# Collective tests for quantum nonlocality

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Pairs of spin-$\frac{1}{2}$ particles are prepared in a Werner state (namely, a mixture of singlet and random components). If the random component is large enough, the statistical results of spin measurements that may be performed on each pair separately can be reproduced by an algorithm involving local ''hidden'' variables. However, if several such pairs are tested simultaneously, a violation of the Clauser-Horne-Shimony-Holt inequality may occur, and no local hidden variable model is compatible with the results. [S1050-2947(96)11409-8]

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## I. INTRODUCTION

From the early days of quantum mechanics, the question has often been raised whether an underlying ''subquantum'' theory, which would be deterministic or even stochastic, was viable. Such a theory would presumably involve additional ''hidden'' variables, and the statistical predictions of quantum theory would be reproduced by performing suitable averages over these hidden variables.

A fundamental theorem was proved by Bell [1], who showed that if the constraint of *locality* was imposed on the hidden variables (namely, if the hidden variables of two distant quantum systems would themselves be separable into two distinct subsets), then there was an upper bound to the correlations of results of measurements that could be performed on the two distant systems. That upper bound, mathematically expressed by Bell's inequality [1], is violated by some states in quantum mechanics, for example the singlet state of two spin-$\frac{1}{2}$ particles.

A variant of Bell's inequality, more general and more useful for experimental tests, was later derived by Clauser, Horne, Shimony, and Holt (CHSH) [2]. It can be written

$$|\langle AB\rangle+\langle AB'\rangle+\langle A'B\rangle-\langle A'B'\rangle|\leqslant 2. \tag{1}$$

On the left-hand side, $A$ and $A'$ are two operators that can be measured by the first observer, conventionally called Alice. These operators do not commute (so that Alice has to choose whether to measure $A$ or $A'$) and each one is normalized to unit norm (the norm of an operator is defined as the largest absolute value of any of its eigenvalues). Likewise, $B$ and $B'$ are two normalized noncommuting operators, any one of which can be measured by another, distant observer (Bob). Note that each one of the *expectation* values in Eq. (1) can be calculated by means of quantum theory, if the quantum state is known, and is also experimentally observable, by repeating the measurements sufficiently many times, starting each time with identically prepared pairs of quantum systems.

The validity of the CHSH inequality, for *all* combinations of measurements independently performed on both systems, is a necessary condition for the possible existence of a local hidden variable (LHV) model for the results of these measurements. It is not in general a sufficient condition, except in some simple cases, for example when each observer is testing a two-state system, and has only two alternative tests to choose from [3]. For more general situations, counterexamples can be found, such that the inequality (1) holds for any two pairs of correlation coefficients, and yet the nonexistence of a LHV model can be proved [4]. The purpose of the present paper is to show that, even if a well defined LHV model exists that reproduces all the statistical properties of pairs of particles when each pair is tested separately, there may be no extension of such a model that is valid when several pairs are tested simultaneously.

Note that the difficulty appears only in the case of *mixed* quantum states. For pure states, it is easily shown that the CHSH inequality is violated by any nonfactorable state [5,6], while on the other hand a factorable state trivially admits a (contextual) LHV model [7]. For a pair of spin-$\frac{1}{2}$ particles with a given mixed density matrix, there is an explicit formula [8] which gives the maximum value of the left-hand side of Eq. (1), for any measurements that can be chosen by Alice and Bob [see Eq. (12) below]. However, even if that maximum value is less than 2, so that the CHSH inequality holds, this does not prove as yet that a LHV model is admissible, as will be shown in this paper.

For quantum systems whose states lie in higher dimensional vector spaces, even less is known [9]. Some time ago, Werner [10] constructed a density matrix $\rho_W$ for a pair of spin-$j$ particles, with paradoxical properties. Werner's state $\rho_W$ cannot be written as a sum of direct products of density matrices, $\Sigma_j c_j \rho_{Aj}\otimes\rho_{Bj}$, where $\rho_{Aj}$ and $\rho_{Bj}$ refer to the two distant particles (the indices $A$ and $B$ stand for Alice and Bob, respectively). Therefore, genuinely quantal correlations are involved in $\rho_W$. Nevertheless, for any pair of ideal local measurements performed on the two particles, the correlations derived from $\rho_W$ not only satisfy the CHSH inequality, but, as Werner showed [10], it is possible to introduce an explicit LHV model that correctly reproduces all the observable correlations for these ideal measurements.

