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Bounding the Set of Classical Correlations of a Many-Body System

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We present a method to certify the presence of Bell correlations in experimentally observed statistics, and to obtain new Bell inequalities. Our approach is based on relaxing the conditions defining the set of correlations obeying a local hidden variable model, yielding a convergent hierarchy of semidefinite programs (SDP's). Because the size of these SDP's is independent of the number of parties involved, this technique allows us to characterize correlations in many-body systems. As an example, we illustrate our method with the experimental data presented in Science **352**, 441 (2016).

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Introduction.—Local measurements on quantum systems can display correlations that may not be explained by any local hidden variable model (LHVM) [1] or, in other words, that cannot be reproduced by local deterministic strategies (LDS), even if assisted by shared randomness [2]. Bell inequalities bound the space of LHVM or "classical" correlations, and correlations that violate a Bell inequality are termed nonlocal. Besides their fundamental interest, nonlocal correlations are a key resource enabling novel quantum information processing tasks [3].

Finding all Bell inequalities is an extremely demanding problem [4], which is NP complete even in the bipartite scenario [5]. For this reason, complete lists of Bell inequalities exist only for the simplest scenarios, e.g., not beyond three parties [6–10].

In the multipartite case one needs to relax the condition of membership in the LHVM set, for example, by looking for Bell inequalities of a particular form. A natural choice is to exploit the symmetries of the physical system of interest [e.g., permutational invariance (PI) [11] or translational invariance (TI) [12]]. Moreover, to make them experimentally practical, it is desirable to ask for additional features such as being composed of low-order correlators only (see Refs. [13,14] and [12,15–17], for the PI and TI cases, respectively). In the PI case, this approach has recently allowed for the detection of Bell correlations in a Bose-Einstein condensate of 480 atoms [18] and in a thermal ensemble of 5×10^5 atoms [19].

The usual technique to find Bell inequalities is via the characterization of the set of LHVM correlations. From a geometrical point of view this set is a polytope, i.e., a bounded convex set that can be described by a finite number of vertices, or, equivalently, by the intersection of a finite number of half-spaces. The vertices of the LHVM polytope can be listed, as they correspond to LDS, and from them the Bell inequalities defining the half-spaces can be computed. Unfortunately, going from one description to the other is extremely inefficient, due to the (double) exponential scaling

of its complexity in the number of parties [20]. Restricting the search to Bell inequalities of a particular form results in (i) a better scaling [12,14] and (ii) Bell inequalities that can be tested experimentally via collective observables, such as total spin components [13,18,19]. However, this approach of characterizing the LHVM polytope is still prohibitive when the number of parties is large, e.g., because a complete list of the vertices is inaccessible and because one has to infer classes of inequalities from a small number of parties [12–15], leaving potentially useful ones undiscovered.

In this work, we present a technique to approximate the set of LHVM correlations from the outside. Our technique can be seen as checking all Bell inequalities of a specific form with a single test. It is based on a hierarchy of semidefinite programs (SDP's) aproximating convex hulls of semialgebraic sets [21–24]. One key advantage of our method is that, contrary to other existing SDP's hierarchies [25,26], the number of parties enters as a parameter in the SDP's, without affecting their size. Moreover, in all cases we considered, our hierarchy shows convergence to a relaxation of the LHVM set already at its lowest level. In summary, the method we propose provides an efficient sufficient condition for a set of correlations to be nonlocal, and it yields a certificate of nonlocality by providing the Bell inequality that is violated.

Overview of the method.—We consider the Bell scenario in which each of N observers performs one of d possible measurements on their share of the system. For simplicity, we are going to assume that every measurement yields outcomes ± 1 , keeping the generalization to more outcomes for later. Let $\mathcal{M}_k^{(i)}$ be the kth measurement of the *i*th party. We are interested in Bell correlations that can be revealed by PI Bell inequalities composed of at most K-body correlators, i.e., inequalities of the form

$$\sum_{k \le K} \sum_{j_1 \le \dots \le j_k} \alpha_{j_1 \dots j_k} \mathcal{S}_{j_1 \dots j_k} + \beta_C \ge 0, \tag{1}$$

where $\alpha_{j_1...j_k} \in \mathbb{R}$, $\beta_C \in \mathbb{R}$ is the so-called classical bound, and $S_{j_1...j_k}$ are the PI correlators defined as

$$\mathcal{S}_{j_1\dots j_k} = \sum_{\substack{i_1,\dots,i_k=1\\\text{all}^r \text{ sdifferent}}}^N \langle \mathcal{M}_{j_1}^{(i_1)}\dots \mathcal{M}_{j_k}^{(i_k)} \rangle.$$
(2)

