Theoretical formulation of finite-dimensional discrete phase spaces: II. On the uncertainty principle for Schwinger unitary operators

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Abstract

We introduce a self-consistent theoretical framework associated with the Schwinger unitary operators whose basic mathematical rules embrace a new uncertainty principle that generalizes and strengthens the Massar-Spindel inequality. Among other remarkable virtues, this quantum-algebraic approach exhibits a sound connection with the Wiener-Kinchin theorem for signal processing, which permits us to determine an effective tighter bound that not only imposes a new subtle set of restrictions upon the selective process of signals and wavelets bases, but also represents an important complement for property testing of unitary operators. Moreover, we establish a hierarchy of tighter bounds, which interpolates between the tightest bound and the Massar-Spindel inequality, as well as its respective link with the discrete Weyl function and tomographic reconstructions of finite quantum states. We also show how the Harper Hamiltonian and discrete Fourier operators can be combined to construct finite ground states which yield the tightest bound of a given finite-dimensional state vector space. Such results touch on some fundamental questions inherent to quantum mechanics and their implications in quantum information theory.

1 Introduction

Initially introduced by Schwinger [1] for treating finite quantum systems characterized by discrete degrees of freedom immersed in a finite-dimensional complex Hilbert space [2], the unitary operators gained their first immediate application in the formal description of Pauli operators. Ever since, an expressive number of manuscripts [3] proposed similar theoretical frameworks with intrinsic mathematical virtues and concrete applications in a wide family of
physical systems — here supported by a finite space of states. With regards to these state spaces, it is worth mentioning that certain algebraic approaches related to quantum representations of finite-dimensional discrete phase spaces were constructed from this context in the past [4], and tailored in order to properly describe the quasiprobability distribution functions [5] in complete analogy with their continuous counterparts [6]. Thus, applications associated with the discrete distribution functions covering different topics of particular interest in physics — e.g., quantum information theory and quantum computation [7,8], as well as the qualitative description of spin-tunneling effects [9], open quantum systems [10] and magnetic molecules [11], among others — emerge from these approaches as a natural extension of an important robust mathematical tool.

Although the efforts in constructing a sound theoretical framework to deal with finite-dimensional discrete phase spaces have recently achieved great advances (e.g., see Ref. [12]), certain fundamental questions particularly associated with the factorization properties of finite spaces [13], uncertainty principle [14] and property testing [15] for the unitary operators still remain without satisfactory answers in the literature (indeed, some of them represent open problems which do not share the same rhythm of progress). In this paper, we focus on the problem of deriving a general uncertainty principle for Schwinger unitary operators in physics. In what follows, we discuss the relevance of such a principle and, subsequently, briefly review the results obtained by Massar and Spindel [14] on this specific subject.

To begin with, it is necessary to remember that, through an original algebraic approach which encompasses the description of finite quantum systems, Weyl [16] was the first to describe quantum kinematics as an Abelian group of ray rotations in the system space. According to Weyl: “The kinematical structure of a physical system is expressed by an irreducible Abelian group of unitary ray rotations in system space. The real elements of the algebra of this group are the physical quantities of the system; the representation of the abstract group by rotations of system space associates with each such quantity a definite Hermitian form which ‘represents’ it.” With respect to the particular case of finite state vector space, one of Weyl’s most significant achievements was that the observation of pairs of unitary rotation operators obey special commutation relations (bringing, as a result, the roots of unity) which are the unitary counterparts of the fundamental Heisenberg relations. Moreover, it is worth mentioning that such a ray representation of the Abelian group of rotations can be connected with some representations of the generalized Clifford algebra, this fact being thoroughly explored by Ramakrishnan and coworkers [17] through extensive studies of certain physical problems. Still within the aforementioned Weyl approach for quantum kinematics, let us briefly mention that some authors have also addressed the problem of discussing quantum mechanics in finite-dimensional state vector spaces, where the coordinate and
momentum operators (characterized by discrete spectra) play an essential role in this context [18].

Although both Weyl and Schwinger’s theoretical approaches have made seminal and complementary contributions upon the scope of unitary operators in finite physical systems, the relevance of a general uncertainty principle for such operators has not been clearly discussed or even mentioned with due emphasis in the past. Reflecting on this, Massar and Spindel [14] have recently established a first uncertainty principle for the discrete Fourier transform [19] whose range of applications in physics covers, among other topics, the Pauli operators, the coordinate and momentum operators with finite discrete spectra, the modular variables, as well as signal processing. Furthermore, their result can also be employed to determine a modified discrete version of the Heisenberg-Kennard-Robertson (HKR) uncertainty principle which resembles the generalized uncertainty principle (GUP) in the quantum-gravity framework [12]. However, if one adopts an essentially pragmatic point of view, certain natural questions arise: “Can Massar-Spindel inequality be recognized as a ‘generalized uncertainty principle’ for all finite quantum states?” If not, “What is the reliable starting point for obtaining a realistic description of this generalized uncertainty principle?”

The main goal of this paper is to present a self-consistent theoretical framework for the Schwinger unitary operators which embodies, within other virtues, an important set of convenient inherent mathematical properties that allows us to construct suitable answers for the aforementioned questions. This theoretical framework, constituted of numerical and analytical results, can be interpreted as a “generalized version” of that one by Massar and Spindel, with immediate applications in quantum information theory and quantum computation, as well as in foundations of quantum mechanics. Next, we emphasize certain essential points of our particular construction process: (i) Numerical computations related to a huge number (\(\geq 10^6\)) of randomly generated finite states demonstrate the existence of a nontrivial hierarchical relation among the different bounds, the Massar-Spindel inequality being considered in such a case as a zeroth-order approximation. (ii) The existence of a tightest bound for different dimensions of state vector space leads us to produce a sufficient number of formal results related to the Hermitian trigonometric operators (defined through well-known specific combinations of unitary operators) and their corresponding Robertson-Schrödinger (RS) uncertainty principles [20], which culminates in the formulation of a new inequality which takes into account the quantum correlation effects. This tighter bound represents a new and important paradigm for signal processing with straightforward implications on finite quantum states [21] and discrete approaches in GUP [22]. (iii) Numerical and analytical approaches [23,24] confirm the special link between the ground state inherent to the Harper Hamiltonian and the tightest bound for any Hilbert space dimensions. Finally, (iv) the connection with tomographic measurements
of finite quantum states via discrete Weyl function represents, in this case, a
*tour de force* in our investigative journey on unitary operators that allows to
join both the Weyl and Schwinger quantum-algebraic approaches in an elegant
way.

This paper is structured as follows. In Section 2, we fix a preliminary ma-
thematical background on the Schwinger unitary operators, which allows us
to discuss the implications and limitations of the Massar-Spindel inequal-
ity for signal processing. In Section 3, we introduce four Hermitian trigonomet-
ric operators through effective combinations of the Schwinger unitary ope-
rators. Together, these operators provide a self-consistent quantum-algebraic
framework, leading us to determine a new tighter bound for Massar-Spindel
inequality. Section 4 is dedicated to discuss certain important aspects of the
tightest bounds and their respective kinematical link with the Harper Ha-
miltonian. In addition, Section 5 presents an elegant mathematical procedure
for measuring a particular family of expectation values — here mapped upon
finite-dimensional discrete phase spaces and related to the unitary operators
under investigation — via discrete Weyl function. Section 6 contains our sum-
mary and conclusions. Finally, Appendix A concerns the Harper functions and
their respective connection with the tightest bounds verified in the numerical
calculations.

2 Preliminaries

In order to make the presentation of this section more clear and self-contained,
we begin by reviewing some essential mathematical prerequisites related to
the Schwinger unitary operators. Only then we establish the Massar-Spindel
inequality and its inherent limitations.

2.1 Schwinger unitary operators

**Definition (Schwinger).** Let \( \{U, V\} \) be a pair of unitary operators defined
in a \( N \)-dimensional state vector space, and \( \{|u_\alpha\rangle, |v_\beta\rangle\} \) denote their respective
orthonormal eigenvectors related by the inner product \( \langle u_\alpha | v_\beta \rangle = \frac{1}{\sqrt{N}} \omega^{\alpha \beta} \) with
\( \omega := \exp \left( \frac{2 \pi i}{N} \right) \). The general properties

\[
U^n |u_\alpha\rangle = \omega^{\alpha n} |u_\alpha\rangle, \quad V^\xi |v_\beta\rangle = \omega^{\beta \xi} |v_\beta\rangle, \quad U^n |v_\beta\rangle = |v_{\beta+n}\rangle, \quad V^\xi |u_\alpha\rangle = |u_{\alpha-\xi}\rangle,
\]

together with the fundamental relations

\[
U^N = 1, \quad V^N = 1, \quad V^\xi U^n = \omega^{n \xi} U^n V^\xi,
\]


constitute an important set of mathematical rules that are related to the
generalized Clifford algebra [17]. Here, the discrete labels \( \{\alpha, \beta, \eta, \xi\} \) obey
the arithmetic modulo \( N \) and \( \langle u_\alpha | v_\beta \rangle \) represents a symmetrical finite Fourier
kernel. A compilation of results and properties associated with \( U \) and \( V \) can be found in Ref. [1].

In the following, let \( \rho \) describe a set of physical systems labeled by a finite
space of states, whereas \( \mathcal{V}_U := 1 - |\langle U \rangle|^2 \) and \( \mathcal{V}_V := 1 - |\langle V \rangle|^2 \) denote the
variances related to the respective unitary operators \( U \) and \( V \) — in this
case, \( \langle U \rangle \) and \( \langle V \rangle \) represent the mean values of \( U \) and \( V \) defined in a \( N \)-
dimensional state vectors space. Since \( \rho \) refers to a normalized density opera-
tor, the Cauchy-Schwarz inequality allows us to prove that
\( |\langle U \rangle|^2 \) and \( |\langle V \rangle|^2 \)
are restricted to the closed interval \([0, 1]\); consequently, both the variances are
trivially bounded by \( 0 \leq \mathcal{V}_U(\mathcal{V}_V) \leq 1 \). Indeed, the upper and lower bounds are
promptly reached when one considers the localized bases \( \{|u_\alpha\rangle\langle u_\alpha|\}_{0 \leq \alpha \leq N-1} \) and
\( \{|v_\beta\rangle\langle v_\beta|\}_{0 \leq \beta \leq N-1} \), i.e., for a given \( \rho = |u_\alpha\rangle\langle u_\alpha| \Rightarrow \mathcal{V}_U = 0 \) and \( \mathcal{V}_V = 1 \);
otherwise, if \( \rho = |v_\beta\rangle\langle v_\beta| \Rightarrow \mathcal{V}_U = 1 \) and \( \mathcal{V}_V = 0 \). Furthermore, note that \( \mathcal{V}_U \)
and \( \mathcal{V}_V \) are invariant under phase transformations, namely, \( U \rightarrow e^{i\varphi} U \) and
\( V \rightarrow e^{i\theta} V \) for any \( \{\varphi, \theta\} \in \mathbb{R} \).

