Uncertainty and symmetry bounds for the quantum total detection probability

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We investigate a generic discrete quantum system prepared in state $|\psi_{\text{in}}\rangle$ under repeated detection attempts, aimed to find the particle in state $|d\rangle$, for example, a quantum walker on a finite graph searching for a node. For the corresponding classical random walk, the total detection probability P_{det} is unity. Due to destructive interference, one may find initial states $|\psi_{\text{in}}\rangle$ with $P_{\text{det}} < 1$. We first obtain an uncertainty relation which yields insight on this deviation from classical behavior, showing the relation between P_{det} and energy fluctuations: $\Delta P \text{Var}[\hat{H}]_d \geq |\langle d | [\hat{H}, \hat{D}] | \psi_{\text{in}} \rangle|^2$, where $\Delta P = P_{\text{det}} - |\langle \psi_{\text{in}} | d \rangle|^2$ and $\hat{D} = |d\rangle\langle d|$ is the measurement projector. Secondly, exploiting symmetry we show that $P_{\text{det}} \leq 1/\nu$, where the integer ν is the number of states equivalent to the initial state. These bounds are compared with the exact solution for small systems, obtained from an analysis of the dark and bright subspaces, showing the usefulness of the approach. The upper bound works well even in large systems, and we show how to tighten the lower bound in this case.

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The dynamics of quantum systems that evolve unitarily but are subject to repeated monitoring using projective measurements have gained recent attention partly driven by increasing interest in quantum information [1–19]. The investigation of a single particle on a finite graph, i.e., a quantum walker [20–29], prepared and detected in the states $|\psi_{\text{in}}\rangle$ and $|d\rangle$, respectively, was promoted as a basic model in the context of quantum search [1,2,4,20,30–38]. Both states may (or may not) be localized in the graph node basis. The key quantifier of this process of unitary evolution mingled with wave function collapse is the total detection probability P_{det} . This is the fraction of particles in the statistical ensemble which are eventually detected. Previous work [1,39–42] showed how nondetectable initial states (*dark* states) may render the quantum search impossible, such that $P_{\text{det}}(\psi_{\text{in}}) = 0$. Likewise, a general initial condition may yield a total detection probability P_{det} less than unity, in stark contrast to a classical random search on the same structure for which P_{det} is always one [43,44]. However, while P_{det} is known explicitly for some specific examples [1,12], general principles leading to its estimation are still missing. In this paper we provide three insights on P_{det} : an uncertainty principle, symmetry arguments, and an exact solution.

The exact solution relies on decomposing the Hilbert space into mutually orthogonal dark and bright subspaces. These are examples of Zeno subspaces [41,42,45], a dynamical separation of the total Hilbert space, which usually appears in the presence of singular coupling or in *rapidly* measured systems. Here, they are relevant for arbitrary detection frequencies

possibly far away from the regime of the quantum Zeno effect [46,47]. This formal solution requires a full diagonalization of the Hamiltonian, involving considerable effort. Therefore, we also present bounds on P_{det} , that give physical insight into the problem. The lower bound is an uncertainty relation and the upper bound exploits symmetry.

Heisenberg's uncertainty relation is probably the most profound signature of quantum reality's deviations from classical Newtonian mechanics [48]. Here we show something very different: how P_{det} of a quantum walk deviates from the corresponding probability of detecting a classical random walk, which is unity. Our uncertainty relation connects this deviation with energy fluctuations and the commutator of $\hat{H}$ and the measurement projector. It follows from the collapse postulate.

