given

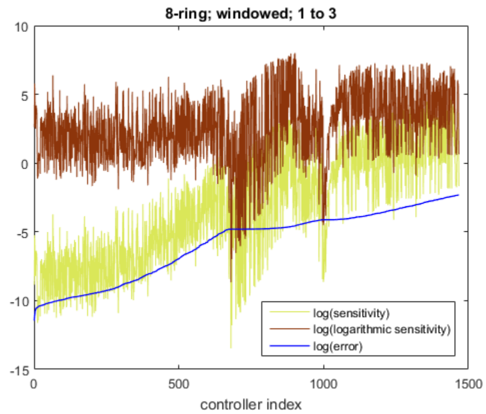

Figure 3: Sensitivity versus logarithmic sensitivity. While the sensitivity is increasing with the error with a Kendall τ of 0.6153, the behavior of the log-sensitivity is less trivial; nevertheless the Jonckheere-Terpstra test rejects the hypothesis of nonincrease of the log-sensitivity.

a case-study $(N_s, (|\mathrm{IN}\rangle, |\mathrm{OUT}\rangle))$ out of a total number of 108 case-studies, the number N of time-windowed optimization runs, or controllers, were between 114 and 1998, with an average of 939 controllers.

Note that we do not have a sampling of the set of *all* controllers. The set of controllers is the subset of those locally optimal controllers computed by the search algorithm and achieving an error not exceeding 0.1.

The major difficulty is that the challenging landscape and the potential for the solution to be trapped in some local minimums make the (absolute and logarithmic) sensitivity versus error plots quite noisy, as shown by Fig. 3, where controllers are ordered by increasing error. Despite this noisy behavior, the graph of Fig. 3 suggests a positive correlation between the sensitivity and the error (for this particular example). This observation is consistent with classical control; it is indeed easily seen that $dS = -S(dL)S$, meaning that if the error vanishes ($S = 0$) so does the sensitivity ($dS = 0$). However, the correlation between the logarithmic sensitivity $\left|\frac{d\mathrm{prob}}{dJ}\frac{1}{1-\mathrm{prob}}\right|$ relative to J-coupling uncertainties in H and the error is not so obvious. In order to make an *objective* statement about whether the logarithmic sensitivity versus error plot is increasing, decreasing, or inconclusive, we used two rank correlation test statistics: the Kendall τ [17] and the Jonckheere-Terpstra statistics [10, 28].

3.2 Kendall τ

Given a set of independent, dependent variables pairs $\{(x_i, y_i)\}_{i=1}^N$, where $\{x_i\}_{i=1}^N$, $\{y_i\}_{i=1}^N$ are samples of random variables $\mathbf{x}$, $\mathbf{y}$, resp., the (estimate of the) Kendall τ is

$$\tau = \frac{\text{number of concordant pairs} - \text{number of discordant pairs}}{N(N-1)/2} \in [-1, 1],$$

where a concordant pair is typically $(x_i < x_j \,\&\, y_i < y_j)$ and a discordant pair is $(x_i < x_j \,\&\, y_i > y_j)$. The preceding assumes that there are no ties [27]. A Kendall tau in $(0, 1]$ means that the plot of y versus x is increasing—in the control context where $\mathbf{x}$ is the error and $\mathbf{y}$ the sensitivity, small (large) error implies small (large) sensitivity, a bit against traditional control wisdom.

The mean and variance of Kendall τ are, respectively [29],

$$\mu(\tau) = 0, \quad \mathrm{var}(\tau) = \frac{2(2N+5)}{9N(N-1)}.$$

For large data set, the τ statistics

$$Z_\tau = \frac{\tau}{\sigma_\tau}$$

is approximately normal, from which a test of significance can be drawn [1].

A crucial condition is that the samples $\{y_i\}_{i=1}^N$ of $\mathbf{y}$ must be independent. This assumption can be justified by the randomness of the numerical optimizer running in an extremely complicated landscape. In case of "persistent data," there is a tendency towards an inflated value of the variance of τ [7].

For the error versus sensitivity averaged over a small interval around t_f, the average Kendall τ over *all* rings from 3 to 20 spins and *all* transfers is 0.4535, indicating positive correlation, with a standard deviation of 0.2113, with an average p of 0.001115741. However, for the logarithmic sensitivity, we obtained the less convincing values $\mu(\tau) = 0.1925$ and $\sigma_\tau = 0.2503$, with an average p of 0.338925.