2.2 Massar-Spindel inequality

This inequality is based on the Wiener-Kinchin theorem for signal processing
and provides a constraint between the values of \( \langle V^\xi \rangle \) (correlation function)
and \( \langle U^\eta \rangle \) (discrete Fourier transform of the intensity time series). Accord-
ing to Massar and Spindel: 'This kind of constraint should prove useful in signal
processing, as it constrains what kinds of signals are possible, or what kind of
wavelet bases one can construct.' We state this result in the theorem below
(proved in the supplementary material from Ref. [14]), for then proceeding
with a numerical study of its content and first implications.

**Theorem (Massar and Spindel).** Let \( \bar{U} \) and \( \bar{V} \) denote two unitary operators
such that \( \bar{U} \bar{V} = e^{i\Phi} \bar{V} \bar{U} \) and \( \bar{U}^\dagger \bar{V} = e^{-i\Phi} \bar{V} \bar{U}^\dagger \) with \( \Phi \in [0, \pi) \). The variances
\( \mathcal{V}_\pi \) and \( \mathcal{V}_\varphi \) — here defined for a given quantum state \( \rho \) and limited to the closed
interval \([0, 1]\) — satisfy the inequality
\[
(1 + 2A) \mathcal{V}_\pi \mathcal{V}_\varphi \geq A^2 (1 - \mathcal{V}_\pi - \mathcal{V}_\varphi)
\]
where \( A = \tan \left( \frac{\Phi}{2} \right) \). The saturation is reached for localized bases.
previous subsection) and \( \{ \mathbf{U}, \mathbf{V} \} \). A first immediate link yields the relation \( \mathbf{U} = \mathbf{U} \) and \( \mathbf{V} = \mathbf{V} \) for \( \Phi = -\frac{2\pi}{N} \), which implies in the apparent violation of Eq. (1) since \( \Phi \not\in [0, \pi) \). The second connection establishes the alternative relation \( \mathbf{U} = \mathbf{V} \) and \( \mathbf{V} = \mathbf{U} \) with \( \Phi = \frac{2\pi}{N} \), this result being responsible for validating the Massar-Spindel inequality. It is important to mention that the apparent problem detected in the first situation can be properly circumvented making \( \Phi \to -\Phi \) and \( A \to -A \) with \( \Phi = \frac{2\pi}{N} \) fixed. That is, the modified bound

\[
(1 - 2A) \mathcal{V}_U \mathcal{V}_V \geq A^2 (1 - \mathcal{V}_U - \mathcal{V}_V)
\]

holds for any \( A = \tan \left( \frac{\pi}{N} \right) \) and integer \( N \in [2, \infty) \).

For the sake of simplicity and convenience, let us now introduce the shift operator \( \Delta \mathcal{O} \equiv \mathcal{O} - \langle \mathcal{O} \rangle \) with \( \langle \mathcal{O} \rangle \neq 0 \) for a given arbitrary unitary operator \( \mathcal{O} \) and density operator \( \rho \), which leads to define\(^1\) its non-unitary counterpart as follows [25]:

\[
\delta \mathcal{O} := \frac{\Delta \mathcal{O}}{\langle \mathcal{O} \rangle} = \frac{\mathcal{O} - \langle \mathcal{O} \rangle}{\langle \mathcal{O} \rangle}.
\]

Following, it is straightforward to show that both the variances \( \mathcal{V}_\mathcal{O} \) and \( \mathcal{V}_{\delta \mathcal{O}} \) are related through the expressions

\[
\mathcal{V}_{\delta \mathcal{O}} = \frac{\mathcal{V}_\mathcal{O}}{1 - \mathcal{V}_\mathcal{O}} \quad (0 \leq \mathcal{V}_{\delta \mathcal{O}} < \infty) \quad \text{and} \quad \mathcal{V}_\mathcal{O} = \frac{\mathcal{V}_{\delta \mathcal{O}}}{1 + \mathcal{V}_{\delta \mathcal{O}}},
\]

which substituted into inequality (1) for \( \mathbf{U} = \mathbf{V} \) and \( \mathbf{V} = \mathbf{U} \) gives

\[
\mathcal{V}_{\delta U} \mathcal{V}_{\delta V} \geq \varepsilon^2 \quad \text{with} \quad \varepsilon = \frac{A}{1 + A}.
\]

To illustrate Eq. (4) and corroborate the analytic results obtained by Massar and Spindel, let us introduce the parameters \( \mathcal{S}_{\delta U} = \varepsilon^{-1} \mathcal{V}_{\delta U} \) and \( \mathcal{S}_{\delta V} = \varepsilon^{-1} \mathcal{V}_{\delta V} \) such that \( \mathcal{S}_{\delta U} \mathcal{S}_{\delta V} \geq 1 \). This particular inequality defines a region in the two-dimensional space limited by the rectangular hyperbola \( \mathcal{S}_{\delta V} = \mathcal{S}_{\delta U}^{-1} \) that preserves the original equation \( \mathcal{V}_{\delta U} \mathcal{V}_{\delta V} \geq \varepsilon^2 \). Figure 1 shows the plots of \( \mathcal{S}_{\delta V} \) versus \( \mathcal{S}_{\delta U} \) for approximately \( 10^6 \) states of randomly generated \( \rho \), within the visualization window \( 0 < \mathcal{S}_{\delta U}, \mathcal{S}_{\delta V} \leq 10 \), with (a) \( N = 2 \) (\( \varepsilon \to 1 \)), (b) \( N = 3 \), (c) \( N = 4 \), and (d) \( N = 5 \). Note that, excepting picture (a), all the subsequent

\footnote{It is important to note a certain level of arbitrariness in this definition because there is no specification whatsoever of which density operator \( \rho \) is used to evaluate the mean value in the denominator of Eq. (2). Henceforth, this arbitrariness will be removed by exploring the fact that, in our computations, the operator \( \delta \mathcal{O} \) will always appear as an argument of a variance function — in such a situation, we will understand that the expectation value \( \langle \mathcal{O} \rangle \) is computed with respect to the same state used in the computation of \( \langle \delta \mathcal{O} \rangle \).}
Fig. 1. Plots of $S_{\delta V}$ versus $S_{\delta U}$ for different values of $N$ — 2 (a), 3 (b), 4 (c), and 5 (d) — with approximately $10^6$ randomly generated states, illustrating the Massar-Spindel inequality ($S_{\delta U}S_{\delta V} \geq 1$) for the Schwinger unitary operators. Note that $0 < S_{\delta U}, S_{\delta V} \leq 10$ characterizes a particular visualization window which leads us to guess the existence of a tightest bound (see dashed curves) for each value of dimension $N$, since the distance between the saturation curve $S_{\delta U}S_{\delta V} = 1$ (solid line) and the cloud of points — generated by numerical calculations — increases for $N > 2$. The dot-dashed curves showed in pictures (b,c,d) represent the intermediate inequality $S_{\delta U}S_{\delta V} \geq 1 + \sin\left(\frac{2\pi}{N}\right)$, this result being considered as a first approximation to our initial intents.

cases exhibit a gap between the distribution of states and the rectangular hyperbola, the size of such a gap being dependent on the value of $N$ (such an evidence motivates the search for a tightest bound that corroborates the numerical calculations). In fact, the dashed lines in (b,c,d) describe hyperbolic curves of the form $S_{\delta U}S_{\delta V} = x$, where the value of $x$ was chosen as the smallest value of $S_{\delta U}S_{\delta V}$ amongst the ones computed with the randomly sampled states. Later in this paper, a more rigorous procedure for obtaining such values will be outlined. Finally, let us briefly mention that the dot-dashed lines exhibited in these pictures correspond to the intermediate result $S_{\delta U}S_{\delta V} \geq 1 + \sin\left(\frac{2\pi}{N}\right)$, which will be properly demonstrated in the next section.
3 A Hierarchy of Tighter Bounds

In the first part of this paper, we established a basic theoretical framework related to the Schwinger unitary operators where the Massar-Spindel inequality and its inherent limitations occupied an important place in our discussion on uncertainty principles for physical systems labeled by a finite space of states. At this moment, let us clarify some fundamental points raised by those results: (i) the aforementioned state spaces consist of \(N\)-dimensional Hilbert spaces; (ii) the Massar-Spindel inequality represents a “zeroth-order approximation” in the hierarchy of uncertainty principles; and finally, (iii) the results obtained from the numerical calculations reveal certain unexplored intrinsic properties of some finite quantum states \([26, 27]\) with potential applications in quantum information theory and quantum computation. In this second part, we begin the construction of a solid algebraic framework based on the RS uncertainty principle, which leads us, in a first moment, to determine a self-consistent set of results for the unitary operators \(U\) and \(V\) that permits to generalize the Massar-Spindel inequality. Indeed, these results represent an important tool in our search for tighter bounds (see numerical evidence exhibited in Fig. 1), whose intermediate uncertainty principles will constitute a hierarchical relation between the Massar-Spindel inequality and the tightest bound.

3.1 Quantum-algebraic framework

Let \(\{A, B\}\) denote a pair of Hermitian operators defined in a \(N\)-dimensional state vectors space which obey the RS uncertainty principle [20]

\[
\mathcal{V}_A \mathcal{V}_B \geq \mathcal{E}(A, B) + \frac{1}{4} |\langle [A, B] \rangle|^2, \tag{5}
\]

where \(\mathcal{E}(A, B) := \langle \frac{1}{2} \{A, B\} \rangle - \langle A \rangle \langle B \rangle\) represents the covariance function, and \([A, B] (\{A, B\})\) corresponds to the commutator (anticommutator) between \(A\) and \(B\). Next, since \(U\) and \(V\) are generally non-Hermitian operators, let us consider the cartesian decomposition of an arbitrary non-Hermitian operator

\[\mathcal{V}_C = \mathcal{V}_A - \frac{\mathcal{E}(A, B)}{2 \mathcal{V}_B} B\]

with \(\mathcal{V}_B \neq 0\) and \(\mathcal{V}_C \geq 0\), it turns immediate to obtain the relation \(\mathcal{V}_C = \mathcal{V}_A - \frac{\mathcal{E}(A, B)}{2 \mathcal{V}_B}\), which demonstrates the previous result for \(\mathcal{E}(A, B)\). Moreover, let us also state a very useful result for both the commutation and anticommutation relations between \(A\) and \(B\), that is \(|\langle [A, B] \rangle|^2 + |\langle \{A, B\} \rangle|^2 = 4|\langle AB \rangle|^2\).
\( \mathcal{O} \) into its ‘real’ and ‘imaginary’ parts as follows [28]:

\[
\mathcal{O} = \left( \frac{\mathcal{O} + \mathcal{O}^\dagger}{2} \right) + i \left( \frac{\mathcal{O} - \mathcal{O}^\dagger}{2i} \right) = \text{Re}[\mathcal{O}] + i \text{Im}[\mathcal{O}].
\]

Note that \( \text{Re}[\mathcal{O}] \) and \( \text{Im}[\mathcal{O}] \) represent two Hermitian operators that comply with the RS uncertainty principle and allow to introduce, in particular, the cosine and sine operators through the Schwinger unitary operators.

