Many-box locality

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There is an ongoing search for a physical or operational definition for quantum mechanics. Several informational principles have been proposed which are satisfied by a theory less restrictive than quantum mechanics. Here, we introduce the principle of "many-box locality," which is a refined version of the previously proposed "macroscopic locality." These principles are based on coarse graining the statistics of several copies of a given box. The set of behaviors satisfying many-box locality for N boxes is denoted L_N^{MB}. We study these sets in the bipartite scenario with two binary measurements, in relation with the sets $\mathcal{Q}$ and $\mathcal{Q}_{1+AB}$ of quantum and "almost quantum" correlations, respectively. We find that the L_N^{MB} sets are, in general, not convex. For unbiased marginals, by working in the Fourier space we can prove analytically that $L_N^{MB} \subsetneq \mathcal{Q}$ for any finite N, while $L_\infty^{MB} = \mathcal{Q}$. Then, with suitably developed numerical tools, we find an example of a point that belongs to L_{16}^{MB} but not to $\mathcal{Q}_{1+AB}$. Among the problems that remain open is whether $\mathcal{Q} \subset L_\infty^{MB}$.

I. INTRODUCTION

The definition of quantum physics is most frequently reduced to a description of its mathematical formalism: Physical systems are described by vector spaces, and their properties by subspaces. The desire for a more physical, or operational, or even philosophical foundation for this definition is an ongoing task. Two programs have reported significant advances in the last decade.

The first program is a revival of the attempts left pending in the approach called "quantum logic" Quantum physics is put in the context of generalized probabilistic theories, then singled out through a small set of axioms. Breakthrough was achieved by realizing that one needs an axiom about composite systems, i.e., one that captures some aspects of entanglement. This program has achieved the goal of reconstructing the Hilbert space structure (see [1] for a review).

Another program has been inspired by the work on Bell nonlocality. There, the basic mathematical object comprises the correlations among the outcomes of measurements on separated systems. One could try and find a physical principle that would allow exactly the set of correlations predicted by quantum theory. The pioneering attempt in this direction was that of Popescu and Rohrlich [2], who asked whether no-signaling could be such a principle and found it defines a much larger set of correlations. This no-signaling set became then the arena, in which the quantum set had to be recovered by further constraints. The main principles proposed to date, inspired either by information theory or by physics, are nontrivial communication complexity [3], no advantage for nonlocal computation [4], information causality (IC) [5],

macroscopic locality (ML) [6], and local orthogonality [7]. Each defines a set of correlations which touches the quantum set in a nontrivial way. For most of them, we do not have a compact characterization but (pending a general proof for IC) we know that they are larger than a set that is strictly larger than the quantum set [8]. In other words, the principle defining quantum physics in this program is still being sought [9,10].

In this paper we explore the principle of many-box locality (MBL) that is a refinement of ML. ML is probably the most physical of the principles listed above. The starting point is the fact that we do not see violation of Bell inequalities in the macroscopic world. The formalization considers that one cannot observe the outcome of individual sources of correlations (*boxes*), but only the coarse graining of the outcomes of N of them [see Fig. 1(b)]. Then, a second coarse graining is considered: The outcomes of N boxes are known with a precision $\sqrt{N}$. Under these coarse-graining assumptions, one can characterize exactly the set of correlations identified by ML in the limit $N \to \infty$: It coincides with the first step of the Navascués-Pironio-Acín hierarchy of semidefinite relaxations [11]. A similar work by Rohrlich [12] shows that in the infinite N limit, some nonlocal boxes can even be activated to signal if weak measurements are possible for these boxes. By forbidding this possibility of activation of signaling, the Tsirelson's bound is recovered.

The second coarse graining is certainly very reasonable in practice, but one may question whether it fits in a fundamental principle: We may never be able to distinguish 10^{23} from $10^{23} + 1$, but nature may not be defined by our limitations. MBL is defined by keeping the first coarse graining of ML, but not the second one. Besides, we shall discuss the set of achievable correlations also for finite N, whereas ML was directly phrased for the infinite limit.

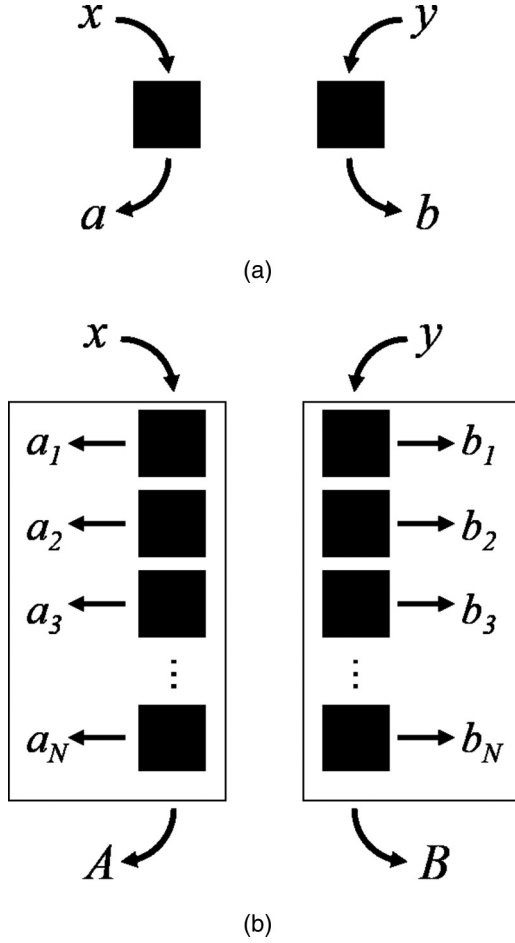*Corresponding author: caiyu01@gmail.com

(a)

(b)

FIG. 1. Comparison between the usual Bell scenario and the many-box scenario. (a) The usual Bell scenario. We called this a "box." (b) The many-box scenario. An "N-box" is formed by combining N boxes together in a particular way: All individual boxes are identical and independent, the same setting is provided to each box, and the outcome of each box is cumulated to produce the outcome of the many box; i.e., $A = \sum_i a_i$, $B = \sum_i b_i$.

II. PRELIMINARY NOTIONS

In this section, we first introduce the Bell scenario. Then three sets of correlations of interest will be introduced: the no-signaling set $\mathcal{NS}$, the quantum set $\mathcal{Q}$, the local set $\mathcal{L}$, as well as Bell inequalities. For simplicity, we introduce these notions in bipartite scenarios, but these can be generalized to any general Bell scenarios including multipartite ones.

A. Bell scenario and behaviors

Consider two parties Alice and Bob at distinct locations. Each has a measurement device, which shall be treated as a black box with the input $x \in \mathcal{X} = \{1,2,\ldots,M_A\}$ and $y \in \mathcal{Y} = \{1,2,\ldots,M_B\}$ and the output $a \in \mathcal{A} = \{1,2,\ldots,m_A\}$ and $b \in \mathcal{B} = \{1,2,\ldots,m_B\}$, for Alice and Bob, respectively. We refer to this as the (M_A,M_B,m_A,m_B) *Bell scenario*.