The issue with the Kendall τ is that, when it comes to the data y increasing in an oscillatory fashion under an increase of x, the Kendall τ will find quite a few discordant pairs, even when on an average y is obviously increasing. One remedy would be to smooth over y and rerun the Kendall τ with the smoothed data. This of course would lead to a τ depending on the way the y data has been smoothed over. Here we propose a different solution. The range of values of x is decomposed in a certain number of groups and a Kendall τ like counting is made between groups, but not inside groups. This removes some of the discordant pairs and lead to a better figure of merit. This is the gist of the Jonckheere-Terpstra test as it is applied to the present robust control problem.

3.3 Jonckheere-Terpstra test

Consider an independent variable, here the error $x = 1 - \mathrm{prob}$ where prob is the transfer success probability, and a dependent variable, here the logarithmic sensitivity of the probability relative to coupling errors $y = \left| \frac{d\mathrm{prob}}{dJ} \frac{1}{1-\mathrm{prob}} \right|$, where J is the near-neighbor spin coupling strength. We want to show that $y(x)$ is statistically an increasing function ("positive correlation" between x and y). The range of values of $x = 1 - \mathrm{prob}$ is decomposed in a certain number of groups such that the independent variable increases along the groups. To be formal, consider a partitioning of the values of the independent variable

$$\{x_i\}_{i=1}^N = X_1 \sqcup X_2 \sqcup ... \sqcup X_I$$

such that $\forall x_i \in X_i$, $\forall x_j \in X_j$ with $i < j$, we have $x_i \leq x_j$ with at least one strict inequality. With this grouping of the values of the independent variable, we construct a grouping of the corresponding values of the dependent variable:

$$\{y_i\}_{i=1}^N = Y_1 \cup Y_2 \cup ... \cup Y_I, \quad Y_i := y(X_i).$$

In each group of dependent variables, we compute the *median* of the population:

$$\widetilde{Y}_1,\ \widetilde{Y}_2,\ ...,\ \widetilde{Y}_I.$$

In the Jonckheere-Terpstra test [10, 28], the Null Hypothesis is

$$H_0 : \widetilde{Y}_1 = \widetilde{Y}_2 = ... = \widetilde{Y}_I$$

and the Alternative Hypothesis is

$$H_A : \widetilde{Y}_1 \leq \widetilde{Y}_2 \leq ... \leq \widetilde{Y}_I, \quad \text{with at least a strict inequality.}$$

The Jonckheere-Terpstra is a test for the Alternative Hypothesis. It is robust and avoids the noise in the log sensitivity because it argues on the medians. (The difficult part, though, is how to group the values of $1 - \text{prob}$).

The statistics is derived from a counting of the number of cases favorable to the increasing property of y relative to x (the number of concordant pairs in the Kendall tau language). Precisely, we start with the Mann-Whitney U-statistics associated with the pair (i, j) of groups:

$$U_{ij} = \sum_{k=1}^{n_i} \sum_{\ell=1}^{n_j} \Phi(Y_j(\ell) - Y_i(k)), \quad i < j, \tag{6}$$

where

$$\Phi(z) = \begin{cases} 1 & \text{if} \quad z > 0 \\ 1/2 & \text{if} \quad z = 0 \\ 0 & \text{if} \quad z < 0 \end{cases} \quad \text{(ties are counted as 1/2)}$$

and $n_i = |Y_i|$ and $Y_i(k)$ denotes the kth element in Y_i. Defining $U = \sum_{i<j} U_{ij}$, the Jonckheere-Terpstra (JT) standardized test statistics is

$$Z = \frac{U - E(U)}{\sqrt{\text{var}(U)}},$$

where, assuming that there are no ties [21], the mean and the variance are, respectively,

$$\begin{aligned} E(U) &= \frac{N^2 - \sum_{i=1}^{I} n_i^2}{4}, \\ \text{var}(U) &= \frac{N^2(2N+3) - \sum_{i=1}^{I} n_i^2(2n_i+3)}{72}, \end{aligned}$$

where $N = \sum_{i=1}^{I} n_i$. For a large data set, the above is approximately a normal distribution from which $p = \int_z^\infty f_Z(z)dz$ is computed.