**Definition.** Let \( \{ C_U, S_U, C_V, S_V \} \) denote four Hermitian operators written in terms of simple combinations associated with \( U \) and \( V \), i.e., \( C_U := \text{Re}[U] \), \( S_U := \text{Im}[U] \), \( C_V := \text{Re}[V] \), and \( S_V := \text{Im}[V] \). The commutation relations involving these operators exhibit a direct connection with certain anticommutation relations:

\[
\begin{align*}
[C_U, C_V] &= iA \{ S_U, S_V \}, \\
[C_U, S_V] &= -iA \{ C_U, C_V \}, \\
[S_U, S_V] &= iA \{ C_U, C_V \}, \\
[S_U, C_V] &= -iA \{ C_U, S_V \},
\end{align*}
\]

where the parameter \( A \) was previously defined in Eq. (1). These results lead us, in principle, to conclude that partial information on two particular elements of the set is not complete, since the complementary elements are also necessary to fully characterize the commutator \([U, V]\). In this sense, let us now consider the four RS uncertainty principles below:

\[
\begin{align*}
\mathcal{V}_{C_U} \mathcal{V}_{C_V} &\geq \mathcal{C}^2(C_U, C_V) + \frac{1}{4} |\langle [C_U, C_V] \rangle|^2, \\
\mathcal{V}_{C_U} \mathcal{V}_{S_V} &\geq \mathcal{C}^2(C_U, S_V) + \frac{1}{4} |\langle [C_U, S_V] \rangle|^2, \\
\mathcal{V}_{S_U} \mathcal{V}_{C_V} &\geq \mathcal{C}^2(S_U, C_V) + \frac{1}{4} |\langle [S_U, C_V] \rangle|^2, \\
\mathcal{V}_{S_U} \mathcal{V}_{S_V} &\geq \mathcal{C}^2(S_U, S_V) + \frac{1}{4} |\langle [S_U, S_V] \rangle|^2.
\end{align*}
\]

In addition, the extra result \( C_{U(V)}^2 + S_{U(V)}^2 = 1 \) resembles a well-known mathematical property associated with the trigonometric functions cosine and sine. For this reason, these Hermitian operators will be henceforth termed ‘cosine’ and ‘sine’ operators, whose respective variances can be shown to obey the mathematical identity

\[
(\mathcal{V}_{C_U} + \mathcal{V}_{S_U})(\mathcal{V}_{C_V} + \mathcal{V}_{S_V}) = \mathcal{V}_{U} \mathcal{V}_{V}.
\]

To make complete this definition, it is interesting to observe that certain combinations of \( \langle C_{U(V)} \rangle^2 \) and \( \langle S_{U(V)} \rangle^2 \) also yield the additional result

\[
(\langle C_U \rangle^2 + \langle S_U \rangle^2)(\langle C_V \rangle^2 + \langle S_V \rangle^2) = (1 - \mathcal{V}_U)(1 - \mathcal{V}_V),
\]
which proves itself useful in our subsequent calculations.

Next, by means of mathematical remarks, we establish an important set of other useful results for the sine and cosine operators, whose relevance is intrinsically connected with the hierarchy relations involving the uncertainty principles related to \( U \) and \( V \) which generalize the Massar-Spindel inequality. It is worth mentioning that some proofs demand a logical sequence of algebraic manipulations to be detailed in the text.

**Remark 1.** Although the sine and cosine operators are genuinely defined for unitary operators, we shall employ, in due time, the same definition for a general operator \( X \) as well. In this general case, it can be easily demonstrated that the following properties hold:

\[
\langle C_X^2 \rangle + \langle S_X^2 \rangle = \frac{1}{2} \langle [X, X^\dagger] \rangle, \quad (C_X)^2 + (S_X)^2 = |\langle X \rangle|^2, \quad \mathcal{C}_X + \mathcal{S}_X = \mathcal{C}(X, X^\dagger).
\]

Note that for a normal operator \( N \) (which satisfies \([N, N^\dagger] = 0\)), the covariance function between \( N \) and \( N^\dagger \) matches the variance of \( N \), namely, \( \mathcal{C}_N + \mathcal{S}_N = \mathcal{V}_N \).

**Remark 2.** Let us initially consider the sum of all aforementioned RS uncertainty principles for the sine and cosine operators, as well as the connection between the commutation and anticommutation relations of such Hermitian operators. Adequate algebraic manipulations allow, in principle, to obtain an inequality for the product \( \mathcal{V}_U \mathcal{V}_V \) with remarkable mathematical features, i.e.,

\[
(1 + A^2) \mathcal{V}_U \mathcal{V}_V \geq (1 + A^2) \mathcal{F}(U, V) + A^2 \mathcal{H}(U, V)
\]

where

\[
\mathcal{F}(U, V) = C^2(C_U, C_V) + C^2(C_U, S_V) + C^2(S_U, C_V) + C^2(S_U, S_V),
\]

\[
\mathcal{H}(U, V) = |\langle C_U C_V \rangle|^2 + |\langle C_U S_V \rangle|^2 + |\langle S_U C_V \rangle|^2 + |\langle S_U S_V \rangle|^2.
\]

Note that \( \mathcal{F} \) and \( \mathcal{H} \) show a nontrivial dependence on the unitary operators \( U \) and \( V \), which will be properly discussed in the subsequent remarks. Moreover, if compared with Massar-Spindel inequality (1), such a result yields subtle additional corrections that will depend explicitly on the dimension of the state space.

For completeness sake, let us now establish a first numerical evaluation on the functions \( \mathcal{F} \) and \( \mathcal{H} \). Figure 2 exhibits the plots of \( \mathcal{F} \) versus \( \mathcal{H} \) for (a) \( N = 4 \) and (b) \( N = 5 \) with the same number of normalized random states used in the previous figure. Since the solid line represents \( \mathcal{F} = \mathcal{H} \) in both the situations, this preliminary numerical search demonstrates a greater contribution coming
Fig. 2. Plots of $F(U,V)$ versus $H(U,V)$ with $10^6$ states of randomly generated $\rho$ for two different values of dimension $N$, namely, (a) $N = 4$ and (b) $N = 5$. The solid line corresponds to the case $F = H$ in both the pictures, where the limit situation $F = H = 0$ describes the localized bases. Our numerical computations demonstrate that, in principle, the contributions due to $H$ are more significant than those coming from $F$ for a large number of random states.

from $H$ than from $F$ for most states of low dimension $N$. This fact appeals for a detailed formal investigation on the origins of such contributions, in which each term of $F$ and $H$ would be examined separately.

**Remark 3.** Important mathematical properties of $H(U,V)$ are easily attained examining each of its terms separately: for instance, to calculate the modulus squared of $\langle C_U C_V \rangle$, we initially expand the cosine operators $C_U$ and $C_V$ in terms of the Schwinger unitary operators $U$ and $V$; the next step consists in decomposing the resulting terms into their real and imaginary Hermitian parts, whose final expression assumes the form

$$\langle C_U C_V \rangle = \frac{1}{4} \left( \langle C_{UV} \rangle + \langle C_{UV^t} \rangle + \langle C_{U^tV} \rangle + \langle C_{U^tV^t} \rangle \right)$$

$$+ \frac{1}{4} \left( \langle S_{UV} \rangle + \langle S_{UV^t} \rangle + \langle S_{U^tV} \rangle + \langle S_{U^tV^t} \rangle \right).$$

Once the remaining terms are obtained in the same way, some algebraic simplification gives rise to the following expression for $H$:

$$H(U,V) = \frac{1}{4} \left( \langle C_{UV} \rangle^2 + \langle C_{UV^t} \rangle^2 + \langle C_{U^tV} \rangle^2 + \langle C_{U^tV^t} \rangle^2 \right)$$

$$+ \frac{1}{4} \left( \langle S_{UV} \rangle^2 + \langle S_{UV^t} \rangle^2 + \langle S_{U^tV} \rangle^2 + \langle S_{U^tV^t} \rangle^2 \right).$$

However, this result does not represent a convenient form of $H$ since the proper summation of $\langle C_o \rangle^2 + \langle S_o \rangle^2 = 1 - \mathcal{Y}_o$ with $\langle C_o^2 \rangle + \langle S_o^2 \rangle = 1$ (in this situation,
one considers all possible matches of $\mathcal{O} \equiv UV, UV^\dagger, U^\dagger V, U^\dagger V^\dagger$) permits us to derive a simplified expression for such a function that includes the variances $\mathcal{V}_{uv}$ and $\mathcal{V}_{uv^\dagger}$. Indeed, since $\mathcal{V}_{uv} \equiv \mathcal{V}_{uv^\dagger}$ and $\mathcal{V}_{uv^\dagger} \equiv \mathcal{V}_{uv}$, it turns immediate to prove that

$$\mathcal{H}(U, V) = 1 - \frac{1}{2} (\mathcal{V}_{uv} + \mathcal{V}_{uv^\dagger}) = |\langle UV \rangle|^2 + |\langle UV^\dagger \rangle|^2$$

which is invariant under the transformations $U \to e^{i\phi} U$ and $V \to e^{i\theta} V$ for $\{\phi, \theta\} \in \mathbb{R}$.

**Remark 4.** Note that Eq. (11) represents a lower bound for any element of $3$

$$\left\{ |\langle C_u C_v \rangle|^2, |\langle C_u S_v \rangle|^2, |\langle S_u C_v \rangle|^2, |\langle S_u S_v \rangle|^2 \right\} \geq \frac{1}{4} \mathcal{H}(U, V),$$

this fact being discussed by Massar and Spindel [14] through different mathematical arguments. In fact, the authors demonstrated that for a given choice of phases of the Schwinger unitary operators, the restrictions $\langle C_v(v) \rangle \in \mathbb{R}_+ \Rightarrow \langle S_v(v) \rangle = 0$ select a set $\{\rho\}$ of finite quantum states for which the inequality

$$|\langle C_u C_v \rangle| \geq \sqrt{(1 - \mathcal{V}_u)(1 - \mathcal{V}_v)}$$

can be formally verified and also numerically tested. Despite the correlations between $U$ and $V$ do not appear in such an expression, the comparison with $\mathcal{H}$ is unavoidable in this case, since correlations represent an important quantum effect that deserve our attention. The saturation is reached in both the situations for localized bases.