Symmetry and degeneracy play an important part in the physics of dark states and are a crucial mechanism leading to $P_{\text{det}} < 1$ [3]. Consider an initial state which is a superposition of two energy eigenstates, $|\psi_{\text{in}}\rangle = N(\langle d|E\rangle|E'\rangle - \langle d|E'\rangle|E\rangle)$. When $|E\rangle$ and $|E'\rangle$ belong to the same energy level, i.e., $\hat{H}|E\rangle = E|E\rangle$ and $\hat{H}|E'\rangle = E|E'\rangle$, the time evolution of $|\psi_{\text{in}}\rangle$ is a simple phase factor e^{-itE} (here $\hbar = 1$). It follows that $\langle d|e^{-it\hat{H}}|\psi_{\text{in}}\rangle = 0$ forever. Hence this is a dark state. Importantly, degeneracy is a signature of $\hat{H}$'s symmetry, so dark states are deeply connected to the symmetry of the problem. Below we exploit this to find a simple bound on P_{det} .

Model. We consider quantum systems with discrete states, e.g., quantum walks on finite graphs. The system is initially in state $|\psi_{\text{in}}\rangle$. We use projective stroboscopic measurements at times $\tau, 2\tau, \dots$ in an attempt to detect the particle in state $|d\rangle$; see Fig. 1 and Refs. [5,12,13]. The detection could be performed on a node of the graph, though any state $|d\rangle$ is acceptable. Between the measurement attempts the evolution is unitary, described with $\hat{U}(\tau) = \exp(-i\tau\hat{H})$. The string of measurements yields a sequence no, no, $\dots$ and in the n th attempt a yes. The time $n\tau$ marks the first detected arrival time in state $|d\rangle$. In some measurement sequences, the particle

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FIG. 1. A quantum walker resides on the nodes of a graph and moves unitarily along its edges, here a ring (left). Every τ time units a detector tests whether the particle is at node $|d\rangle$ collapsing the wave function (right). The first successful detection attempt (click) defines an arrival time and stops the protocol. P_{det} is the probability that the detector clicks at all. Here, the initial state is localized.

is not detected at all ($n = \infty$). Each measurement satisfies the collapse postulate [49]: if the wave function is $|\psi\rangle$ right before measurement, the amplitude of detection is $\langle d|\psi\rangle$. Successful detection terminates the experiment. Unsuccessful detection zeros the amplitude $\langle d|\psi\rangle$, the wave function is renormalized, and the unitary evolution continues until the next measurement. Mathematically, the measurement is described by the projector $\hat{D} = |d\rangle\langle d|$ [see Eq. (8) below]. Repeating this protocol many times, P_{det} is the fraction of runs in which the detector clicked yes at all. It is closely related to the Pólya number and the recurrence of the walk [5,29,50]. If $P_{\text{det}} < 1$, the mean $\langle n \rangle$ diverges and the corresponding search problem is ill posed. Furthermore, the time-of-arrival problem [51–56] can also be tackled using stroboscopic measurements. General quantum walks have been experimentally realized photonically [21,28,57], with trapped ions [23] and in optical lattices [22,58]. Reference [59] reported the measurement of P_{det} in a photonic walk.

Uncertainty relation. Reference [1] showed how the detector’s action separates the Hilbert space of a finite system into a “bright” and a “dark” subspace: $\mathcal{H} = \mathcal{H}_B \oplus \mathcal{H}_D$. Any initial condition within the bright/dark subspace is detected with probability one/zero, respectively. We present a proof of this fundamental result in Ref. [60]. For the dark, as for the bright space, we can find a basis in terms of the eigenstates of $\hat{H}$, denoted $\{|E_j^B\rangle\}$ and $\{|E_j^D\rangle\}$, respectively. The subspaces are thus orthogonal and invariant under $\hat{H}$ and $\hat{D}$.