Note that in the case the classical limitations are likely to hold, the Jonckheere-Terpstra test should be organized around the Alternative Hypothesis

$$\widetilde{Y}_1 \geq \widetilde{Y}_2 \geq ... \geq \widetilde{Y}_I,$$

that is, the log sensitivity is decreasing with increasing error. The test is analogous to the classical one, but in the opposite tail. Rejection of the Null Hypothesis in favor of the above Alternative Hypothesis is more likely to happen with the instantaneous performance optimizing controllers. This is left to a further paper.

There are some conditions for the Jonckheere-Terpstra test to be applicable

1. **Independence of observations:** The initial values chosen for the optimization of the fidelity relative to D are a random sampling of the domain of controllers. In most cases, the difference between the initial D-value and the maximum fidelity D-solution is small. Therefore, it appears that the random sampling should result into a random sampling over the attraction domains for the optimization algorithm. However, if the size of the domain of attraction is notably larger than the mesh of the random sampling of the space of controllers, then there is a bias. If not, then the random initial value sampling matches a random sampling of the maximum fidelity locally optimal controllers. Numerical experiments seem to indicate that the same controller is not found twice over the runs. So this

would indicate that the attraction domains are much smaller than the sampling density and that a random sampling of the space of initial controllers should lead to a random sampling of the resulting sensitivity/error data.

2. **Same group distribution shape:** The distributions of observations in each group must have the same shape and variability. This allows the Jonckheere-Terpstra test to be a test on the medians.

3.4 Some related tests

There are many extensions/refinements of the Jonckheere-Terpstra test [26]. In case of small data sets, a modified version of (6) is proposed as

$$U_{ij} = (j-i)\sum_{k=1}^{n_i}\sum_{\ell=1}^{n_j}\Phi(Y_j(\ell)-Y_i(k)), \quad i<j.$$

Another recently proposed version [26] is

$$U_{ij} = (r_{j\ell}-r_{ik})\sum_{k=1}^{n_i}\sum_{\ell=1}^{n_j}\Phi(Y_j(\ell)-Y_i(k)), \quad i<j,$$

where $r_{j\ell}, r_{ik}$ denote the position (rank) of $Y_j(\ell), Y_i(k)$ in the combined data. Finally, yet another extension proposes a confidence interval [23].

It was observed that the first refinement of the Mann-Whitney U-statistics does not change the overall results and conclusion.

4 Results

4.1 Independence of observations

Here the observations are essentially the many (log)sensitivities achieved by the D-controllers obtained by running the optimization algorithm in the landscape. As already said, for the Jonckheere-Terpstra test to be applicable, observations need to be "independent." A qualitative argument in favor of the randomness of the results of the search algorithm was presented in the preceding section, but a quantitative analysis stills needs to be set up.

For numerical as opposed to categorical variables, independence is usually understood as independence of time-successive observations. Along those lines, we will mention the von Neumann ratio test [30, 31]. Here, however, there is no time variable that can be associated with the outcomes of the search algorithm. This can be explained by the way the results were derived. 2000 independent optimization tasks were created for each routing problem (or "case-study" as defined previously by a number of spins N_s and a target spin $|\mathrm{OUT}\rangle$). These were sent to a cluster and executed in parallel, such that the sequence in which the results came out actually purely depends on the cluster cores and the scheduler used. Tasks were all mixed across all problems, with some rerun if a machine went down, etc. Each individual task selected an independent initial bias diagonal D-controller and initial time according to a uniform distribution. So the initial values are iid (using Matlab's pseudo-random number generator) and as already argued this should lead to random (log)sensitivity results.