In each run of the experiment, each party chooses a input at random and obtains an outcome. After repeating the experiment sufficiently many times, one can reconstruct the

family of $M_A \times M_B$ probability distributions,

$$\mathcal{P}_{\mathcal{X},\mathcal{Y}} = \{P(a,b|x,y), a \in \mathcal{A}, b \in \mathcal{B}\}_{x \in \mathcal{X}, y \in \mathcal{Y}},$$

with $P(a,b|x,y) \geqslant 0$ for all a,b,x,y and $\sum_{a,b} P(a,b|x,y) = 1$ for all x,y. It has become customary to refer to the $\mathcal{P}_{\mathcal{X},\mathcal{Y}}$ as to a *behavior*. For the purpose of this paper, we need to define three sets of behaviors: no-signaling ($\mathcal{NS}$), quantum ($\mathcal{Q}$), and local ($\mathcal{L}$). They are strictly included into one another according to $\mathcal{L} \subsetneq \mathcal{Q} \subsetneq \mathcal{NS}$. In this paper, we will be focusing on $(2,2,d,d)$ scenarios, though the notions in this section apply to any Bell scenarios.

B. The no-signaling set

A behavior $\mathcal{P}$ is said to be no-signaling (NS) if it satisfies

$$\sum_{b \in \mathcal{B}} P(a,b|x,y) \equiv P(a|x,y) = P(a|x),$$

$$\sum_{a \in \mathcal{A}} P(a,b|x,y) \equiv P(b|x,y) = P(b|y), \tag{1}$$

for all x,y. The set of no-signaling behaviors $\mathcal{NS}$ is defined by a finite number of linear constraints, namely the positivity constraints $0 \leqslant P(a,b|x,y) \leqslant 1$, the normalization constraints $\sum_{a,b} P(a,b|x,y) = 1$, and the no-signaling constraints (1). Because of this, it has a compact characterization: It is a *polytope*, i.e., a convex set with finitely many extremal points.

Let us represent no-signaling behaviors in the $(2,2,d,d)$ Bell scenario in the Collins-Gisin form [13],

$$\mathcal{P}_{\mathcal{X},\mathcal{Y}} := \left(\begin{array}{c||c|c} 1 & P(b|y=0) & P(b|y=1) \\ \hline\hline P(a|x=0) & P(a,b|0,0) & P(a,b|0,1) \\ \hline P(a|x=1) & P(a,b|1,0) & P(a,b|1,1) \end{array} \right),$$

where $a,b \in \{0,1,\ldots,d-2\}$. Notice that a $(2,2,d,d)$ no-signaling behavior is fully specified by $4d(d-1)$ numbers, whereas a generic behavior in the same scenario would require $4(d^2-1)$ numbers.

C. The quantum set

For a given bipartite Bell scenario, the *quantum set* $\mathcal{Q}$ of behaviors is the set of all the $\mathcal{P}_{\mathcal{X},\mathcal{Y}}$ that can be obtained with quantum theory. That is, $\mathcal{P}_{\mathcal{X},\mathcal{Y}} \in \mathcal{Q}$ if there exist a quantum state $|\psi\rangle$ and two sets of measurement operators $\{E_A^{a|x}, a \in \mathcal{A}, x \in \mathcal{X}\}$ and $\{E_B^{b|y}, b \in \mathcal{B}, y \in \mathcal{Y}\}$, such that $[E_A^{a|x}, E_B^{b|y}] = 0$, $\sum_a E_A^{a|x} = \mathbb{I}$, $\sum_b E_B^{b|y} = \mathbb{I}$, and

$$P(a,b|x,y) = \langle\psi|E_A^{a|x} E_B^{b|y}|\psi\rangle \tag{2}$$

for all a,b,x,y. Notice that, since no restriction is made on the dimension of the Hilbert space, the state can be taken to be pure and the measurement operators projective.

The quantum set is convex but not a polytope. So far, no compact characterization of the quantum set is known. In this paper, we shall use the hierarchy of semidefinite programs proposed by Navascués-Pironio-Acín (NPA) [11] as an outer approximation of $\mathcal{Q}$. Each level j of the hierarchy defines a set of behaviors larger than the quantum set, such that $\mathcal{Q}_{j+1} \subseteq \mathcal{Q}_j$; the hierarchy converges to the quantum set, i.e., $\mathcal{Q}_{j \to \infty} = \mathcal{Q}$.

D. The local set

A local deterministic behavior is one in which the outputs a and b are determined by the inputs x and y, respectively:

$$P_{LD}(a,b|x,y) = \delta_{a=f_i(x)}\delta_{b=f_j(y)}. \tag{3}$$

There are $m_A^{M_A} m_B^{M_B}$ local deterministic behaviors. As an example that will be used later, in the (2,2,2,2) scenario, the behavior corresponding to deterministically outputting $a = 1$ and $b = 1$ for both inputs is represented by

$$\mathcal{P}_{LD_1} = \begin{pmatrix} 1 & \| & 0 & | & 0 \\ \hline 0 & \| & 0 & | & 0 \\ \hline 0 & \| & 0 & | & 0 \end{pmatrix}. \tag{4}$$

A behavior $\mathcal{P}$ is said to be local if and only if it can be described as a *convex combination of local deterministic behaviors*,

$$\mathcal{P} = \sum_i c_i \mathcal{P}_{LD_i}, \tag{5}$$

where $c_i \geqslant 0$, $\sum_i c_i = 1$. Thus, the local set $\mathcal{L}$ is also a polytope, with the local deterministic behaviors as extremal points.

The local polytope shares some facets with $\mathcal{NS}$, defined by the positivity, normalization and no-signaling constraints. Its proper facets are *Bell inequalities C*,

$$C \cdot \mathcal{P} \equiv \sum_{a,b,x,y} C(a,b,x,y)P(a,b|x,y) \leqslant V, \tag{6}$$

where V is called the local value. In other words, a behavior is local if and only if none of the Bell inequalities is violated. To test whether a given point is local, it is not necessary to list all the Bell inequalities explicitly for that scenario. Rather, one can solve the linear program

$$
\begin{aligned}
\text{maximize} \quad & v, \\
\text{subject to} \quad & \mathcal{P}(v) = v\mathcal{P} + (1-v)\mathcal{P}_{\text{mix}}, \\
& \mathcal{P}(v) = \sum_i t_i \mathcal{P}_{LD_i}, \\
& t_i \geqslant 0, \sum_i t_i = 1,
\end{aligned} \tag{7}
$$

where $\mathcal{P}_{\text{mix}}(a,b|x,y) = 1/d^2, \forall\, a,b,x,y$, is the maximally mixed distribution. We call the returned value $v_{\max}$ the local parameter. The behavior $\mathcal{P}$ is local if $v_{\max} \geqslant 1$, nonlocal if $v_{\max} < 1$. As a by-product of this optimization, a certificate is provided in either case. If the test distribution is local, it will return us a valid decomposition in terms of local deterministic points. Otherwise, it will return a Bell inequality that is violated by the test distribution as a consequence of Farkas' lemma [14].