Reference [5] [and Eq. (13) below] showed that the particular state $|\psi_{\text{in}}\rangle = |d\rangle$ is bright. Since $|d\rangle$ is bright, it is orthogonal to every dark state, i.e., $\langle E_j^D|d\rangle = 0$. Therefore, $\hat{H}^s|d\rangle$ is also bright, because $\langle E_j^D|\hat{H}^s|d\rangle = (E_j)^s \langle E_j^D|d\rangle = 0$, where s is any positive integer. P_{det} is the overlap of $|\psi_{\text{in}}\rangle$ with $\mathcal{H}_B$, so given any orthonormal basis $\{|\beta_l\rangle\}$ of $\mathcal{H}_B$ we have

$$P_{\text{det}} = \sum_l |\langle \beta_l | \psi_{\text{in}} \rangle|^2. \quad (1)$$

To obtain a useful bound, we create a pair of orthonormal bright states from $|d\rangle$ and $\hat{H}^s|d\rangle$:

$$|\beta_1\rangle = |d\rangle, \quad |\beta_2\rangle = N[\mathbb{1} - |d\rangle\langle d|]\hat{H}^s|d\rangle. \quad (2)$$

The normalization $|N|^{-2} = \text{Var}[\hat{H}^s]_d = \langle d|\hat{H}^{2s}|d\rangle - [\langle d|\hat{H}^s|d\rangle]^2$ is related to the energy fluctuations in the detected state. As each term in the sum Eq. (1) is non-negative, a lower

bound is reached by omitting some of the bright states:

$$P_{\text{det}} \geq |\langle \beta_1 | \psi_{\text{in}} \rangle|^2 + |\langle \beta_2 | \psi_{\text{in}} \rangle|^2. \quad (3)$$

We now define the difference between the probability of detection after repeated measurements from the probability of detection at preparation:

$$\Delta P = P_{\text{det}} - |\langle d | \psi_{\text{in}} \rangle|^2. \quad (4)$$

Using Eqs. (2) and (3) we find

$$\Delta P \text{Var}[\hat{H}^s]_d \geq |\langle d | [\hat{H}^s, \hat{D}] | \psi_{\text{in}} \rangle|^2. \quad (5)$$

Figure 2 shows this uncertainty bound $P_{\text{det}} \geq P_{\text{det}}^{\text{unc}}$ for several graphs. Some remarks are in place. First, after the successful detection, the system is in its final state $|\psi_f\rangle = |d\rangle$.¹ This means that we may rewrite the uncertainty principle, say for $s = 1$, as

$$\Delta P \text{Var}[\hat{H}]_{\psi_f} \geq |\langle \psi_f | [\hat{H}, \hat{D}] | \psi_{\text{in}} \rangle|^2. \quad (6)$$

The fluctuations of energy are actually in the *final state* of the particle. So, Eqs. (5) and (6) are relations between the initial condition and the finally selected state. Importantly, after the system is projected into its final state, and the detector turned off, the fluctuation of energy $\text{Var}[\hat{H}]_{\psi_f}$ is a constant of motion. The energy measurement can be made at any time after the detection. Notably, Eqs. (5) and (6) do not depend on τ .

Path-counting approach. We consider the standard quantum walk with $\hat{H} = \hat{A}$, where $\hat{A}$ is the adjacency matrix of some graph. Hence there are no on-site energies, and all bonds in the system are identical, namely $\hat{H}_{ii} = 0$ and $\hat{H}_{ij} = 1$ if site i and j are connected and zero otherwise. We are interested in a particle starting on vertex $|\psi_{\text{in}}\rangle = |r\rangle$ and the detection on another vertex $|d\rangle$. Notice that $\langle d | \hat{H}^s | r \rangle = \mathcal{N}_{r \rightarrow d}(s)$ is the number of paths of length s starting on $|r\rangle$ and ending at $|d\rangle$. Then using Eq. (5), we find

$$P_{\text{det}}(r) \geq P_{\text{det}}^{\text{unc}} = \frac{|\mathcal{N}_{r \rightarrow d}(s)|^2}{\mathcal{N}_{d \rightarrow d}(2s) - [\mathcal{N}_{d \rightarrow d}(s)]^2}. \quad (7)$$

We must choose s here larger or equal to the distance ξ between $|r\rangle$ and $|d\rangle$; otherwise, one gets the trivial $P_{\text{det}} \geq 0$.