Even though the results cannot be ordered time-wise, it is nevertheless possible to order the log sensitivities consistently with increasing error, from which the nonparametric *rank* version of the von Neumann test [4] can be run. More specifically, we ran the rank ratio test for each group. Inside the ith group, the test statistics is

$$\mathrm{RVN}_i = \frac{\sum_{k=1}^{n_i-1}(R_k - R_{k+1})^2}{\sum_{k=1}^{n_i}(R_i - \bar{R})^2},$$

where R_k is the rank (following increasing values) of the kth log-sensitivity observation in group i. The threshold values of RVN_i to achieve various levels of confidence of independence are cataloged in [4, Table 2]. Naturally, some correlation should be expected as the data is on the average increasing. However, the rank test still reveals randomness. For example, for a 7-ring with target spin 3, and 15 groups for a total of 1515 observations, the rank ratio test yields,

$$\begin{aligned}\mathrm{RVN} = &\\ &1.9315\ 2.4791\ 1.8281\ 2.2123\ 1.6447\ 2.2917\ 1.5993\ 1.6046\ 1.7265\ 1.2411\\ &1.5564\ 1.5317\ 2.1542\ 1.8349\ 1.5842\end{aligned}$$

From [4, Table 2] of the thresholds of the β-function statistic, and observing that each group contains about 100 observations, any value ≥ 1.67 would indicate randomness with 95% confidence. Clearly, randomness is present in most of the groups.

4.2 Statistical analysis of error versus log-sensitivity relation

Here we consider all case-studies of rings with $N_s = 3$ to $N_s = 20$ spins, with transport $|\mathrm{IN}\rangle = |1\rangle \to |\mathrm{OUT}\rangle$, with $|\mathrm{OUT}\rangle$ ranging from $|1\rangle$ (Anderson localization) to $\lceil \frac{N_s}{2} \rceil$. This totals to an amount of 108 cases. By symmetry, this covers all cases of transfer of excitation from any spin to any other spin in networks of $N_s = 3, 4, \cdots, 20$ spins.

In each case-study among the 108 cases, we have N pairs $\{x_i, y_i\}_{i=1}^N$. The ith value of the independent variable x_i is the log of the error, $\log(1 - \mathrm{prob}_i)$, where prob_i is the probability of successful $|\mathrm{IN}\rangle \to |\mathrm{OUT}\rangle$ transfer of the ith controller. (The log of the error allows for clearer graphing of the results yet it does not affect the ranking). The errors are in increasing order $x_i \leq x_j$ for $i < j$. The dependent variable takes values

$$y_i = y(x_i) = \frac{1}{2}\log\left(\sum_k \left|\frac{d\mathrm{prob}_i}{dJ_{k,k+1}}\frac{1}{1-\mathrm{prob}_i}\right|^2\right),$$

where $J_{k,k+1}$ is the k-$(k+1)$ spin coupling strength and the sum is extended over all couplings. In our data base, N ranges from 114 up to 1998. The set of pairs is divided into I groups, $\{(X_i, Y_i)\}_{i=1}^I$, where we took $I = 3, 10, 100$.

For each data set $\{x_i, y_i\}_{i=1}^N$ corresponding to a certain number of spins and a certain $|\mathrm{IN}\rangle \to |\mathrm{OUT}\rangle$ transfer, the JT statistics z and the p value were computed along with a "reject/accept" decision based on a confidence level $\alpha = 0.05$. The average results over all case studies are shown in Table 1.

From Table 1 the following conclusions can already be drawn:

1. There is not much difference between the $I = 3$, 10 and 100 cases, except for the outlier $\min Z$, $I = 100$, due to a case where $N = 150$ where the arrangement of the data in 100 groups does not make much sense.
2. The mean p-value is borderline between "accept" H_0 (no disagreement with classical limitations) and "reject" H_0 (disagreement with classical limitations), with a slight tipping of the balance toward "reject." (Recall that $\alpha = 0.05$).

Table 1: Statistics over whole data base of Jonckheere-Terpstra analysis of error versus logarithmic sensitivity (The $\min p = 0$ is up to 4 decimals).

I	$\min Z$	$\mu(Z)$	$\max Z$	σ_Z	$\min p$	$\mu(p)$	$\max p$	σ_p
3	0.0472	11.3055	33.0028	11.1729	0	0.0617	0.4812	0.1182
10	0.0433	12.1213	34.7227	12.1481	0	0.0595	0.4827	0.1156
100	0.364	12.2425	35.0389	12.3419	0	0.0630	0.4855	0.1235

3. $\min p = 0$ (up to 4 decimals) means that there are cases in strong disagreement with classical limitations—the log sensitivity increases with the error.
4. $\max p \approx 0.48 \gg 0.05$ means that there are cases where there is not enough evidence to disagree with the classical limitations—meaning that the log sensitivity does not have trend relative to an increase error.
5. Comparing Kendall τ with Jonckheere-Terpstra, it is absolutely obvious that $\mu(p_{\text{Jonckheere}-\text{Terpstra}}) \ll \mu(p_{\text{Kendall }\tau})$. Clearly the Jonckheere-Terpstra test implicitly filters the oscillatory logarithmic sensitivity data and renders a result with significantly higher confidence than the Kendall τ.