III. MANY-BOX LOCALITY: DEFINITION AND TOOLS

In this section, we first introduce the notion of many-box coarse graining and MBL. Second, we introduce the tool of Fourier transform that would be useful for this study.

A. Definition of many-box locality

Here, for simplicity, we will define many-box locality in the (2,2,2,2) scenario, though it can be generalized to any Bell scenario, including multipartite ones. Consider N identical (2,2,2,2) boxes, each described by $\mathcal{P}(a,b|x,y)$. In any run, all the boxes take the same inputs x and y, but each produces independently the output $a_i, b_i \in \{0,1\}, i = 1, \ldots, N$. Besides, we do not keep all the information on the output, but just the locally coarse-grained variables $A = \sum_i a_i$ and $B = \sum_i b_i$. By construction, $A \in \{0,1,\ldots,N\}$ and $B \in \{0,1,\ldots,N\}$. In other words, the coarse-grained variables define a $(2,2,N+1,N+1)$ scenario.

The behavior of these variables will be denoted by $\mathcal{P}^{*N}$, called the *N-box coarse graining of $\mathcal{P}$*. It is not difficult to write the explicit form of $\mathcal{P}^{*N}$ given $P(a,b|x,y)$,

$$
\begin{aligned}
P^{*N}(A,B|x,y) = \sum_{k=0}^{N} & \binom{N}{A-k, B-k, k, N-A-B+k} \\
& \times P(00|x,y)^{N-A-B+k} P(01|x,y)^{B-k} \\
& \times P(10|x,y)^{A-k} P(11|x,y)^k,
\end{aligned} \tag{8}
$$

where $\binom{N}{n_1,n_2,n_3,n_4} = \frac{N!}{n_1!n_2!n_3!n_4!}$. In particular, the marginals are given by

$$P^{*N}(A|x) = \binom{N}{A} P(a=1|x)^A P(a=0|x)^{N-A},$$

$$P^{*N}(B|y) = \binom{N}{B} P(b=1|x)^B P(b=0|x)^{N-B}.$$

We introduce the notion of MBL sets.

Definition 1. A behavior $\mathcal{P}$ is said to be N-box local ($\mathcal{P} \in L_N^{MB}$) if $\mathcal{P}^{*N}$ is local in the $(2,2,N+1,N+1)$ scenario. Notice that the sets L_N^{MB} are defined in the original scenario (2,2,2,2).

By construction, the coarse-graining procedure obeys the composition rule

$$\mathcal{P}^{*(N_1+N_2)} = \mathcal{P}^{*N_1} * \mathcal{P}^{*N_2}. \tag{9}$$

From it, one can straightforwardly prove the following inclusion relations.

Proposition 1. If $\mathcal{P} \in \bigcap_j L_{N_j}^{MB}$, then $\mathcal{P} \in L_{N(\vec{q})}^{MB}$, with $N(\vec{q}) = \sum_j q_j N_j$, for all $\vec{q} = (q_1, q_2, \ldots)$, with $q_j \in \mathbb{N}$.

Indeed, local decompositions for both $\mathcal{P}^{*N_1}$ and $\mathcal{P}^{*N_2}$ directly define a local decomposition for $\mathcal{P}^{*(N_1+N_2)}$. As a corollary, if a probability distribution is both 2-box and 3-box local, then it is N-box local for any $N \geqslant 2$, since any N can be decomposed as a sum of multiples of two and three.

Beyond this proposition, we have not been able to find general properties for the L_N^{MB} sets. Properties that might have been conjectured, e.g., convexity or the inclusion $L_N^{MB} \subseteq L_{N+1}^{MB}$, do not hold, as forthcoming counterexamples will demonstrate.

B. Fourier transform

The coarse-grained behaviors $\mathcal{P}^{*N}$ are obtained by *convolution* of N copies of $\mathcal{P}$. This observation suggests studying the problem in its Fourier transformed version.

First, we define the Fourier transform of a behavior:

Definition 2. The Fourier transform of order r, where $r \geqslant d$, of a behavior $\mathcal{P}$, denoted $\mathcal{F}_r[\mathcal{P}]$, is defined as

$$\mathcal{F}_r[\mathcal{P}](k,l|x,y) = \tilde{P}_r(k,l|x,y)$$
$$:= \sum_{a,b=0}^{r-1} e^{\frac{2\pi i}{r}(ak+bl)} P(a,b|x,y),$$

for any x,y, where $k,l \in \{0,1,\ldots,r-1\}$.

Similarly, we define the inverse Fourier transform of a Bell expression C:

Definition 3. The inverse Fourier transform of order r, where $r \geqslant d$, of a Bell expression C, denoted $\mathcal{F}_r^{-1}[C]$, is defined as

$$\mathcal{F}_r^{-1}[C](k,l,x,y) = \tilde{C}_r(k,l,x,y)$$
$$:= \frac{1}{r^2} \sum_{a,b=0}^{r-1} e^{-\frac{2\pi i}{r}(ak+bl)} C(a,b,x,y),$$

for any $x,y \in \{0,1\}$, where $k,l \in \{0,1,\ldots,r-1\}$.

Note that the Fourier transform is only well behaved when $r \geqslant d$. So this is always assumed for the rest of the paper, and the subscript r is dropped for simplicity.

Due do the linearity of Fourier transform, Bell violation is preserved; that is,

$$\mathcal{F}_r^{-1}[C] \cdot \mathcal{F}_r[\mathcal{P}] = \sum_{k,l,x,y} \tilde{C}_r(k,l,x,y) \tilde{P}_r(k,l|x,y)$$
$$= \sum_{a,b,x,y} C(a,b,x,y) P(a,b|x,y) = C \cdot \mathcal{P}. \quad (10)$$

Another property of the Fourier transform follows from the convolution theorem, applied repeatedly:

$$\mathcal{F}_r[\mathcal{P}^{*N}] = (\mathcal{F}_r[\mathcal{P}])^N. \quad (11)$$

The N-box coarse graining manifests as raising to the Nth power the Fourier transformed probability.