Our task is to certify that given experimental data $\vec{S}_{K}^{*} = (S_{0}^{*}, S_{1}^{*}, ...)$ cannot be described by LHVM, or, in other words, we want to construct a Bell inequality of the form of Eq. (1) that is violated for \vec{S}_{K}^{*} , thus confirming the presence of Bell correlations. In order to achieve this, we perform two mild relaxations of the membership conditions to the LHVM set, which we show to become negligible as *N* increases. This yields a hierarchy of SDP's of the form

$$\max_{\substack{y_j \in \mathbb{R} \\ \text{s.t. } \tilde{\Gamma}(\vec{y}) \succeq 0 \\ y_0 = 1 \\ y_j = (\vec{\mathcal{S}}_K^*)_j, \end{cases}$$
(3)

where y_0 and the y_j corresponding to \vec{S}_K^* are fixed, while the remaining y_j are free real parameters that can be varied until the moment matrix $\tilde{\Gamma}$ (that we are going to show how to construct) is positive semidefinite. If the SDP (3) is infeasible, its dual yields the coefficients $\alpha_{j_1...j_k}$ and a (relaxed) classical bound β_C of a Bell inequality of the form of Eq. (1) that certifies that \vec{S}_K^* is nonlocal. Note the crucial fact that the number of parties *N* enters as a parameter in $\tilde{\Gamma}$, therefore, not affecting the size of the SDP. Our method can be seen as a way to check infinitely many Bell inequalities of the form of Eq. (1) at once. We now illustrate our method in more detail.

Details of the method.—If the observed statistics \vec{S}_K^* satisfy a LHVM, they belong to the LHVM polytope (projected) in the space of *K*-body symmetric correlators, \mathbb{P}_K^s . Its vertices correspond to LDS, satisfying

$$\langle \mathcal{M}_{j_1}^{(i_1)} \dots \mathcal{M}_{j_k}^{(i_k)} \rangle = \langle \mathcal{M}_{j_1}^{(i_1)} \rangle \cdots \langle \mathcal{M}_{j_k}^{(i_k)} \rangle \quad \text{(local)}, \tag{4}$$

$$\langle \mathcal{M}_j^{(i)} \rangle = \pm 1 \quad \forall \ i, j \quad (\text{deterministic}).$$
 (5)

Fortunately, the PI condition reduces the number of vertices from exponential to polynomial in *N*, because only the amount of parties following the same LDS is relevant [13,14]. For this reason, it is natural to introduce $m = 2^d$ variables $\vec{x} = (x_1, ..., x_m)$, where x_i counts how many parties follow the *i*th LDS. Note that the x_i satisfy

$$\sum_{i=1}^{m} x_i = N, \qquad x_i \in \mathbb{Z}_{\ge 0}.$$
 (6)

Using this parametrization, at every vertex Eq. (2) can be written as a polynomial of degree *k* in *m* variables with real coefficients, i.e., $S_{j_1...j_k} \in \mathbb{R}[\vec{x}]_k$ (see Ref. [13] and the example). Denoting with \vec{S}_K the vector of such correlations up to degree *K*, we express \mathbb{P}_K^S as the convex hull (CH) of \vec{S}_K evaluated on the parameter region defined by Eq. (6):

$$\mathbb{P}_{K}^{S} = \operatorname{CH}\left\{\vec{\mathcal{S}}_{K}(\vec{x}) \text{ s.t. } \sum_{i} x_{i} = N, x_{i} \in \mathbb{Z}_{\geq 0}\right\}.$$
(7)