The upshot is that a simple relation like the classical $S + T = I$ cannot, in general, be expected in the quantum transport setup—except for the Anderson localization case, that is, holding a state of excitation at a single spin, or securing a successful "transfer" $|1\rangle \to |1\rangle$. In this case indeed p is consistently vanishing up to 4 decimals, rejecting the no trend hypothesis in the log sensitivity and pointing towards an increase of the log sensitivity with the error. This anti-classical behavior is not surprising, as the Anderson localization is probably the quantum transport case that most significantly departs from classical concepts.

4.3 Case studies

4.3.1 Case-study: Anderson localization: "reject" classical limitation

We consider the case of an 11-ring with the $|1\rangle \to |1\rangle$ "transfer." Fig. 4 shows that the various figures of merit are not conflicting—quite to the contrary, they are consistent. The detail of the experiment is shown in Table 2. Clearly, the "reject" decision is consistent with the visual appearance of the log sensitivity plot.

Table 2: Details of the 11-ring Anderson localization experiment.

I	Kendall tau	Z	p	Null Hypothesis
3	0.4483	26.5509	0	"rejected"
10	0.4483	29.5768	0	"rejected"
100	0.4483	29.8896	0	"rejected"

4.3.2 Case study: "reject" classical limitation

Anderson localization is not the only case where an anti-classical behavior is observed, as shown by the strongly increasing trend of the log sensitivity in the case of a 5-ring under $|1\rangle \to |2\rangle$

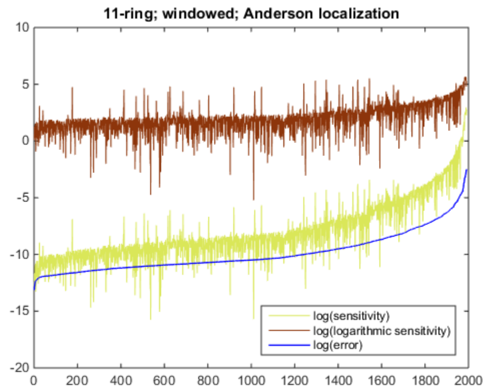

Figure 4: Various nonconflicting figures of merit of an 11-ring under Anderson localization around spin 1.

transport shown in Figure 5. The details of the analysis is shown in Table 3.

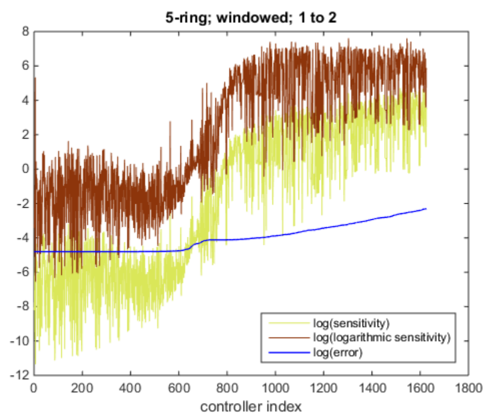

Figure 5: Strong increasing trend of the log sensitivity of a 5-ring under $|1\rangle \to |2\rangle$ transport.

4.3.3 Case-study: borderline "accept/reject" classical limitation

As "borderline" case, we choose a 14-ring with $|1\rangle \to |6\rangle$ transfer. The log sensitivity plot of Fig. 6 shows first an increasing trend and then a decreasing trend relative to the error, which explains the mixed "accept/reject" decision shown in Table 4.

4.3.4 Case study: "accept" classical limitation

Here we consider one of the best illustrative case of no increase of the log sensitivity. We consider the case of a 15-ring with the $|1\rangle \to |6\rangle$ transfer. Fig. 7 shows that the logarithmic

Table 3: Details of the 5-ring under $|1\rangle \to |2\rangle$ transport experiment.