We can now analyze many-box locality in the Fourier transformed space. $\mathcal{P}^{*N}$ is local if and only if it satisfies all the Bell inequalities in the $(2,2,N+1,N+1)$ scenario, $C_i \cdot \mathcal{P}^{*N} \leqslant V_i$. By linearity and the convolution theorem, for the Fourier transformed probability, we have

$$\tilde{C}_i \cdot \widetilde{\mathcal{P}^{*N}} = \tilde{C}_i \cdot \tilde{\mathcal{P}}^N \leqslant V_i \quad (12)$$

for all i. Note that each Bell inequality (C_i, V_i) defines an Nth-degree polynomial inequality for single-box behavior $\mathcal{P}$. Thus, on the boundary of L_N^{MB}, one or more such polynomial inequalities are saturated. We summarize this in the following.

Proposition 2. Let $\mathcal{R}_i^N := \{\mathcal{P} \mid \tilde{C}_i \cdot \tilde{P}^N \leqslant V_i\}$. Then $L_N^{MB} = \bigcap_{i \in I} \mathcal{R}_i^N$, where $\{(C_i, V_i)\}_{i \in I}$ is the set of all the Bell inequalities of the $(2,2,N+1,N+1)$ scenario. Behaviors on the boundary of L_N^{MB} must saturate one or several Bell inequalities:

$$\mathcal{P} \in bd\big(L_N^{MB}\big) \Rightarrow \exists i \in I, \quad \text{such that } \tilde{C}_i \cdot \tilde{\mathcal{P}}^N = V_i.$$

This provides a systematic way to compute the boundary of L_N^{MB}. However, this is not tractable for large N due to the (at least) exponentially increasing number of Bell inequalities in the $(2,2,N+1,N+1)$ scenario. The task is now to find

the relevant set of Bell inequalities that defines the border of the L_N^{MB} sets. As we will see in the following sections, in some cases we could guess the relevant set of Bell inequalities, hence characterizing the L_N^{MB} set; otherwise, any particular set of Bell inequalities will provide an upper bound to the L_N^{MB} set.

IV. RESULTS ON L_N^{MB} IN THE (2,2,2,2) SCENARIO

Now we address explicitly the characterization of L_N^{MB} in the (2,2,2,2) Bell scenario. We start by plotting some of the L_N^{MB} in some slices, by solving the linear optimization (7). These plots show that the shape of the sets and their inclusion is not trivial. Then we present one case in which the tool of Fourier transforms can be used to find the boundary of L_∞^{MB} in a special slice. Finally, we discuss the relation between MBL and the sets $\mathcal{Q}_n$ of the NPA hierarchy, including $\mathcal{Q}_1$ that defines ML.

A. Numerical plots

To have a better understanding of these L_N^{MB} sets, in this section, we start with numerical plots of L_N^{MB} sets. We first show L_2^{MB} and L_3^{MB} in a three-dimensional slice of the $\mathcal{NS}$ polytope. Then, we show L_N^{MB} for N up to 10 in a two-dimensional slice.

The local polytope in the (2,2,2,2) scenario is characterized by its 16 extremal points, $\mathcal{P}_{LD_i}, i = 1, 2, \cdots, 16$. Its nontrivial facets consists of eight Clauser-Horne-Shimony-Holt (CHSH) [15] inequalities, for example,

$$C_1 \equiv E_{00} + E_{01} + E_{10} - E_{11} \leqslant 2,$$
$$C_2 \equiv -E_{00} + E_{01} + E_{10} + E_{11} \leqslant 2, \quad (13)$$

where

$$E_{xy} = P(a = b|x,y) - P(a \neq b|x,y).$$

No-signaling probability distribution that violates each CHSH inequality to its algebraic maximum is known as a Popescu-Rohrlich box (PR box). For the two CHSHs mentioned above, we have the corresponding PR boxes,

$$\mathcal{P}_{PR_1} = \begin{pmatrix} 1 & \| & 1/2 & 1/2 \\ \hline 1/2 & \| & 1/2 & 1/2 \\ \hline 1/2 & \| & 1/2 & 0 \end{pmatrix}, \quad (14)$$

and

$$\mathcal{P}_{PR_2} = \begin{pmatrix} 1 & \| & 1/2 & 1/2 \\ \hline 1/2 & \| & 0 & 1/2 \\ \hline 1/2 & \| & 1/2 & 1/2 \end{pmatrix}. \quad (15)$$

We are going to parametrize the slice under consideration with $\mathcal{P}_{PR_1}$, $\mathcal{P}_{PR_2}$, $\mathcal{P}_{LD_1}$, and $\mathcal{P}_{mix}$:

$$\mathcal{P}(\alpha,\beta,\gamma)$$
$$= \alpha \mathcal{P}_{PR_1} + \beta \mathcal{P}_{PR_2} + \gamma \mathcal{P}_{LD_1} + (1 - \alpha - \beta - \gamma)\mathcal{P}_{mix}$$
$$= \begin{pmatrix} 1 & \| & (1-\gamma)/2 & (1-\gamma)/2 \\ \hline (1-\gamma)/2 & \| & (1+\alpha-\beta-\gamma)/4 & (1+\alpha+\beta-\gamma)/4 \\ \hline (1-\gamma)/2 & \| & (1+\alpha+\beta-\gamma)/4 & (1-\alpha+\beta-\gamma)/4 \end{pmatrix}.$$
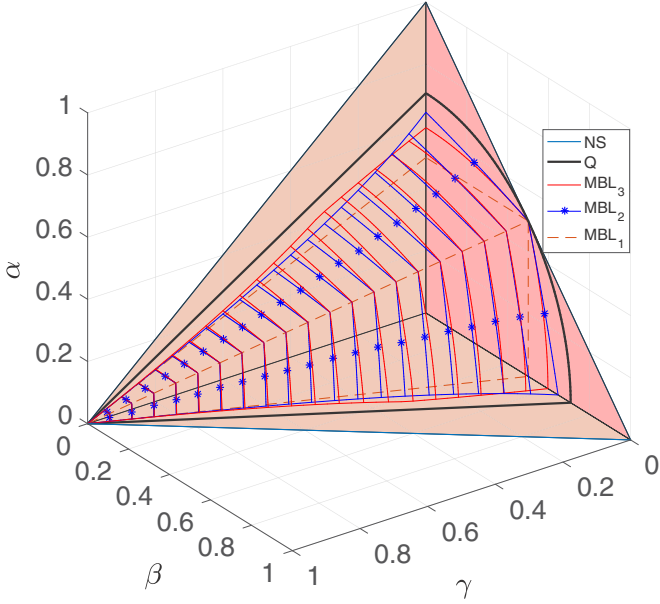$$(16)$$

FIG. 2. The L_1^{MB}, L_2^{MB}, and L_3^{MB} in the no-signaling set. The region inside the dashed brown lines is the set L_1^{MB}, which is the local set. Here, the thick black, the blue with star markers, and the red lines are the boundary of Q, L_2^{MB}, and L_3^{MB}, respectively.