For a pair of spin-$\frac{1}{2}$ particles, Werner's state is

$$\rho_W=\frac{1}{2}\left(\rho_{\text{singlet}}+\frac{1}{4}\mathbb{1}\right), \tag{2}$$

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namely, an equal weight mixture of a singlet state (which maximally violates the CHSH inequality) and a totally uncorrelated random state. Note that this mixture is rotationally invariant. A manifestly nonclassical property of $\rho_W$ was discovered by Popescu [11], who showed that such a particle pair could be used for teleportation of a quantum state [12], albeit with a fidelity less than if a pure singlet were employed for that purpose. This nonclassical property came as a surprise, and it was the first indication that the existence of a formal LHV model was not a complete description of this system. Indeed, the abstract LHV model that was proposed by Werner deals only with pairs of ideal measurements of the von Neumann type. It is not a complete theory, because it does not predict what happens if other measuring methods are chosen. In particular, Werner's algorithm becomes ambiguous for spin $>\frac{1}{2}$, when we consider the measurement of projection operators of rank 2 or higher [13]. The algorithm must then be supplemented by further rules.

This ambiguity was exploited by Popescu [14] in the following way. Instead of measuring complete sets of orthogonal projection operators of rank 1, as discussed in Werner's article, Alice and Bob first measure suitably chosen (and mutually agreed) projection operators of rank 2, say $P_A$ and $P_B$. If one of them gets a null result, the experiment is considered to have failed, and they test another Werner pair. Only if both Alice and Bob find the result 1 for $P_A$ and $P_B$ do they proceed by independently choosing projection operators of rank 1, in the subspaces spanned by $P_A$ and $P_B$, respectively. Popescu then shows that if the initial Hilbert space (for each particle) has dimension 5 or higher, the correlation of the final results violates the CHSH inequality. In other words, Werner's hidden variable model, which worked for single ideal measurements, is incapable of reproducing the results of several *consecutive* measurements (and of course no other hidden variable model would be acceptable).

Popescu's measuring method [14] does not lead to a violation of the CHSH inequality in spaces having fewer than $5\times5$ dimensions. Nonetheless, such a violation can be produced with the simplest Werner pairs, made of two-state systems, by combining several pairs together. In order to achieve this result, Alice and Bob must first ''purify'' the Werner state, and distill, from a large set of Werner pairs, a subset of almost pure singlets [15–18]. In the discussion of that purification procedure, the notion of ''Werner state'' has to be generalized from its original definition (2) to

$$\rho_W = x\rho_{\text{singlet}} + \frac{1}{4}(1-x)\mathbb{1}. \tag{3}$$

This state consists of a singlet fraction $x$ and a random (totally uncorrelated) fraction $(1-x)$. States of this type were first considered by Blank and Exner [19]. Note that the random fraction $(1-x)$ also includes singlets, mixed in equal proportions with the three triplet components. Another commonly used measure of entanglement is the ''fidelity''

$$F = (3x+1)/4, \tag{4}$$

which is the *total* fraction of singlets [15–18].

In the present work, I shall not consider the fractional distillation of singlets—a multistage process—but the result of a single simultaneous observation of several Werner pairs. Namely, if there are $n$ such pairs, Alice and Bob perform their tests on quantum systems consisting of $n$ particles (each system is described by a vector space of dimension $2^n$). To understand why new results may be obtained by means of such collective tests, let us recall how the statistical interpretation of the quantum formalism is related to actual statistical tests. When we say that a physical system has a density matrix $\rho$, this means that we may mentally construct a *Gibbs ensemble* of such systems, namely an infinite set of conceptual replicas of it, all prepared in the same way [20]. This mental process is not the same thing as actually preparing a large number of such systems, say $N$ of them. The latter preparation gives a *Maxwell ensemble* (for example, a gas made of $N$ identical molecules). If we test individually the various members of a Maxwell ensemble, we may approach, in the limit $N\to\infty$, the statistical properties computed for the Gibbs ensemble. I emphasize that the latter is a pure theoretical construct, needed for the sole purpose of statistical reasoning.