I	Kendall tau	Z	p	Null Hypothesis
3	0.58	33.0028	0	"rejected"
10	0.58	34.7227	0	"rejected"
100	0.58	35.0389	0	"rejected"

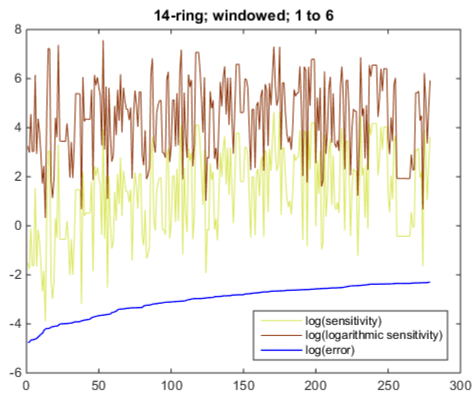

Figure 6: The mixed increase followed by decrease behavior of the logarithmic sensitivity relative to the error in a 14-ring under $|1\rangle \to |6\rangle$ transport.

sensitivity has no trend compared with the error, as confirmed by the details of Table 2 and the "admit" the Null Hypothesis decision.

5 Discussion: Dependency of error versus log-sensitivity relation on $(|\mathrm{IN}\rangle, |\mathrm{OUT}\rangle)$

In the previous study, the data incorporated *all* cases, up to symmetry, of $|\mathrm{IN}\rangle \to |\mathrm{OUT}\rangle$ transfers, for all N_s ranging from 3 to 20, with an overall "positive correlation" between error and log sensitivity. Here we examine how much the classical/anti-classical behavior depends on the relative position of the $|\mathrm{IN}\rangle$ and $|\mathrm{OUT}\rangle$ spins. The overall Jonckheere-Terpstra Z-data with $|\mathrm{IN}\rangle = |1\rangle$ of Section 4.2 is divided into three $|\mathrm{OUT}\rangle$-groups ($I = 3$) that roughly correspond to a decomposition of the right half of the ring into 3 equally-sized sectors:

- Y_1: $120^\circ < \mathrm{angle}(|1\rangle, |\mathrm{OUT}\rangle) < 180^\circ + \epsilon$,
- Y_2: $60^\circ < \mathrm{angle}(|1\rangle, |\mathrm{OUT}\rangle) < 120^\circ$,
- Y_3: $0^\circ < \mathrm{angle}(|1\rangle, |\mathrm{OUT}\rangle) < 60^\circ$,

as illustrated in Fig. 8. If N_s is not divisible by 3, we arrange the N_s-spin data such that $|Y_3| \geq |Y_2| \geq |Y_1|$ with at least a strict inequality. The more specific grouping of the data is shown in the contingency Table 6.

Table 4: Details of the 14-ring $|1\rangle \to |6\rangle$ transport experiment.

I	Kendall tau	Z	p	Null Hypothesis
3	0.0575	1.4875	0.0684	"accept"
10	0.0575	1.5144	0.065	"accept"
100	0.0575	1.6696	0.0475	"reject"

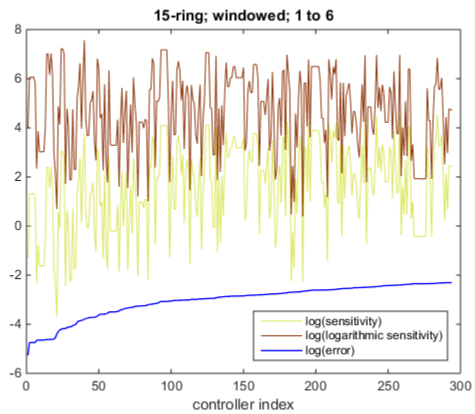

Figure 7: The "no trend" behavior of the logarithmic sensitivity relative to the error in a 15-ring under $|1\rangle \to |6\rangle$ transport.

The Jonckheere-Terpstra test rejects the Null Hypothesis of no trend with $Z = 7.6283$ and $p = 0.0000$ (up to 4 decimals). Therefore when the spins of excitation states $|\text{IN}\rangle$ and $|\text{OUT}\rangle$ are no too far apart, the design behaves anti-classically (error and log sensitivity increasing together). When they become so far as to be nearly anti-podal, then the design behaves classically with the conflict between error and log sensitivity.