Thanks to the symmetry of PR boxes, we only need to discuss the case where $\alpha, \beta \geqslant 0$. We first consider the region $\gamma \geqslant 0$. The positivity constraint is given by $\alpha + \beta + \gamma \leqslant 1$. The local polytope is constrained by two CHSH inequalities, $2\alpha + \gamma \leqslant 1$ and $2\beta + \gamma \leqslant 1$. The quantum set is well characterized for the planes $\alpha = 0$, $\beta = 0$, and $\gamma = 0$ by $\sqrt{2}\beta + \gamma = 1$, $\sqrt{2}\alpha + \gamma = 1$, and $\alpha^2 + \beta^2 = 1/2$, respectively (the first two by [16], and the last is the well-known Tsirelson-Landau-Masanes arcsine inequality [17–19]). We conjecture that in the region $\alpha, \beta, \gamma > 0$, the quantum set is given by

$$\alpha^2 + \beta^2 \leqslant (1 - \gamma)^2/2. \tag{17}$$

In Fig. 2, L_1^{MB}, L_2^{MB}, and L_3^{MB} are plotted for the region $\alpha, \beta, \gamma \geqslant 0$, as well as $\mathcal{N}$, $\mathcal{Q}$, and $\mathcal{L}$. By definition, L_1^{MB} is simply the local set $\mathcal{L}$. L_2^{MB} and L_3^{MB} are obtained by solving the optimization (7). We would like to highlight two qualitative features about these MBL sets. First, L_N^{MB} sets are not convex as we can see from the figure. Mathematically, it says that to show $\mu\mathcal{P}_1 + (1-\mu)\mathcal{P}_2 \in L_N^{MB}$, knowing $\mathcal{P}_1 \in L_N^{MB}$ and $\mathcal{P}_2 \in L_N^{MB}$ is not sufficient. Second, in general, L_N^{MB} is not contained in L_{N+1}^{MB}, as we can see in the figure, L_2^{MB} is not contained in L_3^{MB}. For example, $\mathcal{P}(\alpha) = \mathcal{P}(\alpha, 0, 0)$ is in L_2^{MB} but not L_3^{MB} for $\sqrt{7} - 2 < \alpha \leqslant (1 + \sqrt{2})^{1/3} - (1 + \sqrt{2})^{-1/3}$.

In Figs. 3 and 4, the L_N^{MB} sets are plotted in two 2D slices corresponding to $\gamma = 0$ and $\beta = 0$. Note that for $\gamma < 0$, the positivity constraint becomes $\alpha + \beta - 3\gamma \leqslant 1$ and the quantum boundary is well approximated by the second level of the NPA hierarchy, $\mathcal{Q}_2$. From the figures, we can see that for up to $N = 10$, the L_N^{MB} are contained in the quantum set $\mathcal{Q}$. The general trend of the sets are increasing with N. Though the inclusion relation $L_N^{MB} \subseteq L_{N+1}^{MB}$ is not true, $L_N^{MB} \subseteq L_{N+2}^{MB}$ is conjectured to hold for both even and odd N.
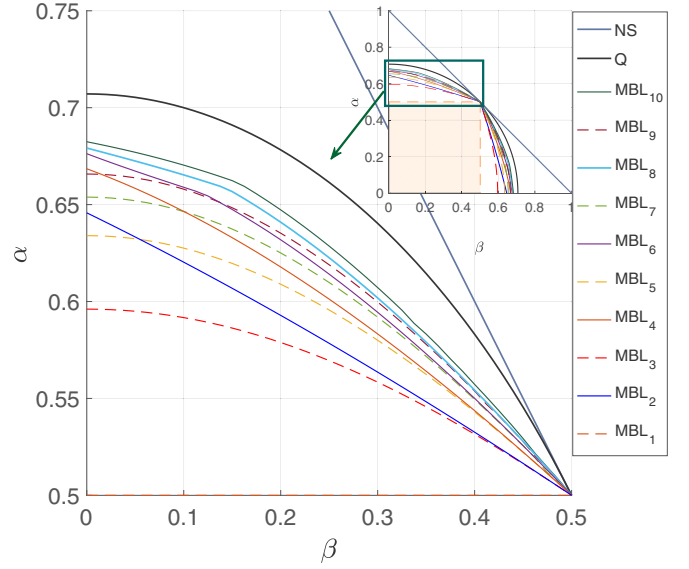

FIG. 3. The boundary of the L_N^{MB} sets in the plane $\gamma = 0$ for N from 2 to 10. Here, solid lines from top to bottom are NS, Q, L_{10}^{MB}, L_8^{MB}, L_6^{MB}, L_4^{MB}, L_2^{MB}, respectively, and dashed lines from top to bottom are L_9^{MB}, L_7^{MB}, L_5^{MB}, L_3^{MB}, L_1^{MB}, respectively. Note that the shaded is the set MBL_1, i.e., the local set. In particular, we magnify the region inside the green rectangle box to show more details.

In the next section, we present some analytic results, especially for the case for $N \to \infty$.

B. $L_\infty^{MB} = \mathcal{Q}$ for unbiased marginals

In Fig. 3 in the previous section, the numerical plots for the boundary of the L_N^{MB} sets for N odd are reasonably smooth. A closer inspection at the dual of the linear program (7) reveals that the relevant inequality has a special form. For odd N where the number of outcome $d = N + 1$ is even, the relevant inequality that defines the boundary of L_N^{MB} is the so-called *half-half* lifting [20] of CHSH. It is equivalent to first coarse graining the d outcomes in to a binary outcome, such that Alice (Bob) assigns $+$ if $A \geqslant \frac{d}{2}$ ($B \geqslant \frac{d}{2}$), $-$ otherwise, then
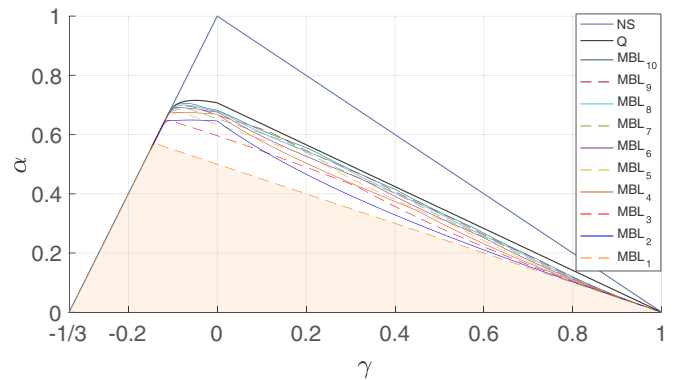

FIG. 4. The boundary of the L_N^{MB} sets in the plane $\beta = 0$ for N from 2 to 10. Here, solid lines, from top to bottom, are NS, Q, L_{10}^{MB}, L_8^{MB}, L_6^{MB}, L_4^{MB}, L_2^{MB}, respectively, and dashed lines from top to bottom are L_9^{MB}, L_7^{MB}, L_5^{MB}, L_3^{MB}, L_1^{MB}, respectively. Note that the shaded area is the set L_1^{MB}, i.e., the local set.

applying the CHSH inequality. Using the array notation for inequalities, expressed in terms of full probabilities, we can also write

$$
C_{\text{half}} = \left(\begin{array}{c|c} -\mathcal{J} & \mathcal{J} \\ \hline \mathcal{J} & \mathcal{J} \end{array} \right), \quad \mathcal{J} = \begin{pmatrix} J & -J \\ -J & J \end{pmatrix},
$$

and J is a matrix of ones of size $d/2 \times d/2$.