Now, once there actually is a Maxwell ensemble, we may also test its constituent systems two by two, three by three, etc. In that case, we effectively consider a new kind of physical system, which consists of two, or three, or more, of the former ''physical systems.'' If the mathematical representation of the states of the old systems was a density matrix $\rho$, then the representation of the new systems is given by a tensor product, such as $\rho\otimes\rho$, $\rho\otimes\rho\otimes\rho$, etc. The purpose of this paper is to show that even if the density matrices $\rho$ obey the CHSH inequality, it is possible that $\rho\otimes\rho$, $\rho\otimes\rho\otimes\rho$, etc., violate that inequality, when we measure suitably chosen operators.

## II. PROTOCOL FOR COLLECTIVE TESTS

In the case of Werner pairs that are considered here, each one of the two observers has $n$ particles (one particle from each Werner pair). The two observers then proceed as follows. First, they subject their $n$-particle systems to suitably chosen local unitary transformations, $U$ for Alice and $V$ for Bob. (This is always possible, in principle, by using a multiport [21] or a similar device.) Then, they test whether each one of the particles labeled 2, 3, ..., $n$ has spin up (for simplicity, it is assumed that all the particles are distinguishable, and can be labeled unambiguously). Note that any other test that they can perform is unitarily equivalent to the one for spins up, as this involves only a redefinition of the matrices $U$ and $V$. If any one of the $2(n-1)$ particles tested by Alice and Bob shows spin down, the experiment is considered to have failed, and the two observers must start again with $n$ new Werner pairs. A similar elimination of ''bad'' samples is also inherent to Popescu's protocol [14], or to any experimental procedure where a failure of one of the detectors to fire is handled by discarding the results registered by all the other detectors: only when *all* the detectors fire are their results included in the statistics. This obviously requires an exchange of *classical* information between the observers.

Note that, instead of the unitary transformations $U$ and $V$, Alice and Bob could use more general *nonunitary* transformations, involving selective absorption [22]. The latter can sometimes be used to enhance nonlocality, but they

would not help in the present case, because Werner states are rotationally symmetric. Still another possibility would be for Alice and Bob to use a positive operator valued measure (POVM) [23], by including in their apparatuses auxiliary quantum systems, independently prepared by each one of them, and then performing local unitary transformations and tests on the *combined* systems. In the present work, such a strategy was examined, as a possible alternative to the simpler one discussed above, and it was found that no advantage resulted from the use of a POVM. This is likely due to the rotational symmetry of Werner states. I shall therefore restrict the following discussion to what happens after *unitary* transformations $U$ and $V$ have been performed on the $n$ particles held by each observer.

The calculations shown below will refer to the case $n=3$, for definiteness. The generalization to any other value of $n$ is straightforward. Spinor indices, for a single spin-$\frac{1}{2}$ particle, will take the values 0 (for the ''up'' component of spin) and 1 (for the ''down'' component). The 16 components of the density matrix of a Werner pair, consisting of a singlet fraction $x$ and a random fraction $(1-x)$, are, in the standard direct product basis;

$$\rho_{mn,st}=xS_{mn,st}+(1-x)\,\delta_{ms}\delta_{nt}/4, \tag{5}$$

where the indices $m$ and $s$ refer to Alice's particle, $n$ and $t$ to Bob's particle, and where the density matrix for a pure singlet is given by

$$S_{01,01}=S_{10,10}=-S_{01,10}=-S_{10,01}=\tfrac{1}{2}\,, \tag{6}$$

and all the other components of $S$ vanish.

When there are three Werner pairs, their combined density matrix is a direct product $\rho\otimes\rho'\otimes\rho''$, or explicitly, $\rho_{mn,st}\rho_{m'n',s't'}\rho_{m''n'',s''t''}$. The result of the unitary transformations $U$ and $V$ is

$$\rho\otimes\rho'\otimes\rho''\rightarrow(U\otimes V)(\rho\otimes\rho'\otimes\rho'')(U^{\dagger}\otimes V^{\dagger}). \tag{7}$$

Explicitly, with all its indices, the $U$ matrix satisfies the unitarity relation

$$\sum_{mm'm''}U_{\mu\mu'\mu'',mm'm''}U^{*}_{\lambda\lambda'\lambda'',mm'm''}=\delta_{\mu\lambda}\delta_{\mu'\lambda'}\delta_{\mu''\lambda''}. \tag{8}$$

In order to avoid any possible ambiguity, Greek indices (whose values are also 0 and 1) are used to label spinor components *after* the unitary transformations. Note that the indices without primes refer to the two particles of the first Werner pair (the only ones that are not tested for spin up) and the primed indices refer to all the other particles (that are tested for spin up). The $V_{\nu\nu'\nu'',nn'n''}$ matrix elements of Bob's unitary transformation satisfy a relationship similar to Eq. (8). The generalization to a larger number of Werner pairs is obvious.