**Remark 5.** Let us now decompose $\mathcal{F}$ into three terms $\mathcal{F}_1, \mathcal{F}_2$ and $\mathcal{F}_3$, whose different contributions will be formally calculated with the help of the mathematical procedure sketched in the previous remarks. We initially consider the term

$$\mathcal{F}_1 = \frac{1}{4} \left( |\langle C_u, C_v \rangle|^2 + |\langle C_u, S_v \rangle|^2 + |\langle S_u, C_v \rangle|^2 + |\langle S_u, S_v \rangle|^2 \right)$$

$^3$ Let $\|U\|_{\text{HS}} = \|V\|_{\text{HS}} = \sqrt{N}$ and $\|C_u(v)\|_{\text{HS}} = \|S_u(v)\|_{\text{HS}} = \sqrt{\frac{N}{2}}$ characterize the Hilbert-Schmidt norms associated with the Schwinger unitary operators and their respective related trigonometric operators, where $\|X\|_{\text{HS}} := \sqrt{\text{Tr}[X^* X]}$ defines the aforementioned norm [28]. The further mathematical property

$$\left\{ \|C_u C_v\|_{\text{HS}}, \|C_u S_v\|_{\text{HS}}, \|S_u C_v\|_{\text{HS}}, \|S_u S_v\|_{\text{HS}} \right\} \leq \frac{N}{2}$$

represents an effective gain in this stage, since it brings out relevant information on the different products of cosine and sine operators used in the text.
responsible for contributions associated with squared mean values of all anti-commutation relations involved in $\mathcal{F}$ through the covariance functions. So, let $\langle\{C_u, C_v\}\rangle$ admit the form

$$
\langle\{C_u, C_v\}\rangle = \frac{1}{4} \left[ (1 + \omega) \left( \langle C_{uv} \rangle + \langle C_{u\dagger v\dagger} \rangle \right) + (1 + \omega^*) \left( \langle C_{uv\dagger} \rangle + \langle C_{u\dagger v} \rangle \right) \right]
$$

in complete analogy with $\langle C_u C_v \rangle$. Writing the remaining mean values in an analogous way, subsequent computations allow to prove that $F_1$ is connected with $\mathcal{H}(U, V)$ through the relation $F_1 = \cos^2 \left( \frac{\Phi}{2} \right) \mathcal{H}$ for $\Phi = \frac{2\pi}{N}$ fixed.

Following, in what concerns the second term

$$
F_2 = \langle C_u \rangle \langle C_v \rangle \langle\{C_u, C_v\}\rangle + \langle C_u \rangle \langle S_v \rangle \langle\{C_u, S_v\}\rangle + \langle S_u \rangle \langle C_v \rangle \langle\{S_u, C_v\}\rangle + \langle S_u \rangle \langle S_v \rangle \langle\{S_u, S_v\}\rangle,
$$

it can be expressed by means of the convenient form

$$
2F_2 = \text{Re}[\langle U \rangle \langle V \rangle] \text{Re}[\langle 1 + \omega \rangle \langle UV \rangle] + \text{Re}[\langle U \rangle \langle V^\dagger \rangle] \text{Re}[\langle 1 + \omega^* \rangle \langle UV^\dagger \rangle] + \text{Im}[\langle U \rangle \langle V \rangle] \text{Im}[\langle 1 + \omega \rangle \langle UV \rangle] + \text{Im}[\langle U \rangle \langle V^\dagger \rangle] \text{Im}[\langle 1 + \omega^* \rangle \langle UV^\dagger \rangle]
$$

which represents an important formal result in our calculations.

Finally, let us briefly mention that $F_3$ coincides with $(1 - \mathcal{K}_u)(1 - \mathcal{K}_v)$ since it is equivalent to the product $(\langle C_u \rangle^2 + \langle S_u \rangle^2)(\langle C_v \rangle^2 + \langle S_v \rangle^2)$; consequently, the function

$$
F(U, V) = F_1(U, V) - F_2(U, V) + F_3(U, V)
$$

(12)

can be immediately obtained. Note that the nontrivial dependence of Eq. (10) on the Schwinger unitary operators is completely justified in these remarks.

This set of mathematical remarks establishes a first solid algebraic framework for the unitary operators $U$ and $V$, whose intrinsic virtues lead us to formulate a theorem which generalizes the Massar-Spindel inequality (1) in order to include the quantum correlation effects between the aforementioned operators. In fact, this theorem consists of an initial compilation of efforts in our future search for the tightest bound, where the correlation function has occupied an important place in the investigative process.
Theorem. Let $U$ and $V$ be two unitary operators defined in a $N$-dimensional state vector space which satisfy the commutation relations $[U, V] = (1 - \omega)UV$ and $[U, V^\dagger] = (1 - \omega^*)UV^\dagger$ for $\omega := \exp\left(\frac{2\pi i}{N}\right)$. Moreover, let $\mathcal{V}_U := 1 - |\langle U \rangle|^2$ and $\mathcal{V}_V := 1 - |\langle V \rangle|^2$ represent the respective variances such that $0 \leq \mathcal{V}_U, \mathcal{V}_V \leq 1$.

The inequality
\begin{equation}
\mathcal{V}_U \mathcal{V}_V \geq F(U, V) + \sin^2\left(\frac{\pi}{N}\right) \mathcal{H}(U, V)
\end{equation}
yields a new bound for $\mathcal{V}_U \mathcal{V}_V$, where the quantum correlation effects related to the unitary operators are taken into account. Note that $F$ and $\mathcal{H}$ were precisely defined and formally studied in the previous mathematical remarks, the saturation $F = \mathcal{H} = 0$ being attained for localized bases.

Next, let us determine some additional results focused on the Hermitian operators $\{C_{\delta U}, S_{\delta U}, C_{\delta V}, S_{\delta V}\}$ in order to yield a set of specific intermediate inequalities whose hierarchical relations correspond to a solid bridge towards the tightest bound.

### 3.2 Hierarchical relations

We start this subsection stating a first important result for the sine and cosine operators $\{C_{\delta U}, S_{\delta U}, C_{\delta V}, S_{\delta V}\}$ defined, in turn, in terms of the non-unitary counterparts $\delta U$ and $\delta V$. This particular result shows how the mean values of their commutation and anticommutation relations are linked with determined correlation functions, namely,

\begin{align*}
\langle [C_{\delta U}, C_{\delta V}] \rangle &= iA \langle [S_{\delta U}, S_{\delta V}] \rangle = 2iA \mathcal{C}(S_{\delta U}, S_{\delta V}), \\
\langle [C_{\delta U}, S_{\delta V}] \rangle &= -iA \langle [S_{\delta U}, C_{\delta V}] \rangle = -2iA \mathcal{C}(S_{\delta U}, C_{\delta V}), \\
\langle S_{\delta U}, C_{\delta V} \rangle &= -iA \langle [C_{\delta U}, S_{\delta V}] \rangle = -2iA \mathcal{C}(C_{\delta U}, S_{\delta V}), \\
\langle [S_{\delta U}, S_{\delta V}] \rangle &= iA \langle [C_{\delta U}, C_{\delta V}] \rangle + 2 = 2iA \mathcal{C}(C_{\delta U}, C_{\delta V}) + 1.
\end{align*}

Following, let us complete this set of results with relations that connect all the covariance functions previously defined with the original framework:

\begin{align*}
F_3 \mathcal{C}(C_{\delta U}, C_{\delta V}) &= \mathcal{C}(C_U, C_V)\langle C_U \rangle \langle C_V \rangle + \mathcal{C}(S_U, S_V)\langle S_U \rangle \langle S_V \rangle \\
&+ \mathcal{C}(C_U, S_V)\langle C_U \rangle \langle S_V \rangle + \mathcal{C}(S_U, C_V)\langle S_U \rangle \langle C_V \rangle, \\
F_3 \mathcal{C}(C_{\delta U}, S_{\delta V}) &= -\mathcal{C}(C_U, C_V)\langle C_U \rangle \langle C_V \rangle + \mathcal{C}(S_U, S_V)\langle S_U \rangle \langle S_V \rangle \\
&+ \mathcal{C}(C_U, S_V)\langle C_U \rangle \langle C_V \rangle - \mathcal{C}(S_U, C_V)\langle S_U \rangle \langle C_V \rangle, \\
F_3 \mathcal{C}(S_{\delta U}, C_{\delta V}) &= -\mathcal{C}(C_U, C_V)\langle S_U \rangle \langle C_V \rangle + \mathcal{C}(S_U, S_V)\langle S_U \rangle \langle C_V \rangle \\
&- \mathcal{C}(C_U, S_V)\langle S_U \rangle \langle C_V \rangle + \mathcal{C}(S_U, C_V)\langle S_U \rangle \langle C_V \rangle, \\
F_3 \mathcal{C}(S_{\delta U}, S_{\delta V}) &= \mathcal{C}(C_U, C_V)\langle S_U \rangle \langle S_V \rangle + \mathcal{C}(S_U, S_V)\langle C_U \rangle \langle C_V \rangle \\
&- \mathcal{C}(C_U, S_V)\langle S_U \rangle \langle C_V \rangle - \mathcal{C}(S_U, C_V)\langle C_U \rangle \langle S_V \rangle.
\end{align*}
These equations enable us to rewrite $F$ in the compact form

$$\frac{F}{F_3} = C^2(C_{\delta U}, C_{\delta V}) + C^2(C_{\delta V}, S_{\delta V}) + C^2(S_{\delta V}, C_{\delta V}) + C^2(S_{\delta U}, S_{\delta V}), \quad (14)$$

while $(\gamma_{C_{\delta U}} + \gamma_{S_{\delta U}})(\gamma_{C_{\delta V}} + \gamma_{S_{\delta V}}) = \gamma_{\delta U} \gamma_{\delta V}$ brings out a completely analogous expression to that established for $\gamma_{\delta U} \gamma_{\delta V}$; consequently,

$$\gamma_{\delta U} \gamma_{\delta V} \geq \frac{F}{F_3} + \sin^2 \left( \frac{\pi}{N} \right) \frac{H}{F_3} \quad (15)$$

represents an alternative form of Eq. (13) since $\gamma_{\delta U} \gamma_{\delta V} \equiv F_3 \gamma_{\delta U} \gamma_{\delta V}$.