Now let us consider the class of behaviors with fully random marginals, that is, $P(a|x) = P(b|y) = \frac{1}{2}$ for all a,b,x,y. Such a behavior can be parametrized by four parameters,

$$
\mathcal{P}_{\text{half}} = \left(\begin{array}{c|c} P(\mu_1) & P(\mu_2) \\ \hline P(\mu_3) & P(\mu_4) \end{array} \right),
$$

where

$$
P(\mu) = \frac{1}{4} \begin{pmatrix} 1+\mu & 1-\mu \\ 1-\mu & 1+\mu \end{pmatrix}.
$$

In the following, we aim to show that, in this slice of fully random marginals, the boundary defined by the half-half lifting, in the limit where N tends to infinity, coincides with that of $\mathcal{Q}_1$. The Fourier transform introduced in Sec. III B will be used in the proofs below.

We start by computing the inner product of $\mathcal{J}$ and $P(\mu)$,

$$
g(\mu) = \mathcal{J} \cdot P(\mu)^{*N},
$$

which in the Fourier-transformed space, following Eq. (12), becomes

$$
g(\mu) = \mathcal{F}^{-1}[\mathcal{J}] \cdot \{\mathcal{F}[P(\mu)]\}^N. \quad (18)
$$

Let us first work out the inverse Fourier transform of the Bell coefficient. Define the d th root of unity as $\omega = e^{\frac{2\pi i}{d}}$, $R_+ = \{0, 1, \ldots \frac{d}{2} - 1\}$, and $R_- = \{\frac{d}{2}, \frac{d}{2} + 1, \ldots, d-1\}$, we have

$$
\mathcal{F}_d^{-1}[\mathcal{J}](k,l)
$$

$$
= \frac{1}{d^2} \left(\sum_{\substack{(a,b) \in \begin{subarray}{c} R_+ \times R_+ \\ R_- \times R_- \end{subarray}}} \omega^{-(ak+bl)} - \sum_{\substack{(a,b) \in \begin{subarray}{c} R_+ \times R_- \\ R_- \times R_+ \end{subarray}}} \omega^{-(ak+bl)} \right)
$$

$$
= \frac{(1 - \omega^{-\frac{dk}{2}})^2 (1 - \omega^{-\frac{dl}{2}})^2}{d^2(1 - \omega^{-k})(1 - \omega^{-l})}. \quad (19)
$$

Then, we focus on the $\mathcal{F}_d^N[P(\mu)]$ term. Since $P(a,b|x,y) = 0$ for $a,b > 1$, only four terms survive:

$$
\mathcal{F}_d[P(\mu)](k,l)
$$

$$
= \frac{1}{4}[(1+\omega^k)(1+\omega^l) + (1-\omega^k)(1-\omega^l)\mu]. \quad (20)
$$

Now we are ready to expand Eq. (18) as a polynomial in μ. After some calculations, we have

$$
g(\mu) = \sum_{m=\text{odd}}^N C(d,m)\mu^m,
$$

where we write $C(d,m)$ in terms of Γ functions:

$$
C(d,m) := \frac{16\Gamma(d)}{4^d \Gamma(m+1)\Gamma(d-m)}
$$

$$
\times \left[\frac{\Gamma(d-m)\Gamma(m)}{\Gamma\left(\frac{d}{2}\right)\Gamma\left(\frac{d-m+1}{2}\right)\Gamma\left(\frac{m+1}{2}\right)} \right]^2.
$$

Only coefficient for odd m survives, $C(d,m) = 0$ for even m because that the denominator diverges to infinity, see the Appendix for more detail.

Furthermore, evaluating the limit when $N \to \infty$, one obtains

$$
C(\infty,m) = \frac{2}{\pi} \frac{1}{m} \frac{(m-2)!!}{(m-1)!!}, \quad (21)
$$

where $(\cdot)!!$ is the double factorial (see the Appendix). Note that this resembles the Taylor expansion of $\arcsin(\mu)$, which reads

$$
\arcsin(\mu) = \sum_{m=\text{odd}}^{\infty} \frac{1}{m} \frac{(m-2)!!}{(m-1)!!} \mu^m. \quad (22)
$$

In conclusion, in the limit of N going to infinity, testing the Bell inequality $C_{\text{half}} \cdot \mathcal{P}^{*N} \leqslant 2$ reduces to testing the Bell inequality

$$
\frac{2}{\pi}[- \arcsin(E_{00}) + \arcsin(E_{01})
$$

$$
+ \arcsin(E_{10}) + \arcsin(E_{11})] \leqslant 2 \quad (23)
$$

on the single-box behavior. Incidentally, Eq. (23) also characterizes the $\mathcal{Q}_1$ set of behaviors.

As a by-product, one can derive the analytic solution of the boundary of L_N^{MB}, for odd N, in the plane $\gamma = 0$. For example, the boundaries of L_N^{MB}, $N = 1, 3, 5$ are shown in the following table.

N	Expression
1	$4\beta = 2$
3	$\beta(3 + 3\alpha^2 + \beta^2) = 2$
5	$\beta[45 + 45\alpha^4 + 10\beta^2 + 9\beta^4 + 30\alpha^2(1 + 3\beta^2)]/16 = 2$

Note that the boundary in the case of $N = 1$ is simply the CHSH-Bell inequality.

C. A sequence of quantum behaviors outside L_N^{MB}

In this section, we present an analytic sequence of quantum behaviors that is N-nonlocal for each N. This family makes use of a different binning of the $N + 1$ outcomes than the half-half binning in the previous section: Instead, we consider that each party outputs the parity of its outcome, e.g., $(-1)^A$ for Alice. We note that this binning requires a full resolution of the outcomes A and B; hence, it is not possible in the context of ML, where the resolution is limited [6].

Consider the probability distribution obtained from measuring the singlet state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

in the following basis:

$$A_0 : \sigma_Z, \qquad\qquad A_1 : \cos(2\theta)\sigma_Z + \sin(2\theta)\sigma_X,$$

$$B_0 : \cos(\theta)\sigma_Z + \sin(\theta)\sigma_X, \quad B_1 : \cos(\theta)\sigma_Z - \sin(\theta)\sigma_X.$$

With these measurements, we can compute the four correlators for a single box:

$$E_{00} = E_{01} = E_{10} = \cos(\theta), \quad E_{11} = \cos(3\theta).$$

Incidentally, this behavior always sits on the boundary of $\mathcal{Q}$, since it satisfies the conditions in Ref. [19].