After the execution of the unitary transformation (7), Alice and Bob have to test that all the particles, except those labeled by the first (unprimed) indices, have their spin up. They discard any set of $n$ Werner pairs where that test fails, even once. The density matrix for the remaining ''successful'' cases is thus obtained by retaining, on the right-hand side of Eq. (7), only the terms whose primed components are zeros, and then renormalizing the resulting matrix to unit trace. This means that only two of the $2^n$ rows of the $U$ matrix, namely those with indices $000\ldots$ and $100\ldots$, are relevant (and likewise for the $V$ matrix). The elimination of all the other rows greatly simplifies the problem of optimizing these matrices. We shall thus write, for brevity,

$$U_{\mu 00,mm'm''}\rightarrow U_{\mu,mm'm''}, \tag{9}$$

where $\mu=0,1$. Then, on the left-hand side of Eq. (8), we effectively have two unknown vectors, $U_0$ and $U_1$, each one with $2^n$ components (labeled by Latin indices $mm'm''$). These vectors have unit norm and are mutually orthogonal. Likewise, Bob has two vectors, $V_0$ and $V_1$. The problem is to optimize these four vectors so as to make the expectation value of the Bell operator [24],

$$C:=AB+AB'+A'B-A'B', \tag{10}$$

as large as possible.

The optimization proceeds as follows. The new density matrix, for the pairs of spin-$\frac{1}{2}$ particles not yet tested by Alice and Bob (that is, for the first pair in each set of $n$ pairs), is

$$(\rho_{\rm new})_{\mu\nu,\sigma\tau}=NU_{\mu,mm'm''}V_{\nu,nn'n''}\rho_{mn,st}\rho_{m'n',s't'}\rho_{m''n'',s''t''}\times U^{*}_{\sigma,ss's''}V^{*}_{\tau,tt't''}, \tag{11}$$

where $N$ is a normalization constant, needed to obtain unit trace ($N^{-1}$ is the probability that all the ''spin up'' tests were successful). We then have [8], for fixed $\rho_{\rm new}$ and all possible choices of $C$,

$$\max[\,{\rm Tr}(C\rho_{\rm new})]=2\sqrt{M}, \tag{12}$$

where $M$ is the sum of the two largest eigenvalues of the real symmetric matrix $T^{\dagger}T$, defined by

$$T_{pq}:={\rm Tr}[(\sigma_p\otimes\sigma_q)\rho_{\rm new}]. \tag{13}$$

Note that the matrix $T_{pq}$ is real, because the Pauli matrices $\sigma_p$ and $\sigma_q$ are Hermitian, but in general it is not symmetric (explicit formulas are given in the Appendix). Our problem is to find the vectors $U_\mu$ and $V_\nu$ that maximize $M$.

At this point, some additional simplifying assumptions are helpful. Since all matrix elements $\rho_{mn,st}$ are real, we shall restrict our search to vectors $U_\mu$ and $V_\nu$ that only have real components. (It is unlikely that higher values of $M$ can be attained by using complex vectors, but this possibility cannot be totally ruled out without a formal proof.)

Furthermore, the situations seen by Alice and Bob are completely symmetric, except for the presence of opposite signs in the standard expression for the singlet state:

$$\psi=\left[\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix}-\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\right]\Big/\sqrt{2}. \tag{14}$$