Now, let us rewrite Eq. (15) according to definitions employed for $S_{\delta U}$ and $S_{\delta V}$ in the previous section,

$$S_{\delta U} S_{\delta V} \geq \left[ 1 + \sin \left( \frac{2\pi}{N} \right) \right] \frac{\csc^2 \left( \frac{\pi}{N} \right) F}{F_3} + \frac{H}{F_3}. \quad (16)$$

From this result, it is relatively easy to derive a number of simpler (but looser) inequalities: for instance, given the non-negativity of $\frac{F}{F_3}$ [cf. Eq. (14)], the first term in the second bracket can be dropped to give

$$S_{\delta U} S_{\delta V} \geq \left[ 1 + \sin \left( \frac{2\pi}{N} \right) \right] \frac{H}{F_3},$$

which corresponds, in such a case, to the HKR uncertainty principle; alternatively, $\frac{H}{F_3}$ can also be dropped (for the same reason, i.e., its non-negativity) in order to yield

$$S_{\delta U} S_{\delta V} \geq \left[ 1 + \sin \left( \frac{2\pi}{N} \right) \right] \csc^2 \left( \frac{\pi}{N} \right) \frac{F}{F_3}.$$

Consequently, such inequalities are then combined in order to give a tighter one,

$$S_{\delta U} S_{\delta V} \geq \left[ 1 + \sin \left( \frac{2\pi}{N} \right) \right] \max \left[ \csc^2 \left( \frac{\pi}{N} \right) \frac{F}{F_3}, \frac{H}{F_3} \right]. \quad (17)$$

At this point, one is led to ask if there exists a general ordering relation between $\csc^2 \left( \frac{\pi}{N} \right) \frac{F}{F_3}$ and $\frac{H}{F_3}$. To answer this question, let us establish a set of numerical calculations associated with the different values of dimension $N$, where, for each specific case, one has approximately $10^6$ randomly generated states. In order to make the presentation of these numerical results more self-contained, Fig. 3 depicts the plots of $\csc^2 \left( \frac{\pi}{N} \right) \frac{F}{F_3}$ versus $\frac{H}{F_3}$ for $N = 2, 3, 4, 6$ and 20. In this case, note that the maximum can indeed arise from either terms, depending on the particular chosen state $\rho$. As a rule of thumb, one has the following: for low dimensional states (e.g., $N = 2, 3$), the term $\frac{H}{F_3}$ usually dominates; however, as the dimension $N$ increases ($N \geq 6$), $\csc^2 \left( \frac{\pi}{N} \right) \frac{F}{F_3}$ becomes the usually dominant term. Finally, if one considers $N = 4$, it is visible that there is not a usually dominant term — in this case, the result of the optimization is strongly dependent on the particular input state.
Fig. 3. Plots of $\csc^2 \left( \frac{\pi}{N} \right) \frac{\mathcal{F}}{F_3}$ versus $\frac{\mathcal{H}}{F_3}$ with, at least, $10^6$ randomly generated states for each different value of dimension $N$. Thus, yellow points depict the $N=2$ case, while red, grey, blue, and green points describe, respectively, the $N=3, 4, 6$, and $20$ situations. Note that $(0, 0)$ is associated with localized bases in this picture, whereas the solid line corresponds to the particular case $\csc^2 \left( \frac{\pi}{N} \right) \frac{\mathcal{F}}{F_3} = \frac{\mathcal{H}}{F_3}$. It is interesting to observe how $\csc^2 \left( \frac{\pi}{N} \right) \frac{\mathcal{F}}{F_3}$ and $\frac{\mathcal{H}}{F_3}$ behave when different dimensions of state vector space are considered in our numerical computations.

As it turns out, inequality (17) can be further strengthened by the addition of yet another (less trivial) lower bound of $\csc^2 \left( \frac{\pi}{N} \right) \frac{\mathcal{F}}{F_3} + \frac{\mathcal{H}}{F_3}$ to the maximization at hand. Just as $\frac{\mathcal{F}}{F_3}$ could be written as in Eq. (14), we can also show that $\frac{\mathcal{H}}{F_3}$ admits the form

$$\frac{\mathcal{H}}{F_3} = \sec^2 \left( \frac{\pi}{N} \right) \left[ 1 + 2\mathcal{G}(C_{\delta U}, C_{\delta V}) + \frac{\mathcal{F}}{F_3} \right].$$

(18)

With that in mind, some straightforward manipulation yields

$$\csc^2 \left( \frac{\pi}{N} \right) \frac{\mathcal{F}}{F_3} + \frac{\mathcal{H}}{F_3} = \sec^2 \left( \frac{\pi}{N} \right) (1 + x)^2 + \csc^2 \left( \frac{\pi}{N} \right) x^2$$

$$+ 4 \csc^2 \left( \frac{2\pi}{N} \right) \left( \frac{\mathcal{F}}{F_3} - x^2 \right)$$

$$\geq \sec^2 \left( \frac{\pi}{N} \right) (1 + x)^2 + \csc^2 \left( \frac{\pi}{N} \right) x^2$$

for $x \equiv \mathcal{G}(C_{\delta U}, C_{\delta V})$, where the inequality follows from fact that $\frac{\mathcal{F}}{F_3} \geq x^2$ [cf. Eq. (14)]. A mathematical virtue of this lower bound is that it depends only on the covariance $\mathcal{G}(C_{\delta U}, C_{\delta V})$, whereas $\frac{\mathcal{F}}{F_3}$ and $\frac{\mathcal{H}}{F_3}$ depend on the covariances of all combinations among $C_{\delta U}, C_{\delta V}, S_{\delta U}$ and $S_{\delta V}$. As a result, we may now write

$$S_{\delta U} S_{\delta V} \geq \left[ 1 + \sin \left( \frac{2\pi}{N} \right) \right] \max \left[ 1 + \mathcal{G}(x; N), \csc^2 \left( \frac{\pi}{N} \right) \frac{\mathcal{F}}{F_3}, \frac{\mathcal{H}}{F_3} \right]$$

(19)
with \( G(x; N) := 4 \csc^2 \left( \frac{2\pi}{N} \right) x^2 + 2 \sec^2 \left( \frac{\pi}{N} \right) x + \tan^2 \left( \frac{\pi}{N} \right) \). Note that \( 1 + G(x; N) \) coincides, in such a situation, with \( \sec^2 \left( \frac{\pi}{N} \right) (1 + x)^2 + \csc^2 \left( \frac{\pi}{N} \right) x^2 \). Once again, numerical calculations demonstrate that there is not a general ordering between the arguments of the maximization of such an equation.

It is worth stressing that both bounds of Eqs. (16) and (19) explicitly depend on the Hilbert space dimension, as well as on the particular state under consideration. Henceforth, we further lose the bound (19) to provide yet another bound, but now a state-independent one (i.e., solely dependent on the Hilbert space dimension). In this way, let us initially consider the inequality

\[
S_{\delta U} S_{\delta V} \geq \left[ 1 + \sin \left( \frac{2\pi}{N} \right) \right] \left[ 1 + G(x; N) \right].
\]

So, for a given \( N \), \( G(x; N) \) describes a parabola with upwards concavity and minimum value equal to 0 \((y\)-coordinate of the vertex), namely, \( G(x; N) \geq 0 \), which implies that

\[
S_{\delta U} S_{\delta V} \geq 1 + \sin \left( \frac{2\pi}{N} \right).
\]

Despite of all the mathematical assumptions used in the relaxation process of inequality (16), the bound above is still tighter than the one proposed in Ref. [14], which is now trivially proved by disregarding the sine function in the inequality (20), that is, \( S_{\delta U} S_{\delta V} \geq 1 \).

**Hierarchy.** The tightest bound of the product \( S_{\delta U} S_{\delta V} \) is particularly related to an underlying minimization problem — see Appendix A. Although this problem seems simple at first glance [23], let us now establish a set of inequalities which characterizes an important hierarchical relation among certain formal results mentioned in the body of the text:

\[
S_{\delta U} S_{\delta V} \geq R_1 \geq R_2 \geq R_3 \geq R_4 \geq 1,
\]

where \( R_1 \equiv \) tightest bound, \( R_2 = \) RHS of Eq. (16), \( R_3 = \) RHS of Eq. (19), and finally, \( R_4 = \) RHS of Eq. (20). Note that \( S_{\delta U} S_{\delta V} \geq 1 \) describes the loosest bound, which is precisely the inequality of Massar and Spindel [14].

### 4 The tightest bound

Massar and Spindel [14] relied on the works of Jackiw and Opatrný [23] to provide a numerical recipe that implicitly produces the tightest bound for the cloud of points depicted in Fig. 1. In this section, we review such a procedure while applying it to explicitly construct closed-form expressions for the tightest bound here related to physical systems characterized by a low-dimensional space of states.
Generally, the tightest bound can be obtained by the following reasoning:

\[ S_{\delta U} S_{\delta V} \geq \min_{|\psi\rangle} S_{\delta U} S_{\delta V} = \varepsilon^{-2} \min_{|\psi\rangle} \mathcal{V}_{\delta U} \mathcal{V}_{\delta V} = \varepsilon^{-2} \mathcal{V}_{\delta U}^{(0)} \mathcal{V}_{\delta V}^{(0)} = \left[ \varepsilon^{-1} \mathcal{V}_{\delta U}^{(0)} \right]^2 = S_{\delta U}^{(0)} . \]

In such a case, the super-index \((0)\) indicates that the corresponding normalized discrete wavefunction is associated with the nondegenerate ground state \(|\psi_0\rangle\), which minimizes the product \(\mathcal{V}_{\delta U} \mathcal{V}_{\delta V}\). In fact, this ground state will also minimize \(\mathcal{V}_{\delta U} \mathcal{V}_{\delta V}\), since \(\mathcal{V}_{\delta U}\) is monotonically increasing with \(\mathcal{V}_{\delta U}\) [cf. Eq. (3)] — this observation justifies the second equality. Besides, both the variances evaluated with respect to the ground state satisfy \(\mathcal{V}_{\delta U}^{(0)} = \mathcal{V}_{\delta V}^{(0)}\), which justifies the third equality.

Now, let us establish a sequence of mathematical steps based on the respective eigenvalues and eigenvectors of the Harper Hamiltonian [24]

\[ H = -\sin(\theta) C_U - \cos(\theta) C_V \]

for \(0 \leq \theta \leq \frac{\pi}{2}\). Initially, we look for the smallest eigenvalue of such a Hermitian operator, as well as for its corresponding eigenvector in a given fixed \(N\)-dimensional state vector space. Since the eigenvalues and eigenvectors related to the Harper Hamiltonian are dependent on the angle \(\theta\), let us consider that eigenvector evaluated at the first step in order to estimate the maximum of \(\cos(\theta)|\langle U| + \sin(\theta)|\langle V|\) for all \(\theta \in \left[0, \frac{\pi}{2}\right]\) — which exactly coincides with the smallest eigenvalue in this case. In particular, such a mathematical procedure allows us to obtain, through numerical evaluations, the value of \(\theta = \frac{\pi}{4}\) for any dimension \(N\), and also to characterize the ground state \(|\psi_0\rangle \equiv |0\rangle_N\) with well-defined mathematical properties (see Appendix A for possible connection with Harper functions).