First relaxation.—According to Eq. (7), \mathbb{P}_{K}^{S} is defined as the convex hull of a finite set of points, therefore, not exploiting the inherent algebraic structure present in the polynomials $\vec{S}_{K}(\vec{x})$. The first relaxation we introduce consists of dropping the condition $x_i \in \mathbb{Z}_{\geq 0}$, and considering instead $x_i \in \mathbb{R}_{\geq 0}$, which gives rise to the set

$$\widetilde{\mathbb{P}_{K}^{S}} = \operatorname{CH}\left\{\vec{\mathcal{S}}_{K}(\vec{x}) \text{ s.t. } \sum_{i} x_{i} = N, x_{i} \in \mathbb{R}_{\geq 0}\right\}.$$
(8)

Note that $\vec{S}_K(\vec{x})$ with $\vec{x} \in \mathbb{R}^m$ interpolates the vertices of \mathbb{P}^S_K , implying $\mathbb{P}^S_K \subseteq \widetilde{\mathbb{P}^S_K}$. As a consequence, if a set of correlations lies outside $\widetilde{\mathbb{P}^S_K}$, it also lies outside \mathbb{P}^S_K , and therefore it is nonlocal.

The correlators $\overline{S}_K(\vec{x})$ can be expressed as a set of equations $f_i(\vec{S}_K) = 0$, and similarly the non-negativity constraints $x_j \ge 0$ can be expressed as a set of constraints in \vec{S}_K , by a set of inequalities $g_j(\vec{S}_K) \ge 0$ (see the example). In what follows, we refer to the set of solutions of a system of polynomial equations $f_i(\vec{S}_K) = 0$ as an algebraic set. Moreover, if an algebraic set is further restricted by polynomial non-negativity constraints $g_j(\vec{S}_K) \ge 0$, as is the case for $\widetilde{\mathbb{P}}_K^{\tilde{S}}$ in Eq. (8), we shall call such a set semialgebraic.

Second relaxation.—Deciding membership in the CH of a (semi)algebraic set \mathcal{V} is NP hard [23]. However, there exist efficient approximations for CH(\mathcal{V}) from the outside [21–24]. The idea behind these methods is to reduce the membership problem in CH(\mathcal{V}) to that of a multivariate polynomial being non-negative, which can be relaxed to determining whether such polynomial can be expressed as a sum of squares (s.o.s.) [27]. While the first condition is NP hard, the second can be efficiently checked using a SDP, as we are going to show.

Following this approach, the main idea behind our method is to construct linear polynomials $l(\vec{S}_K) \in \mathbb{R}[\vec{S}_K]_1$ satisfying $l(\vec{S}_K) \ge 0$ for all $\vec{S}_K \in \mathcal{V}$, i.e., valid Bell inequalities defining half-spaces containing CH(\mathcal{V}).

Starting from the observation that every polynomial of the form $p + \sum_i f_i p_i$, with $p, p_i \in \mathbb{R}[\vec{S}_K]$, takes the same

values when evaluated in \mathcal{V} [because $f_i(\vec{\mathcal{S}}_K) = 0$ for all $\vec{\mathcal{S}}_K \in \mathcal{V}$], we define the ideal *I* generated by f_i as the set

$$I = \left\{ \sum_{i} f_{i} p_{i} \text{ s.t. } p_{i} \in \mathbb{R}[\vec{\mathcal{S}_{K}}] \right\} \subseteq \mathbb{R}[\vec{\mathcal{S}_{K}}], \qquad (9)$$

such that every polynomial in $p + I = \{p + q, q \in I\}$ is equivalent when evaluated in \mathcal{V} . Moreover, the ideal Idefines the set of equivalence classes $\mathbb{R}[\vec{S_K}]/I$, where $p, q \in \mathbb{R}[\vec{S_K}]$ are in the same class if they are equivalent modulo I, i.e., $p \equiv q \mod I$, meaning that $p - q \in I$.

To express $l(\vec{S}_K)$ we consider the following ansatz:

$$l(\vec{\mathcal{S}}_K) = \sum_{i=0}^m g_i(\vec{\mathcal{S}}_K) \sigma_i(\vec{\mathcal{S}}_K) \mod I, \qquad (10)$$

where $g_0(\vec{S}_K) = 1$, and $\sigma_i(\vec{S}_K)$ are s.o.s. polynomials modulo I [i.e., there exists a s.o.s. polynomial in $\sigma_i(\vec{S}_K) + I$]. For compactness, let us use the shorthand notation g_i and σ_i . Note that since all $g_i \ge 0$ in \mathcal{V} by definition, and s.o.s. are non-negative, the form of Eq. (10) ensures the non-negativity of $l(\vec{S}_K)$ in \mathcal{V} [28].