The opposite signs can be made to become the same by redefining the basis, for example by representing the ''down'' state of Bob's particle by the symbol $\left(\begin{smallmatrix}0\\-1\end{smallmatrix}\right)$, *without* changing the basis used for Alice's particle. This partial change of basis is equivalent to a substitution

$$V_{\nu,nn'n''} \rightarrow (-1)^{\nu+n+n'+n''} V_{\nu,nn'n''}, \tag{15}$$

on Bob's side. The minus signs in Eq. (6) also disappear, and there is then complete symmetry for the two observers. It is therefore plausible that, with that new basis, we have $U_\nu = V_\nu$. Therefore, when we return to the original basis and notations, the optimal $U_\nu$ and $V_\nu$ satisfy

$$V_{\nu,nn'n''} = (-1)^{\nu+n+n'+n''} U_{\nu,nn'n''}. \tag{16}$$

We shall henceforth restrict our search to pairs of vectors that satisfy this relation. (Without imposing this restriction, I checked, for a few values of $x$, that the optimal vectors $U$ and $V$ indeed had that symmetry property, when $n=2$ or 3. However, an exhaustive search for $n=4$ would have exceeded the capacity of my workstation.)

After all the above simplifications, the problem that has to be solved is the following: find two mutually orthogonal unit vectors, $U_0$ and $U_1$, each with $2^n$ real components, that maximize the value of $M(U)$ defined by Eqs. (12) and (13). This is a standard optimization problem, which can be solved numerically, for example by using the Powell algorithm [25]. Some care must, however, be exercised. The orthonormality constraints must be imposed in a way that does not impede the convergence of the iterations. Moreover, there is a continuous infinity of equivalent solutions, because the entire experimental protocol, and therefore all the physical data, are invariant under rotations around the quantization axes (namely, the axes along which the ''spin up'' tests are performed). This means that a substitution

$$\begin{aligned} U_{0,mm'm''} &\rightarrow U_{0,mm'm''}\cos\alpha - U_{1,mm'm''}\sin\alpha, \\ U_{1,mm'm''} &\rightarrow U_{0,mm'm''}\sin\alpha + U_{1,mm'm''}\cos\alpha, \end{aligned} \tag{17}$$

for any real $\alpha$, does not affect the value of $M(U)$. Similar transformations, with arbitrary angles, can also be performed on each one of the $n$ other indices. Therefore the location of a maximum of $M(U)$ is not a *point* in the $(2^{n+1}-3)$-dimensional parameter space, but can lie anywhere on an $(n+1)$-dimensional *manifold*.

Since the function $M(U)$ is bounded, it must have at least one maximum. It may, however, have more than one: there may be several distinct $(n+1)$-dimensional manifolds on which $M(U)$ is locally maximal, each one with a different value of the maximum. A numerical search by the Powell algorithm [25] ends at one of these maxima, but not necessarily at the largest one. The outcome may depend on the initial point of the search. It is therefore imperative to start from numerous randomly chosen points in order to ascertain, with reasonable confidence, that the largest maximum has indeed been found. (A curious difficulty arises from the fact that Alice and Bob can always obtain $\langle C\rangle = 2$, irrespective of the quantum state, simply by measuring the unit operator, so that all their results are $+1$. It is important that the computer program used for optimization be immune to such artifices.)

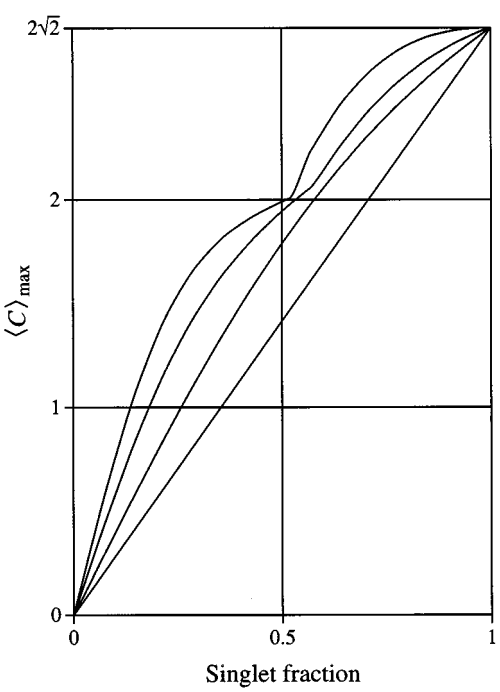


FIG. 1. Maximal expectation value of the Bell operator, versus the singlet fraction in the Werner state, for collective tests performed on several Werner pairs (from bottom to top of the figure, 1, 2, 3, and 4 pairs, respectively). The CHSH inequality is violated when $\langle C\rangle > 2$.