Table 1 illustrates the hierarchical relation depicted in Eq. (21) where, in particular, certain numerical results directly related to the analytical calculations performed for \(\{R_1, R_2, R_3, R_4\}\) with \(N \in [2, 6]\) are exhibited — closed-form expressions for \(S_{\delta U}^{(0)}\) can be viewed in Appendix A and their respective squared values \(R_1 = S_{\delta U}^{(0)}\) compared with those results previously obtained in Fig. 1. Note that for higher dimensions, some numerical methods (for instance, Laguerre method or even Newton-Raphson method) should be applied in order to obtain approximate numerical values for \(S_{\delta U}^{(0)}\) (this statement is supported by the Abel-Galois irreducibility theorem [29], which asserts that polynomial equations of degree \(\geq 5\) do not produce, in general, algebraic solutions, only numerical solutions).
Table 1

Numerical values for \( \{ \mathcal{R}_i \} \)\(^{1 \leq i \leq 4} \) considering the ground state \( \{|0\rangle_N \} \)\(^{2 \leq N \leq 6} \) described in Appendix A. It is important to stress that such results were inferred from their respective exact algebraic counterparts, which illustrate, in principle, not only the hierarchical relation depicted in Eq. (21) but also the quantum-algebraic framework developed in the previous sections. In addition, note that eigenvalues extracted from the Harper Hamiltonian for \( N > 6 \) do not yield easy-to-compute expressions for the tightest bounds \( \mathcal{R}_1 \), this fact being supported by Abel-Galois irreducibility theorem for polynomial equations.

| \( N \) | \( \mathcal{R}_1 \) | \( \mathcal{R}_2 \) | \( \mathcal{R}_3 \) | \( \mathcal{R}_4 \) |
|---|---|---|---|---|
| 2 | 1 | 1 | 1 | 1 |
| 3 | \( \approx 3.254 \) | \( \approx 2.182 \) | \( \approx 1.895 \) | \( \approx 1.866 \) |
| 4 | 4 | 3 | 2 | 2 |
| 5 | \( \approx 3.781 \) | \( \approx 3.469 \) | \( \approx 2.987 \) | \( \approx 1.951 \) |
| 6 | \( \approx 3.348 \) | \( \approx 1.915 \) | \( \approx 1.915 \) | \( \approx 1.866 \) |

5 The connection with discrete Weyl function

How the discrete Weyl function [5] can be employed to measure a particular family of expectation values — for instance, \( \langle U^\alpha V^\beta \rangle \) for \( \{ \alpha, \beta \} \in \mathbb{Z}_N \) — here mapped into finite-dimensional discrete phase spaces? To answer this specific question, we initially recall certain basic mathematical tools which correspond to the central core of that theoretical formulation presented in Ref. [12]. This procedure will lead us to establish a parallel quantum-algebraic framework for those results obtained in Section 3, whose connection with the discrete Weyl function represents a first step towards effective experimental measurements via tomographic reconstructions of finite quantum states [8]. Throughout this section, we will assume \( N \) odd.\(^4\)

The particular set of \( N^2 \) operators \( \{ \Delta(\mu, \nu) \} \)\(^{\mu, \nu = -\ell, \ldots, \ell} \) characterizes a complete orthonormal unitary operator basis which leads us to construct all possible kinematical and/or dynamical quantities belonging to a given \( N \)-dimensional state vector space. For instance, the decomposition of any linear operator \( \mathbf{O} \) in this basis assumes the expression

\[
\mathbf{O} = \frac{1}{N} \sum_{\mu, \nu = -\ell}^{\ell} \theta(\mu, \nu) \Delta(\mu, \nu),
\]

(22)

where \( \theta(\mu, \nu) \equiv \text{Tr}[\Delta(\mu, \nu)\mathbf{O}] \) represent coefficients evaluated through trace

\(^4\) For completeness reasons, it is important to stress that even dimensionalities can also be dealt with simply by working on non-symmetrized intervals.
operation and
\[
\Delta(\mu, \nu) := \frac{1}{N} \sum_{\eta, \xi = -\ell}^{\ell} \omega^{-(\eta \nu - \xi \mu)} D(\eta, \xi)
\] (23)

defines the aforementioned operator basis here expressed in terms of a discrete Fourier transform of the displacement operator
\[
D(\eta, \xi) = \omega^{-\{2^{-1} \eta \xi\}} \sum_{\gamma = -\ell}^{\ell} \omega^{\gamma \eta} \langle u_{\gamma - \xi} \rangle = \omega^{-\{2^{-1} \eta \xi\}} \sum_{\gamma = -\ell}^{\ell} \omega^{-\gamma \xi} \langle v_{\gamma + \eta} \rangle \langle v_{\gamma} \rangle.
\]

In such a case, note that \(\omega^{-\{2^{-1} \eta \xi\}}\) consists of a specific phase whose argument satisfies the mathematical rule \(2\{2^{-1} \eta \xi\} = \eta \xi + kN\) for all \(k \in \mathbb{Z}_N\); furthermore, note that these labels assume integer values in the symmetric interval \([-\ell, \ell]\) with \(\ell = \frac{N-1}{2}\) fixed.

According to expansion (22), the decomposition of any density operator \(\rho\) in the \(\text{mod}(N)\)-invariant unitary operator basis (23) has as coefficients the discrete Wigner function \(\mathcal{W}_\rho(\mu, \nu) := \text{Tr}[\Delta(\mu, \nu) \rho]\), which leads us, in principle, to establish an analytical expression for the mean value \(\langle O \rangle \equiv \text{Tr}[O \rho]\), that is
\[
\langle O \rangle = \frac{1}{N} \sum_{\mu, \nu = -\ell}^{\ell} \mathcal{O}(\mu, \nu) \mathcal{W}_\rho(\mu, \nu).
\] (24)

In what concerns to \(\mathcal{W}_\rho(\mu, \nu)\), it is particularly worth mentioning that such a function is connected to the Weyl function \(\tilde{\mathcal{W}}_\rho(\eta, \xi) := \text{Tr}[D(\eta, \xi) \rho]\) by means of a mere discrete Fourier transform, and its complexity basically depends on the initial quantum state adopted for the physical system under investigation.

To illustrate the mathematical steps used in the evaluation of \(\mathcal{O}(\mu, \nu)\), let us consider those specific combinations of cosine and sine operators exhibited in Section 3, as well as the intermediate result
\[
D^\dagger(\eta, \xi) U^\alpha V^\beta D(\eta, \xi) = \omega^{\alpha \xi + \beta \eta} U^\alpha V^\beta
\]
since the trace operation
\[
\text{Tr}[D(\eta, \xi) U^\alpha V^\beta] = N \omega^{-\{2^{-1} \eta \xi\} + \eta \beta} \delta^{\eta + \alpha, 0} \delta^{\xi - \beta, 0}
\]
will be necessary in the next steps. Thus, after some repetitive calculations, we achieve the set of formal expressions.
\[
\text{Tr}[D(\eta, \xi)C_u C_v] = \frac{N}{4} \omega^{-\{2^{-1}\eta\xi\}} \left( \delta_{\eta+1,0}^{[N]} + \delta_{\eta-1,0}^{[N]} \right) \left( \omega^{-\eta} \delta_{\xi+1,0}^{[N]} + \omega^{\eta} \delta_{\xi-1,0}^{[N]} \right)
\]

\[
\text{Tr}[D(\eta, \xi)C_u S_v] = i \frac{N}{4} \omega^{-\{2^{-1}\eta\xi\}} \left( \delta_{\eta+1,0}^{[N]} + \delta_{\eta-1,0}^{[N]} \right) \left( \omega^{-\eta} \delta_{\xi+1,0}^{[N]} - \omega^{\eta} \delta_{\xi-1,0}^{[N]} \right)
\]

\[
\text{Tr}[D(\eta, \xi)S_u C_v] = -i \frac{N}{4} \omega^{-\{2^{-1}\eta\xi\}} \left( \delta_{\eta+1,0}^{[N]} - \delta_{\eta-1,0}^{[N]} \right) \left( \omega^{-\eta} \delta_{\xi+1,0}^{[N]} + \omega^{\eta} \delta_{\xi-1,0}^{[N]} \right)
\]

\[
\text{Tr}[D(\eta, \xi)S_u S_v] = \frac{N}{4} \omega^{-\{2^{-1}\eta\xi\}} \left( \delta_{\eta+1,0}^{[N]} - \delta_{\eta-1,0}^{[N]} \right) \left( \omega^{-\eta} \delta_{\xi+1,0}^{[N]} - \omega^{\eta} \delta_{\xi-1,0}^{[N]} \right)
\]

which represents, in such a case, the dual counterpart of \(g(\mu, \nu)\) — the superscript \([N]\) on the Kronecker delta denotes that this function is different from zero when its discrete labels are congruent modulo \(N\).

The second and last step consists in computing, for each case above, its respective discrete Fourier transform, which basically depends on the intermediate result

\[
\text{Tr}[\Delta(\mu, \nu)U^\alpha V^\beta] = \omega^{\beta \mu + \alpha \nu - \alpha \beta + \{2^{-1}\alpha \beta\}}
\]

So, the final expressions admit the simple forms

\[
(C_u C_v)(\mu, \nu) = \frac{1}{4} \left[ \left( \omega^{\mu - \nu} + \omega^{-\mu + \nu} \right) \omega^{1-\{2^{-1}\}} + \left( \omega^{\mu + \nu} + \omega^{-\mu - \nu} \right) \omega^{-1+\{2^{-1}\}} \right]
\]

\[
(C_u S_v)(\mu, \nu) = -\frac{i}{4} \left[ \left( \omega^{\mu - \nu} - \omega^{-\mu + \nu} \right) \omega^{1-\{2^{-1}\}} + \left( \omega^{\mu + \nu} - \omega^{-\mu - \nu} \right) \omega^{-1+\{2^{-1}\}} \right]
\]

\[
(S_u C_v)(\mu, \nu) = \frac{i}{4} \left[ \left( \omega^{\mu - \nu} - \omega^{-\mu + \nu} \right) \omega^{1-\{2^{-1}\}} - \left( \omega^{\mu + \nu} - \omega^{-\mu - \nu} \right) \omega^{-1+\{2^{-1}\}} \right]
\]

\[
(S_u S_v)(\mu, \nu) = \frac{1}{4} \left[ \left( \omega^{\mu - \nu} + \omega^{-\mu + \nu} \right) \omega^{1-\{2^{-1}\}} - \left( \omega^{\mu + \nu} + \omega^{-\mu - \nu} \right) \omega^{-1+\{2^{-1}\}} \right]
\]

where \((AB)(\mu, \nu) = \text{Tr}[\Delta(\mu, \nu)AB]\) denotes the above mapped expressions. Consequently, with the aid of Eq. (24), the associated mean values can be promptly obtained: for instance, if one considers \((U^\alpha V^\beta)\), we easily reach the important result

\[
\langle U^\alpha V^\beta \rangle = \omega^{-\alpha \beta + \{2^{-1}\alpha \beta\}} \tilde{\mathcal{W}}_\rho(\alpha, -\beta).
\]