One can test the nonlocality of its N-box coarse graining by the so-called *parity binning* [21] of the CHSH inequality, denoted as C', where

$$C' = \left(\begin{array}{c|c} \mathcal{J}' & \mathcal{J}' \\ \hline \mathcal{J}' & -\mathcal{J}' \end{array} \right), \quad \mathcal{J}'_{i,j} = (-1)^{i+j}.$$

Following parity binning, and because the N box are identical and independent, we can see that the correlation

$$\begin{aligned}
\langle E_{x,y}^{(N)} \rangle = \langle (-1)^{A_x + B_y} \rangle &= \langle (-1)^{\sum_i a_{x,i} + b_{y_i}} \rangle \\
&= \langle (-1)^{a_{x,i} + b_{y,i}} \rangle^N = E_{x,y}^N;
\end{aligned} \tag{24}$$

that is the correlation for the N-box coarse-graining is simply the Nth power of that of a single box. Hence,

$$\begin{aligned}
S_N = C' \mathcal{P}^{*N} &= E_{00}^N + E_{01}^N + E_{10}^N - E_{11}^N \\
&= 3\cos^N(\theta_N) - \cos^N(3\theta_N).
\end{aligned} \tag{25}$$

Let $\theta_N = \frac{\theta_0}{\sqrt{N}}$; this quantity can be larger than 2 for any N with suitable choice of θ_0. Moreover, in the limit of N going to infinity,

$$S_N = 3e^{-\theta_0^2/2} - e^{-(3\theta_0)^2/2},$$

whose maximum $S_N^{\max} = 3^{7/8} - 3^{-9/8} \approx 2.3245$ is achieved with $\theta_0 = \frac{\sqrt{\ln 3}}{2}$.

It is worth emphasizing that the quantum behavior considered here is different for each value of N (i.e., the angle θ_N depends on N). In particular, setting $N = \infty$ produces a local box which belongs to $L_N^{MB} \forall N$. Therefore, this family of behaviors does not constitute an example of quantum behavior that is outside L_∞^{MB}.

D. A nonquantum L_{16}^{MB} behavior

In this section, we present a behavior that is not quantum but nevertheless belongs to the L_{16}^{MB} set: $\mathcal{P}_{\not\in} \notin \mathcal{Q}$ and $\mathcal{P}_{\not\in} \in L_{16}^{MB}$. This point lies in the slice where $\beta = 0$, and is defined by

$$\alpha = 0.287\,569\,286\,421\,973,$$

$$\gamma = 0.505\,748\,781\,260\,095.$$

First be reminded that the boundary of the quantum set is known analytically on this slice for $\alpha, \gamma \geqslant 0$. It is given by the straight line $\gamma = \frac{1}{\sqrt{2}}(1-\alpha)$. One can thus easily check that $\mathcal{P}_{\not\in}$ is not in the quantum set. A direct computation also

demonstrates that this point does not belong to the set of almost quantum correlations: $\mathcal{P}_{\not\in} \notin \mathcal{Q}_{1+AB}$.

In order to test whether this point belongs to the L_{16}^{MB} set, we solved the linear program (7) with $\mathcal{P}_{\not\in}^{*16}$. This linear program involves 83521 extremal points in an 1088-dimensional space and is tractable with standard solvers. However, the local parameter v turns out to be 1 up to machine precision. We thus developed a high-precision linear programming solver to determine whether v is smaller or larger than 1. This solver is available online in the latest version of YALMIP [22,23]. Using this tool, we solve the linear program (7) with 50 digits of precision and find that the local parameter is

$$v = 1 + 7.4 \times 10^{-19},$$

with $t_i \geqslant 0$ (strictly), $\sum t_i = 1 + 9.8 \times 10^{-55}$, and $|\sum_i t_i \mathcal{P}_{LD_i} - (v\mathcal{P}_{\not\in}^{*16} + (1-v)\mathcal{P}_{\mathrm{mix}})|_1 \leqslant 8.8 \times 10^{-36}$. We consider this a convincing numerical proof of a valid decomposition, since v is significantly larger than 1 compared to the precision with which the constraints are satisfied. The full high-precision primal solution to this linear program is provided in the Supplemental Material [24].

In conclusion, we have shown an explicit example of a distribution that lies in L_{16}^{MB} but outside $\mathcal{Q}$ and $\mathcal{Q}_{1+AB}$. Since $L_{16}^{MB} \subseteq L_\infty^{MB}$, this also shows that $\mathcal{Q} \neq L_\infty^{MB}$ and $\mathcal{Q}_{1+AB} \neq L_\infty^{MB}$.

V. DISCUSSION AND OUTLOOK

In this paper we introduced the set of many-box local behaviors L_N^{MB}. Since the MBL principle is less coarse grained than ML, this set is *a priori* stricter than the set of ML, $L_\infty^{MB} \subseteq \mathcal{Q}_1$. We have shown in Sec. IV B that $L_\infty^{MB} = \mathcal{Q}$ in one slice in which $\mathcal{Q}_1 = \mathcal{Q}$ also holds. Also, we found that L_{16}^{MB} contains behaviors which belong neither to $\mathcal{Q}$, nor to the larger set $\mathcal{Q}_{1+AB}$. This shows that $L_\infty^{MB} \nsubseteq \mathcal{Q}_{1+AB}$. In particular, the principle of many-box locality does not identify the quantum set, either for finite or for infinite N.

There are two main open questions. On the one hand, we do not know if MBL is satisfied by all quantum behaviors, i.e., if $\mathcal{Q} \subsetneq L_\infty^{MB}$. The opposite would mean that there exist quantum boxes that remain nonlocal even in the limit of infinitely many copies, in a way that is washed out by the second coarse graining of ML. On the other hand, we do not know whether in some slices L_∞^{MB} comes closer to the quantum set than $\mathcal{Q}_1$ or than $\mathcal{Q}_{1+AB}$. If L_∞^{MB} were equal to $\mathcal{Q}_1$, the second coarse graining of ML does not play any role. If $L_\infty^{MB} \supsetneq \mathcal{Q}_{1+AB}$, many-box locality is a strictly weaker principle than "almost-quantum."

Other technical features of the L_N^{MB} sets, suggested by numerical studies, remain conjectural. First, all the relevant inequality that detects the nonlocality of N-box distributions seems to be liftings of the CHSH inequality; we have not found an example where no liftings of CHSH is violated while a genuine d-outcome Bell inequality is. Second, the inclusion $L_N^{MB} \subseteq L_{N+2}^{MB}$ seems to hold for N both even and odd in all slices that we studied.