Now, given a point $\vec{\mathcal{S}}_{K}^{*}$, our goal is to prove that $l(\vec{\mathcal{S}}_{K}^{*}) < 0$ for some set of σ_{i} . If we succeed in this proof, then we have to conclude that $\vec{\mathcal{S}}_{K}^{*} \notin CH(\mathcal{V}) \supseteq \mathbb{P}_{K}^{S}$, i.e., that the statistics in $\vec{\mathcal{S}}_{K}^{*}$ come from nonlocal correlations.

For computational reasons, we need to bound the maximum degree of the s.o.s. decomposition allowed in $\sigma_i + I$. The higher the degree, the larger the family of $l(\vec{S}_K)$ that can be accessed through Eq. (10), but the more computationally expensive to produce such s.o.s. representation will be. This naturally yields a hierarchy of outer approximations to CH(\mathcal{V}) by increasing the degree of the s.o.s. decomposition of σ_i . To simplify our exposition, we consider here the special case where all $\sigma_i = \sigma$.

To express all σ that are s.o.s. of degree 2μ , modulo I, we adopt the following procedure. First, we select (via a Gröbner basis [29]) a linearly independent set of representatives of $\mathbb{R}[\vec{S}_K]/I$, and we order them in the vector $\vec{b} = (1, S_0, S_1, ...)^T$. Denoting by \vec{b}_{μ} the vector of elements of \vec{b} of degree at most μ , we write $\sigma = \sum_j s_j^2 \mod I$, where s_j are linear combinations of the elements of \vec{b}_{μ} ; i.e., $s_j = \vec{b}_{\mu}^T \vec{a}_j$, with \vec{a}_j real vectors. At this point, by defining the matrix $G = \sum_j \vec{a}_j \vec{a}_j^T$, which is positive semidefinite by construction ($G \succeq 0$), and the moment matrix $\Gamma_i = g_i \vec{b}_{\mu} \vec{b}_{\mu}^T$ mod I, we write

$$g_i \sigma = \Gamma_i \cdot G \mod I, \qquad G \succeq 0.$$
 (11)

Here, $X \cdot Y = \sum_{ab} X_{ab} Y_{ab}$.

When the elements of Γ_i corresponding to \vec{S}_K are replaced by \vec{S}_K^* , only some of its entries are constrained. If the remaining free parameters can be tuned to make $\Gamma_i \geq 0$, Eq. (11) ensures that $g_i \sigma \geq 0$ in \vec{S}_K^* for all σ (that are s.o.s. of degree 2μ , modulo *I*). On the other hand, when $\Gamma_i \geq 0$ for any choice of the free parameters, there exists at least one σ such that $g_i \sigma < 0$ in \vec{S}_K^* [30].

Recall here that our final goal is to prove that there exists a σ such that Eq. (10) gives $l(\vec{S}_{K}^{*}) < 0$. To this end, we write Eq. (10) as $l(\vec{S}_{K}) = \tilde{\Gamma} \cdot \tilde{G} \mod I$, where $\tilde{\Gamma} = \bigoplus_{i=0}^{m} \Gamma_{i}$, and similarly for \tilde{G} . As for Eq. (11), we ask whether $\tilde{\Gamma}$ can be made positive semidefinite at the point \vec{S}_{K}^{*} . To perform this check with a SDP, we first reduce $\tilde{\Gamma}$ modulo *I*, and then linearize it as

$$\tilde{\Gamma} = \sum_{j} y_{j} \tilde{\Gamma}_{j}, \tag{12}$$

where y_j indexes the *j*th element of \vec{b} , and $\tilde{\Gamma}_j$ are constant real matrices embodying the constraints among the entries of $\tilde{\Gamma}$. Now, for the point \vec{S}_K^* , we execute SDP (3) to check the presence of nonlocal correlations.