Now, let us pay attention to \(\langle C_u C_v \rangle\) and its particular link with the discrete Weyl function,

\[
\langle C_u C_v \rangle = \frac{1}{4} \left[ \tilde{\mathcal{W}}_\rho(-1, -1) + \tilde{\mathcal{W}}_\rho(1, 1) \right] \omega^{1-\{2^{-1}\}}
\]

\[
+ \frac{i}{4} \left[ \tilde{\mathcal{W}}_\rho(1, -1) + \tilde{\mathcal{W}}_\rho(-1, 1) \right] \omega^{-1+\{2^{-1}\}}.
\]

This remarkable result states that, for a given \(\rho\) and its respective discrete Weyl function \(\tilde{\mathcal{W}}_\rho(\eta, \xi)\), \(\langle C_u C_v \rangle\) can be promptly inferred from tomography measures upon such a function at specific points of the dual \(N\)-dimensional discrete phase space. Besides, if one applies the triangle inequality for \(|\langle C_u C_v \rangle|\),
both the upper and lower bounds can be easily established in this context,\(^5\)

\[ |\langle C_u C_v \rangle| \leq \frac{1}{4} \left( |\tilde{W}_\rho(-1, -1) + \tilde{W}_\rho(1, 1)| \pm |\tilde{W}_\rho(1, -1) + \tilde{W}_\rho(-1, 1)| \right). \]

Similar procedure leads us to prove that \(|\langle S_u S_v \rangle|\) shares exactly the same bounds, while the remaining quantities are bounded by the inequalities

\[
\{|\langle C_u S_v \rangle|, |\langle S_u C_v \rangle| \| \leq \frac{1}{4} \left( |\tilde{W}_\rho(-1, -1) - \tilde{W}_\rho(1, 1)| \right)
\]

\[ \pm \frac{1}{4} \left( |\tilde{W}_\rho(1, -1) - \tilde{W}_\rho(-1, 1)| \right). \]

As a last note, let us mention that \(Y_u\) and \(Y_v\) can also be expressed in terms of specific Weyl functions with the help of Eq. (25), i.e., \(Y_u = 1 - |\tilde{W}_\rho(1, 0)|^2\) and \(Y_v = 1 - |\tilde{W}_\rho(0, -1)|^2\).

In particular, it is worth stressing that the compilation of results obtained in this section allows us to rewrite inequality (13) into a new quantum-algebraic framework, since \(F(U, V)\) and \(H(U, V)\) now depend on specific combinations of discrete Weyl functions. From an experimental point of view, this observation represents an effective gain towards tomographic measurements in \(N\)-dimensional discrete phase spaces of such a generalized inequality for any finite quantum state \(\rho\) [8].

6 Concluding remarks

Through a well succeeded concatenation of efforts in a recent past \([5,12]\), we have made great advances (from a theoretical point of view) in constructing certain sound quantum-algebraic frameworks for finite-dimensional discrete phase spaces. Since unitary operators represent the basic constituent blocks of these theoretical frameworks (in particular, the Schwinger’s approach for

\(^5\) Let \(A\) and \(B\) characterize two general matrices of same size, as well as \(\rho\) denote the density matrix related to a physical system described by a finite-dimensional state vector space. The additional inequality \([\text{Tr}[AB\rho]]^2 \leq \text{Tr}[AA^\dagger \rho] \text{Tr}[BB^\dagger \rho]\) (see Ref. [27, page 230]) establishes a new upper bound for Eq. (26) since \(\langle C_u C_v \rangle^2 \leq \langle C_u^2 \rangle \langle C_v^2 \rangle\), where

\[ \langle C_u^2 \rangle = \frac{1}{2} + \frac{1}{4} \left[ \tilde{W}_\rho(2, 0) + \tilde{W}_\rho(-2, 0) \right] \]

and

\[ \langle C_v^2 \rangle = \frac{1}{2} + \frac{1}{4} \left[ \tilde{W}_\rho(0, 2) + \tilde{W}_\rho(0, -2) \right]. \]

This complementary result basically represents a step forward in our comprehension on hierarchical relations involving those means values listed in Remark 4.
unitary operators [1]), let us focus our attention on some real and effective gains obtained from this paper whose formal implications deserve to be carefully discussed.

- The Massar-Spindel inequality does not explain the tightest bounds exhibited in Fig. 1 for the product $S_\delta U S_\delta V$ when dimensions $N \geq 3$ are considered in the numerical evaluations. This concrete evidence suggests the implementation of an effective search for different inequalities and new finite quantum states whose implications lead us not only to obtain a reasonable set of improved mathematical results, but also to answer certain important questions that emerge from such an evidence.

- The mathematical background for achieving different inequalities related to the aforementioned unitary operators has the RS uncertainty principle as solid starting-point [12]. The initial algebraic advantage of this investigative approach is the inclusion of that contribution coming from the anticommutation relation between two Hermitian non-commuting operators connected via discrete Fourier transform (and/or also related through the Pontryagin duality [30]). In fact, this particular contribution allows to include, into the algebraic approach, some additional terms — here associated with the mean values of different products of the cosine and sine operators — which are responsible for correlations between the unitary operators. In principle, the theorem derived from this constructive process represents a first important point to be strongly emphasized since Eq. (13) introduces a tighter bound whose mathematical properties depend on the $N$-dimensional state vector space in which the initial quantum state is defined.

- The hierarchical relation (21) derived from the tighter bound characterizes a solid bridge between two ‘distant’ bounds: the first one consists of a zeroth-order approximation that confirms the Massar-Spindel result [14] (however, it does not depend on the initial quantum state or even on the dimension which the state vector space is embedded, these facts being considered as a severe limitation for their result); while the second one describes the tightest bound for the left-hand side of Eq. (13) and depicts the importance of the initial quantum state for a given dimension $N$. This simple (but important) observation justifies our search for finite ground states which quantitatively describe those numerical values obtained in Fig. 1 for the tightest bounds.

- How to construct a finite quantum state which formally explains the tightest bounds verified in the numerical calculations? To answer this fundamental question, it is necessary to establish an adequate mathematical prescription that leads us to obtain a set of normalized eigenfunctions which constitutes a complete orthonormal basis in a $N$-dimensional state vector space. In this sense, Appendix A deals with such a task presenting a reliable mathematical relation between Harper functions and tightest bounds by means of ground states $\{|0\rangle_N\}$ specifically constructed for dimensions $N \in [2, 6]$. These finite quantum states indeed describe perfectly all the numerical values exhibited in Fig. 1 for the tightest bounds, and illustrate the hierarchical relation (21).
as well — see Table 1.

- The bounds determined in this paper for the product $S_\delta U S_\delta V$ exhibit a special link with the theoretical formulation of finite-dimensional discrete phase spaces through the discrete Weyl function. In fact, this connection establishes an interesting link between both the Schwinger and Weyl prescriptions for unitary operators, which leads us to guess on the possibility of experimental observation with the help of tomographic measurements.

Now, let us discuss some pertinent points associated with the uncertainty principle for Schwinger unitary operators. The first point concerns the Harper functions and their remarkable connection with the tightest bounds through the ground states $\{|0\rangle_N\}$ for a given dimension $N$ fixed. Despite the worked-examples in Appendix A belonging to the closed interval $2 \leq N \leq 6$, this fact does not represent any apparent limitation related to the quantum-algebraic framework here exposed. In fact, these results consist of a solid starting point for a future search of $\{\langle u_\alpha|n\rangle\}_{0 \leq n \leq N-1}$ with $\alpha \in \mathbb{Z}_N$, whose general expression will correspond to a new paradigm for finite quantum states with immediate implications in the Fourier analysis on finite groups [19,30] (and/or finite fields [31]), as well as in the analysis of signal processing [32,33]. This particular task is currently in progress and the results will be presented in elsewhere.

The second point focus on the systematic study recently developed in Ref. [15] for property testing of unitary operators, where $D^2(U, V) := 1 - \frac{1}{N} |\text{Tr}[U^\dagger V]|$ represents a ‘normalized distance measure that reflects the average difference between unitary operators’. With respect to this specific measure, Wang shows that both the Clifford and orthogonal groups can be efficiently tested through algorithms with intrinsic mathematical virtues (namely, query complexities independent of the system’s size and one-sided error). Since the results here obtained describe an uncertainty principle for unitary operators, it seems reasonable to investigate how these different — but complementary — approaches can be juxtaposed in order to produce a unified framework for determined tasks in quantum information theory [7].

As a final comment, let us briefly mention that our results also touch on some fundamental questions inherent to quantum mechanics (such as spin-squeezing and entanglement effects [34]), discrete fractional Fourier transform [35], and generalized uncertainty principle into the quantum-gravity context [12].

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A Harper’s equation, quantum Fourier transform, tightest bound and their inherent connections with unitary operators

Definition (Harper functions). Let \( \{ |n\rangle \}_{0 \leq n \leq N-1} \) describe a particular set of eigenvectors defined in a \( N \)-dimensional state vector space that simultaneously diagonalizes both the Hamiltonian (\( H \)) and Fourier (\( \Phi \)) operators, that is, \( H|n\rangle = h_n|n\rangle \) and \( \Phi|n\rangle = f_n|n\rangle \) for a given dimension \( N \) fixed. In such a case, \( \{ h_n, f_n \}_{0 \leq n \leq N-1} \) represents the corresponding set of eigenvalues related to the respective Hamiltonian and Fourier operators. Since

\[
H\Phi|n\rangle = \Phi H|n\rangle = f_n h_n |n\rangle \Rightarrow [H, \Phi]|n\rangle = 0|n\rangle,
\]

the intrinsic mathematical properties associated with the discrete representation \( \{ |u_\alpha\rangle \}_{0 \leq \alpha \leq N-1} \) allow to obtain the general equation

\[
\langle u_\alpha | H \Phi | n \rangle = f_n h_n \langle u_\alpha | n \rangle,
\]

(A.1)

whose solution set \( \{ \langle u_\gamma | n \rangle \} \in \mathbb{R} \) yields a complete orthonormal basis of real eigenfunctions genuinely labelled by discrete variables. The Harper functions are here attained when one considers \( H \) as being a Harper-type operator [32].