APPENDIX: EVALUATION OF $g(\mu)$

In this section, we provide a detailed description of the evaluation of $g(\mu)$.

First, from Eq. (19), it is easy to conclude that $\mathcal{F}_d^{-1}[\mathcal{J}](k,l) = 0$ for k or l even, and

$$\mathcal{F}_d^{-1}[\mathcal{J}](k,l) = \frac{16\omega^{k+l}}{d^2(1-\omega^k)(1-\omega^l)} \quad \text{(A1)}$$

for k,l odd.

Recall the definition of $g(\mu)$ from Eqn. (18), we have

$$g(\mu) = \frac{16}{d^2 4^{d-1}} \sum_{k,l=\text{odd}} \left((1+\omega^k)(1+\omega^l) \right.$$

$$+ (1-\omega^k)(1-\omega^l)\mu)^{d-1} \frac{\omega^{k+l}}{(1-\omega^k)(1-\omega^l)}$$

$$= \frac{16}{d^2 4^{d-1}} \sum_{k,l=\text{odd}} \sum_{m=0}^{d-1} \binom{d-1}{m} \mu^m (1-\omega^k)^{m-1}$$

$$\times (1-\omega^l)^{m-1}(1+\omega^k)^{d-m-1}(1+\omega^l)^{d-m-1}\omega^{k+l}.$$

Here, we exchange the order of sums, and k,l are symmetric, then we have

$$g(\mu) = \frac{16}{d^2 4^{d-1}} \sum_{m=0}^{d-1} \binom{d-1}{m} \mu^m S^2(d,m), \quad \text{(A2)}$$

where

$$S(d,m) = \sum_{k=\text{odd}}^{d-1} (1-\omega^k)^{m-1}(1+\omega^k)^{d-m-1}\omega^k. \quad \text{(A3)}$$

In the following, we aim to simplify $S(d,m)$. First we focus on the case of $m = 0$ and expand $(1+\omega^k)^{d-1}$ in the binomial form. Then, we have

$$S(d,0) = \sum_{k=\text{odd}}^{d-1} \sum_{t=0}^{d-1} \binom{d-1}{t} \frac{\omega^{k(t+1)}}{1-\omega^k}$$

$$= \sum_{t=0}^{d-1} \binom{d-1}{t} \sum_{k=\text{odd}}^{d-1} \frac{\omega^{k(t+1)}}{1-\omega^k}.$$

We apply $\binom{d-1}{t} = \binom{d-1}{d-t-1}$, and obtain that

$$S(d,0) = \sum_{t=0}^{d/2-1} \binom{d-1}{t} \left(\sum_{k=\text{odd}}^{d-1} \frac{\omega^{k(t+1)} + \omega^{k(d-t)}}{1-\omega^k} \right)$$

$$= \sum_{t=0}^{d/2-1} \binom{d-1}{t} \cdot 0 = 0. \quad \text{(A4)}$$

The above equation holds since on the one hand the sum of $(\omega^{k(t+1)} + \omega^{k(d-t)})/(1-\omega^k)$ and its conjugate is 0, which implies that its real part is 0; on the other hand, its imaginary part is 0 because $S(d,0)$ must be a real number.

Then for $m \geqslant 1$, we rewrite $(1-\omega^k)^{m-1}$ and $(1-\omega^k)^{d-1-m}$ in the binomial form, then exchange the order of sum. Afterwards, we know that

$$S(d,m) = \sum_{s=0}^{m-1} \sum_{t=0}^{m-1} (-1)^s \binom{m-1}{s} \binom{d-m-1}{t}$$

$$\times \left(\sum_{k=\text{odd}}^{d-1} \omega^{k(s+t+1)} \right)$$

$$= \sum_{s=0}^{m-1} \sum_{t=0}^{m-1} (-1)^s \binom{m-1}{t} \binom{d-m-1}{s}$$

$$\times \left(\frac{d}{2}(\delta_{s+t+1=0} - \delta_{t=d/2-s-1}) \right)$$

$$= \frac{d}{2} \sum_{s=0}^{m-1} (-1)^{s+1} \binom{m-1}{s} \binom{d-m-1}{d/2-s-1}, \quad \text{(A5)}$$

Here, Eq. (A5) holds since

$$\sum_{k=\text{odd}}^{d-1} \omega^{kt} = \frac{d}{2}(\delta_{t=0} - \delta_{t=d/2}), \quad 1 \leqslant t \leqslant d.$$

Now the summation over s can be evaluated in Mathematica:

$$S(d,m) = -\frac{d}{2} \frac{2^{d-2}\Gamma\left(\frac{d-m}{2}\right)}{\Gamma\left(\frac{d}{2}\right)\Gamma\left(1-\frac{m}{2}\right)}. \quad \text{(A6)}$$

Finally, we obtain that

$$g(\mu) = \sum_{m=\text{odd}}^{N} C(d,m)\mu^m. \quad \text{(A7)}$$

Third, we introduce two properties of Gamma function to calculate $C(\infty,m)$. One is called as the duplication formula:

$$\Gamma(\eta)\Gamma\left(\eta+\frac{1}{2}\right) = 2^{1-2\eta}\sqrt{\pi}\Gamma(2\eta). \quad \text{(A8)}$$

Another one is a equivalent condition:

$$\lim_{n\to\infty} \frac{\Gamma(n+\eta)}{\Gamma(n)n^\eta} = 1. \quad \text{(A9)}$$

Subsequently, we conclude Eq. (21) by applying the duplication formula and the equivalent condition. That is,

$$C(\infty,m) = \lim_{d\to\infty} C(d,m)$$

$$= \frac{16\Gamma^2(m)}{\Gamma(m+1)\Gamma^2\left(\frac{m+1}{2}\right)} \lim_{d\to\infty} \frac{\Gamma(d)\Gamma(d-m)}{4^d \Gamma^2\left(\frac{d}{2}\right)\Gamma^2\left(\frac{d-m+1}{2}\right)}$$

$$= \frac{16\Gamma\left(\frac{m}{2}\right)}{m\sqrt{\pi}2^{1-m}\Gamma\left(\frac{m+1}{2}\right)} \lim_{d\to\infty} \frac{\Gamma\left(\frac{d+1}{2}\right)\Gamma\left(\frac{d-m}{2}\right)}{2^{2+m}\pi\Gamma\left(\frac{d}{2}\right)\Gamma\left(\frac{d-m+1}{2}\right)}$$

$$= \frac{2\Gamma\left(\frac{m}{2}\right)}{m\pi^{3/2}\Gamma\left(\frac{m+1}{2}\right)}. \quad \text{(A10)}$$

Note that only odd m needs to be considered. In this way, Eq. (21) is obtained by the definition of the Gamma function.

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