If SDP (3) is infeasible, $\tilde{\Gamma} \not\geq 0$ independently on the free y_j , which proves that there exist a σ such that $l(\vec{S}_K^*) < 0$, while $l(\vec{S}_K) \geq 0$ for all $\vec{S}_K \in \mathbb{P}_K^S$. Therefore, the infeasibility of SDP (3) certifies that $\vec{S}_K^* \notin CH(\mathcal{V}) \supseteq \mathbb{P}_K^S$, i.e., its nonlocal nature (see the example and Fig. 2).

While the output of SDP (3) is the answer feasible or infeasible, we can also write a SDP to maximize λ subject to $y_0 = 1$ and $y_j = \lambda(\vec{S}_K^*)_j$. The dual formulation of this modified SDP results in the dual variables $\alpha_{j_1...j_k}$ associated to $y_1...y_i$, and β_C associated to y_0 , defining a Bell inequality (1) that provides a certificate for the nonlocality of \vec{S}_K^* [31] (see the example and Fig. 2). In addition, maximizing λ along different directions \vec{S}_K^* results in the points $\lambda_{\max} \vec{S}_K^*$ that can be used to approximate the boundary of \mathbb{P}_K^S , (see Fig. 1).

On the other hand, if SDP (3) is feasible it means that it does not exist a σ that is s.o.s. of degree 2μ , modulo *I*, such that $l(\vec{S}_K^*) < 0$. In this case, we could access a higher level of our hierarchy by increasing μ , which enlarges the class of $l(\vec{S}_K)$ that can be represented [32].

An additional result in Refs. [21,22] ensures that, since the set \mathcal{V} we want to approximate is compact, our hierarchy converges at least asymptotically to $CH(\mathcal{V}) \equiv \widetilde{\mathbb{P}}_{K}^{S}$. Actually, in all examples we studied, we observed numerically that convergence at $\mu = 1$ was already present.

Example.—In the spirit of Refs. [13,18], we consider d = K = 2, giving rise to the set of correlators



FIG. 1. For N = 10 and K = 2, the plane of the symmetric correlations of the form $\alpha \vec{S}_2^{(1)} + \beta \vec{S}_2^{(2)}$, with $\vec{S}_2^{(1)} = (1, -1, 0, -1, 1)^T / \sqrt{4}$ and $\vec{S}_2^{(2)} = (0, -1, -1, 1, 0)^T / \sqrt{3}$. In blue, the intersection of \mathbb{P}_2^S with the plane, computed with a linear program. In red, the boundary of the feasible set of SDP (3) for $\mu = 1$. The gap between the two objects is imputable mainly to the first relaxation, and the small *N* was chosen also to appreciate its size, which remains of the same order while \mathbb{P}_2^S increases with *N* (see also Fig. 2).

 $\vec{S}_2 = (S_0, S_1, S_{00}, S_{01}, S_{11}) \in \mathbb{R}^5$, and *N* parties. In this scenario, there are four LDS parametrized by $x_i \ge 0$ and satisfying $\sum_{i=1}^4 x_i = N$. By expressing the correlators \vec{S}_2 evaluated on a LDS in terms of \vec{x} , we obtain [13]

$$\begin{pmatrix} N\\ S_1\\ S_0\\ Z \end{pmatrix} = \begin{pmatrix} x_1 + x_2 + x_3 + x_4\\ x_1 + x_2 - x_3 - x_4\\ x_1 - x_2 + x_3 - x_4\\ x_1 - x_2 - x_3 + x_4 \end{pmatrix},$$
(13)

$$\begin{pmatrix} S_{00} \\ S_{01} \\ S_{11} \end{pmatrix} = \begin{pmatrix} S_0^2 - N \\ S_0 S_1 - Z \\ S_1^2 - N \end{pmatrix}.$$
 (14)

When *N* is fixed Eqs. (13) are three free parameters, while Eqs. (14) define the ideal *I*, whose generators $\{f_1(\vec{S}_2), f_2(\vec{S}_2)\} = \{S_{00} - S_0^2 + N, S_{11} - S_1^2 + N\}$ form also a Gröbner basis for *I* [29]. Inverting Eq. (13) we obtain four polynomials in \vec{S}_2 that allow us to express the constraints $x_i = g_i(\vec{S}_2) \ge 0$, for instance,

$$g_1(\vec{\mathcal{S}}_2) = [\mathcal{S}_0 + \mathcal{S}_1 + (\mathcal{S}_0 \mathcal{S}_1 - \mathcal{S}_{01}) + (\mathcal{S}_0^2 - \mathcal{S}_{00})]/4 \ge 0.$$

At the first level of our hierarchy, $\mu = 1$, the vector $\vec{b}_1^T = (1, S_0, ..., S_{11})$ generates the five 6×6 moment matrices Γ_i . Combined together, the Γ_i give a 30×30 block-diagonal moment matrix $\tilde{\Gamma}$, in which *N* appears as a parameter, and thus not affecting its size.