As a first application, let us, for now, adopt the discrete Fourier operator

\[
\Phi := \sum_{\beta=0}^{N-1} |v_\beta\rangle \langle u_\beta| = \frac{1}{\sqrt{N}} \sum_{\beta, \beta'=0}^{N-1} \omega^{\beta \beta'} |u_\beta\rangle \langle u_{\beta'}| \Rightarrow \Phi \Phi^\dagger = \Phi^\dagger \Phi = 1,
\]

as well as that Harper Hamiltonian operator previously discussed in Section 4, namely, \( H = -\sin(\theta) C_U - \cos(\theta) C_V \) for \( \theta \in [0, \frac{\pi}{2}] \). Thus, Eq. (A.1) assumes the functional form

\[
\sum_{\beta=0}^{N-1} O(\alpha, \beta; N) \langle u_\beta | n \rangle = f_n h_n \langle u_\alpha | n \rangle,
\]

(A.2)

where

\[
O(\alpha, \beta; N) \equiv \langle u_\alpha | H | v_\beta \rangle = - \left[ \sin(\theta) \cos \left( \frac{2\pi \alpha}{N} \right) + \cos(\theta) \cos \left( \frac{2\pi \beta}{N} \right) \right] \langle u_\alpha | v_\beta \rangle
\]

represents the mapped expression of the Hamiltonian operator in the discrete representations \( \{ |u_\alpha\rangle, |v_\beta\rangle \} \) with \( \langle u_\alpha | v_\beta \rangle = \frac{1}{\sqrt{N}} \omega^{\alpha \beta} \) and \( \omega = \exp \left( \frac{2\pi i}{N} \right) \); besides,

\[\text{For } N \text{ odd and discrete labels assuming integer values in the symmetric interval } [-\ell, \ell] \text{ with } \ell = \frac{N-1}{2} \text{ fixed, it is worth stressing that } \Phi^2 \text{ coincides with that parity operator } P \text{ previously defined in Ref. } [12].\]
\( \{ \langle u_\gamma | n \rangle \} \in \mathbb{R} \) denotes the Harper functions for a given \( N \in \mathbb{N}^* \). In fact, such a result can also be split up into two combined equations as follows:

\[
\sin(\theta) \cos \left( \frac{2\pi \alpha}{N} \right) \langle u_\alpha | n \rangle + \frac{1}{2} \cos(\theta) \left( \langle u_{\alpha-1} | n \rangle + \langle u_{\alpha+1} | n \rangle \right) = -h_n \langle u_\alpha | n \rangle \quad (A.3)
\]

and

\[
\frac{1}{\sqrt{N}} \sum_{\beta=0}^{N-1} \omega^{\alpha \beta} \langle u_\beta | n \rangle = f_n \langle u_\alpha | n \rangle. \quad (A.4)
\]

The first one describes a three-term recurrence relation and also depicts the well-known Harper’s equation, whose link with discrete harmonic oscillator and discrete fractional Fourier transform was already discussed by Barker and coworkers [24]; whilst the second one reflects exactly the eigenvalue problem investigated by Mehta [36] when \( f_n = i^n \) (in this particular case, see Ref. [19] for supplementary material), although his ansatz solution

\[
\langle u_\alpha | n \rangle = N_n (-i)^n \sqrt{\frac{2\pi N}{\pi}} \sum_{\kappa=-\infty}^{\infty} \exp \left( -\frac{\pi N \kappa^2}{4} + \frac{2\pi i N \kappa \alpha}{2} \right) H_n \left( \sqrt{\frac{2\pi}{N}} \kappa \right)
\]

does not represent a complete set of orthonormal eigenfunctions [37] — in such ansatz solution, \( N_n \) corresponds to a normalization constant and \( H_n(z) \) denotes the Hermite polynomials.

Summarizing, Eq. (A.3) yields, in general, a set of real eigenvalues \( \{ h_n \} \) whose respective eigenfunctions \( \{ \langle u_\alpha | n \rangle \} \) constitute a complete orthonormal basis in a \( N \)-dimensional state vector space. In this specific case, both the eigenvalues and eigenfunctions are dependent on the angle variable \( \theta \in [0, \frac{\pi}{2}] \), which leads us to determine the maximum of \( \cos(\theta) |\langle U \rangle| + \sin(\theta) |\langle V \rangle| \) for each particular situation \( h_n \equiv \langle u_\alpha | n \rangle \) with \( N \) fixed. Thus, the global maximum obtained from this mathematical procedure allows not only to fix a given value of \( \theta \), but also to estimate the smallest eigenvalue of the Hermitian operator \( H \); consequently, the corresponding eigenvector will describe the ground state \( |0\rangle \) characterized by \( \theta = \frac{\pi}{4} \) and \( f_0 = +1 \) for any dimension \( N \) (it is worth stressing that theoretical and numerical calculations confirm these results). Next, let us consider the \( N = 2, \ldots, 6 \) cases for \( \theta = \frac{\pi}{4} \) fixed, in order to provide a complete list of results exhibited in Table 1 associated with the normalized ground state.

- Case \( N = 2 \) (prime dimension) and \( h_0 = -1 \). This first example obeys the criterion “easy to calculate”, once the corresponding ground state

\[
|0\rangle_2 = \frac{\sqrt{2} + \sqrt{2}}{2} |u_0\rangle + \frac{\sqrt{2} - \sqrt{2}}{2} |u_1\rangle
\]

\footnote{Such a quantity implicitly defines the boundary — or, more precisely, the convex hull — of the accessible region related to the \( \{|\langle U \rangle|, |\langle V \rangle|\} \)-space [14].}
allows to obtain \( \mathcal{V}_{U(V)} = \frac{1}{2} \) and \( \mathcal{Y}_{\delta U(\delta V)} = 1 \), which implies that \( S_{\delta U}^{(0)} = 1 \).

- Case \( N = 3 \) (prime dimension) and \( h_0 = - \frac{\sqrt{5} + \sqrt{2}}{4} \). This particular example yields certain interesting peculiarities since its respective ground state

\[
|0\rangle_3 = \sqrt{\frac{3 + \sqrt{3}}{6}} |u_0\rangle + \sqrt{\frac{3 - \sqrt{3}}{12}} |u_1\rangle + \sqrt{\frac{3 - \sqrt{3}}{12}} |u_2\rangle
\]

leads to achieve \( \mathcal{V}_{U(V)} = \frac{1}{2} + \frac{2 - \sqrt{3}}{8} \) and \( \mathcal{Y}_{\delta U(\delta V)} = 15 - 8\sqrt{3} \), which corroborate those results obtained by Opatrný [23] for the number and phase operators. Furthermore, it is easy to demonstrate that \( S_{\delta U}^{(0)} = 7 - 3\sqrt{3} \), which justifies the approximated numerical value \( R_1 \approx 3.254 \) exhibited in Table 1.

- Case \( N = 4 \) (even dimension) and \( h_0 = -1 \). In such a situation, the ground state

\[
|0\rangle_4 = \frac{2 + \sqrt{2}}{4} |u_0\rangle + \frac{\sqrt{2}}{4} |u_1\rangle + \frac{2 - \sqrt{2}}{4} |u_2\rangle + \frac{\sqrt{2}}{4} |u_3\rangle
\]

attains those same values of \( \mathcal{V}_{U(V)} \) and \( \mathcal{Y}_{\delta U(\delta V)} \) verified in \( N = 2 \); however, it is worth stressing that \( S_{\delta U}^{(0)} = 2 \), since \( \varepsilon = \frac{1}{2} \) in this particular case.

- Case \( N = 5 \) (prime dimension) and \( h_0 = - \frac{\sqrt{5} + \sqrt{2} + \sqrt{10 + 2\sqrt{21}}}{4} \). For this non-trivial example, the normalized ground state assumes the form

\[
|0\rangle_5 = \frac{1}{\sqrt{1 + 2(a_1^2 + a_2^2)}} (|u_0\rangle + a_1 |u_1\rangle + a_2 |u_2\rangle + a_2 |u_3\rangle + a_1 |u_4\rangle)
\]

with \( a_1 = \frac{\sqrt{5} + \sqrt{2(35 + \sqrt{5})} - 7}{8} \) and \( a_2 = \frac{3\sqrt{5} - \sqrt{2(35 + \sqrt{5})} + 3}{8} \). So, after some lengthy calculations, the exact expression \( \mathcal{Y}_{\delta U(\delta V)} = \frac{45 - 5 - \sqrt{110 + 38\sqrt{5}}}{19 + \sqrt{5} + \sqrt{110 + 38\sqrt{5}}} \) for the variance allows to show that

\[
S_{\delta U}^{(0)} = \left( \frac{5 + \sqrt{25 + 10\sqrt{5}}}{5} \right) \left( \frac{45 - 5 - \sqrt{110 + 38\sqrt{5}}}{19 + \sqrt{5} + \sqrt{110 + 38\sqrt{5}}} \right) \approx 1.9444,
\]

corroborating, in this way, the numerical result \( R_1 \approx 3.781 \) (see Table 1).

- Case \( N = 6 \) (even dimension) and \( h_0 = - \frac{\sqrt{10 + 2\sqrt{21}}}{4} \). Similarly to the previous case, in this situation the ground state admits

\[
|0\rangle_6 = \frac{1}{\sqrt{1 + 2(b_1^2 + b_2^2 + b_3^2)}} (|u_0\rangle + b_1 |u_1\rangle + b_2 |u_2\rangle + b_3 |u_3\rangle + b_2 |u_4\rangle + b_1 |u_5\rangle)
\]

as a solution of Eq. (A.2), where
\[ b_1 = \frac{-2 + \sqrt{5 + \sqrt{21}}}{2} = \frac{-4 + \sqrt{6} + \sqrt{14}}{4} \]
\[ b_2 = \frac{5 + \sqrt{21} - 3 \sqrt{5 + \sqrt{21}}}{2} = \frac{10 - 3 \sqrt{6} - 3 \sqrt{14} + 2 \sqrt{21}}{4} \]
\[ b_3 = -4 + \sqrt{6} - 2 \sqrt{1 + 2 \sqrt{5 + \sqrt{21}}} = -4 + 2 \sqrt{6} + \sqrt{14} - \sqrt{21} \]

represent the respective coefficients. Note that \( V_{\delta V} = 19 - 4 \sqrt{21} \), which implies in \( S_{\delta V} = 19(1 + \sqrt{3}) - 4 \sqrt{42(2 + \sqrt{3})} \approx 1.8297 \) (this result justifies that numerical value \( R_1 \approx 3.348 \) appeared in Table 1 for \( N = 6 \)).

As an initial purpose, these first theoretical results related to the ground state are sufficient to clarify the numerical results depicted in Fig. 1 for the tightest bound. In fact, the results exhibited in this appendix indeed represent a first investigative step towards a general mathematical recipe that presents as a primary product the eigenfunctions \( \{ \langle u_\alpha | n \rangle \}_{0 \leq n \leq N - 1} \), which differ from that Mehta’s ansatz solution.

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