Note that this conclusion is supported *by the available dataset,* which contains only those controllers with a largest error of 0.1. This in particular means we have fewer controllers for the longer distance transitions on the ring, as it was considerably hard to find these. Possibly the conclusion could be invalidated by better optimizers able to find better controllers at long distance transport.

6 Conclusion

As already observed in [25], the quantum transport problem can be re-formulated in the classical control setup only at the expense of a complicated sensitivity matrix $\mathcal{S}(s)$, from which the fundamental limitations, if any, are not easy to come by. Here we have developed a statistical approach to the issue. For *every* ring from 3 to 20 spins and *every* transfer on such ring, a fairly large data set of locally optimal controllers, ordered by increasing order of their error, was constructed. With the controllers at hand, we investigated whether the logarithmic sensitivity increases with the error using the Kendall tau and the Jonckheere-Terpstra tests, with a

Table 5: Details of the 15-ring $|1\rangle \to |6\rangle$ transport experiment.

I	Kendall tau	Z	p	Null Hypothesis
3	-0.0285	0.1789	0.4290	"accept"
10	-0.0285	0.7549	0.2252	"accept"
100	-0.0285	0.2052	0.4200	"accept"

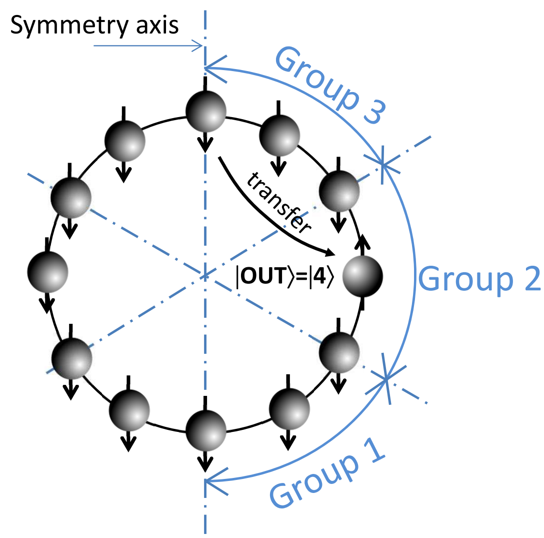

Figure 8: The 3 groups of $|\mathrm{OUT}\rangle$-data to assess dependency classical/anti-classical behavior on $|\mathrm{OUT}\rangle$-position around the ring.

preference for the latter as it gives higher confidence. From the study presented in this paper, it appears that, depending on the case-study, the Jonckheere-Terpstra Null Hypothesis of no trend may or may not be rejected. The latter—rejection of no trend in favor of an increasing trend—is a challenge to the classical limitations that say that the error and the logarithmic sensitivity should be in conflict. By a further analysis, it was shown that for transfers between nearby spins, the classical limitation does not hold, while it is recovered for transfers between distant spins.

The results derived here are based on a data set that retains, among other numerically optimized controllers, only those achieving a probability error no greater than 0.1. Those controllers were confronted with small perturbations of the coupling constants together with a differential formulation of fundamental limitations. Allowing more controllers in the data set along with *large* variations will be considered in a further paper, but a preview that uses structured singular values is already available in [16].

Table 6: Contingency table of data: $[N_s : N_s'] - [|\mathrm{OUT}\rangle : |\mathrm{OUT}\rangle']$ denotes all Z-data, $I = 3$, pertaining to a number of spin between N_s and N_s' with initial spin state $|\mathrm{IN}\rangle = |1\rangle$ and target spin state ranging from $|\mathrm{OUT}\rangle$ to $|\mathrm{OUT}\rangle'$.

Y_1	Y_2	Y_3
$10 - 5$	$[10:12] - [3:4]$	$[10:12] - [1:2]$
$[11:12] - [5:6]$	$[13:14] - [4:5]$	$[13:18] - [1:3]$
$[13:14] - [6:7]$	$[15:18] - [4:6]$	$[19:20] - [1:4]$
$[15:16] - [7:8]$	$[19:20] - [5:7]$	
$[17:18] - [7:9]$		
$[19:20] - [8:10]$		

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