Considering the experimental data presented in Ref. [18], we can conclude that the measured statistics



FIG. 2. Plane generated by $\{S_0, (S_{00} + 2S_{01} + S_{11})\}$. Black circled dot, point (367.6, -525.4) measured experimentally in [18] for N = 476. Blue points, projected vertices of \mathbb{P}_2^{S} . Blue line, bound given by the Bell inequality $-2S_0 + (S_{00} + 2S_{01} + S_{11})/2 + 2N \ge 0$, from Refs. [13,18]. This inequality is tight, meaning that it is also a facet of the projected polytope. Pink region, points where SDP (15) gives $\lambda \ge 1$. Orange dashed line, Bell inequality obtained numerically by solving the dual of SDP (15). The distance between the blue and the orange lines is 1.000 002, meaning that the error of our method compared to the tight classical bound scales as 1/N, and it is imputable mainly to the first relaxation.

 $(S_0^*, S_{00}^* + 2S_{01}^* + S_{11}^*) = (367.6, -525.4)$ contain Bell correlations because the following SDP gives $\lambda < 1$:

$$\max_{y_{j} \in \mathbb{R}} \lambda$$

s.t. $\tilde{\Gamma} \succeq 0$ (15)
 $y_{0} = 1$
 $(y_{1}, y_{3} + 2y_{4} + y_{5}) = \lambda(\mathcal{S}_{0}^{*}, \mathcal{S}_{00}^{*} + 2\mathcal{S}_{01}^{*} + \mathcal{S}_{11}^{*}).$

The dual of SDP (15) gives as a result the dual variables associated to y_0 , y_1 , and $y_3 + 2y_4 + y_5$, which correspond, respectively, to the coefficients of the Bell inequality $\beta_C + \alpha_1 S_0 + \alpha_2 (S_{00} + 2S_{01} + S_{11}) \ge 0$ (see Fig. 2).

Comment on more outcomes.—It is possible to consider the case where measurements have more outcomes by defining the expectation values as, e.g., $\langle \mathcal{M}_j^{(i)} \rangle^{(a)} =$ $2P_i(a|j) - 1$, where $P_i(a|j)$ is the probability that measurement j on party i gives as outcome a, and the symmetrized correlators as, e.g., $\mathcal{S}_j^{(a)} = \sum_{i=1}^N \langle \mathcal{M}_j^{(i)} \rangle^{(a)}$.

Conclusions.—We introduced a method to bound the set of LHVM correlations. Its main advantage, with respect to other techniques, is that there is no scaling with the number of parties, making it particularly suited for the study of nonlocal correlations in many-body systems. Our approach has several applications, some of which were presented here, such as the characterization of experimentally observed correlations or the derivation of new Bell inequalities. Furthermore, it can be easily generalized to scenarios with more measurements settings and outcomes, potentially enlarging the class of systems, and states, where nonlocal correlations could be experimentally detected.

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- [27] Obviously, every s.o.s. polynomial is non-negative, but the converse is false in general. The textbook counter-example is the Motzkin polynomial, $x^4y^2 + x^2y^4 3x^2y^2 + 1$, which is non-negative on \mathbb{R}^2 but it is not a s.o.s. of elements of $\mathbb{R}[x, y]$.
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- [30] For a detailed proof, see the proof of Theorem 5.1 in Ref. [24].
- [31] See Sec. 3.1 of Ref. [26] and, for a detailed derivation, Sec. 4.2 of Ref. [23].
- [32] Note that the matrix Γ for the level μ , is a principal minor of the matrix $\tilde{\Gamma}'$ for the level $\mu' > \mu$. Therefore, if $\tilde{\Gamma}' \succeq 0$ then necessarily $\tilde{\Gamma} \succeq 0$, while the converse is not always true.