## III. RESULTS AND CONCLUSIONS

In all the cases that were examined, it was found that $M(U)$ has one of its maxima for the following simple choice:

$$U_{0,00\ldots} = U_{1,11\ldots} = 1, \tag{18}$$

and all the other components of $U_0$ and $U_1$ vanish. Recall that the ''vectors'' $U_0$ and $U_1$ actually are *rows* $U_{000\ldots}$ and $U_{100\ldots}$ of the $2^n$-dimensional unitary matrix $U$ (the other rows are irrelevant because of the elimination of all the experiments in which a particle failed the spin-up test). In the case $n=2$, one of the unitary matrices having the property (18) is a simple permutation matrix that can be implemented by a ''controlled- NOT'' quantum gate [26]. The corresponding Boolean operation is known as XOR (exclusive OR). For larger values of $n$, matrices that satisfy Eq. (18) will also be called XOR-transformations.

It was found, by numerical calculations, that XOR-transformations always are the optimal ones for $n=2$. They are also optimal for $n=3$ when the singlet fraction $x$ is less than 0.57, and for $n=4$ when $x<0.52$. For larger values of $x$, more complicated forms of $U_0$ and $U_1$ give better results. The existence of two different sets of maxima may be seen in Fig. 1: there are discontinuities in the slopes of the graphs for $n=3$ and 4, which occur at the values of $x$ where the largest maximum of $\langle C\rangle$ passes from one of the manifolds to the other one.

For $n=5$, a complete determination of $U_0$ and $U_1$ requires the optimization of 64 parameters subject to three constraints, more than my workstation could handle. I therefore

considered only XOR-transformations, which are likely to be optimal for $x \lesssim 0.5$. In particular, for $x=0.5$ (the value that was used in Werner's original work [10]), the result is $\langle C \rangle = 2.0087$, and the CHSH inequality is violated. This violation occurs in spite of the existence of an explicit LHV model that gives correct results if the pairs are tested one by one. For $n \to \infty$, we expect the CHSH inequality to be violated for $x > \frac{1}{3}$ (that is, when the fidelity is $F > \frac{1}{2}$), because such pairs can be ''purified'' by the methods of Refs. [15–18].

In summary, it has been shown that, even if a well defined LHV model [10] can correctly predict all the statistical properties of some pairs of particles when the particles are tested separately by two distant observers, a definite nonlocal behavior (namely, a violation of the CHSH inequality) may arise if several pairs are tested simultaneously, provided that the particles held by each observer are allowed to *interact locally before they are tested*. This result is yet another example of the fact that more information can sometimes be extracted by simultaneously testing several identically prepared quantum systems, than by testing each one of them separately [27]. Note that, for such a phenomenon to occur, it is always necessary that the distant observers exchange *classical* information [13].

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## APPENDIX

This appendix explicitly lists all the components of the $T_{pq}$ matrix (13), when the density matrix $\rho_{mn,st}$ is real and symmetric:

$$T_{xx} = \rho_{00,11} + \rho_{01,10} + \rho_{10,01} + \rho_{11,00}, \tag{A1}$$

$$T_{yy} = -\rho_{00,11} + \rho_{01,10} + \rho_{10,01} - \rho_{11,00}, \tag{A2}$$

$$T_{zz} = \rho_{00,00} - \rho_{01,01} - \rho_{10,10} + \rho_{11,11}, \tag{A3}$$

$$T_{xz} = \rho_{00,10} - \rho_{01,11} + \rho_{10,00} - \rho_{11,01}, \tag{A4}$$

$$T_{zx} = \rho_{00,01} + \rho_{01,00} - \rho_{10,11} - \rho_{11,10}. \tag{A5}$$

The other components vanish, because the Hermitian matrices $\sigma_p \otimes \sigma_q$ that have only one $y$-index are antisymmetric (and pure imaginary).

Recall that $M$ in Eq. (12) is the sum of the two largest eigenvalues of $T^\dagger T$. One of the eigenvalues of this matrix obviously is $T_{yy}^2$. The two others are obtained by diagonalizing the symmetric matrix

$$\begin{pmatrix} T_{xx}^2 + T_{zx}^2 & T_{xx}T_{xz} + T_{zx}T_{zz} \\ T_{xz}T_{xx} + T_{zz}T_{zx} & T_{xz}^2 + T_{zz}^2 \end{pmatrix}. \tag{A6}$$

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