Upper bound from symmetry. To complement our lower bound, we use a different approach. The detection probability is by definition $P_{\text{det}} = \sum_{n=1}^{\infty} |\varphi_n|^2$, where φ_n is the amplitude of first detection at the n th attempt [12]. This can be expressed as [8]

$$\varphi_n = \langle d | \hat{U}(\tau) [(\mathbb{1} - \hat{D}) \hat{U}(\tau)]^{n-1} | \psi_{\text{in}} \rangle. \quad (8)$$

Reading this right to left, we see that φ_n is given by the initial condition, followed by steps combining unitary evolution and attempted detection, of which the final, n th detection is successful. It is crucial for our discussion that φ_n is linear with respect to $|\psi_{\text{in}}\rangle$, so it obeys the superposition principle.

We are interested in the total detection probability starting from node $|r\rangle$ and detecting on another $|d\rangle$. In the system we have a set $\{|r_j\rangle\}_{j=1}^v$ of v states, which are equivalent to $|r\rangle$ and

¹Here and all along $|\psi\rangle$ denotes the state of the system/particle along the measurement process, e.g., in the initial of final state, while $|d\rangle$ is the detection state.

Features of Eq. (13). The exact formula exhibits some remarkable properties. We easily see that the initial states $|\psi_{\text{in}}\rangle = |d\rangle$ and $|\psi_{\text{in}}\rangle = N_s \hat{H}^s |d\rangle$ yield $P_{\text{det}} = 1$. Hence, as claimed earlier, these states are bright. Furthermore, the total detection probability is τ independent. The only exception, not considered here in depth, is when $|E_l - E_{l'}|\tau = 0 \bmod 2\pi$, for some pairs of energy levels. They are a unique feature of the stroboscopic detection protocol. These special τ 's are isolated, but still of interest since the statistics exhibit gigantic fluctuations and discontinuous behavior in their vicinity [5,62,63], related to partial revivals of the state function. More importantly, Eq. (13)'s τ independence ensures its general validity, even if one tampers with the detection protocol, for example, by sampling with a Poisson process. The reason is that any initial state $|\psi_{\text{in}}\rangle$ starting in the dark space has zero overlap with the detected state for $t \geq 0$. No measurement protocol can detect this state.

Figure 2 compares our main results, the uncertainty relation (5), and the symmetry bound (11), with the exact result (13) for small systems where the results are apparent to the eye. In some cases both bounds coincide and thus determine the exact results from elementary calculations instead of full diagonalization of $\hat{H}$. Experimental measurement of P_{det} as in Ref. [59] requires the system size to be small compared to the achievable decoherence-free observation time. This motivated our focus on small systems.

a. Large systems. We start discussing our results in large systems with the example of the B -dimensional hypercube. Here, each node is represented by a string of B bits, e.g., $|01011 \dots 0\rangle$, and each transition corresponds to flipping one bit. We detect on node $|d\rangle$ and start at any node $|r_\xi\rangle$ with ξ bits different from $|d\rangle$, i.e., ξ is the Hamming distance between the nodes. Remarkably, the upper bound works perfectly here, coinciding with the exact result $P_{\text{det}}(r_\xi) = 1/\nu = 1/\binom{B}{\xi} = P_{\text{det}}^{\text{sym}}$. What about the lower bound? Equation (7) yields [61]:

$$\frac{\xi! 2^{B-\xi}}{(2\xi-1)!! - [(\xi-1)!!]^2} \leq P_{\text{det}}(r_\xi) = \frac{1}{\nu} = \frac{1}{\binom{B}{\xi}}. \quad (14)$$

The second term in the denominator has to be omitted when ξ is odd. Several strategies to improve the lower bound are compared in the Supplemental Material (SM) [61]. Exploiting the shell structure of a graph leads to a much better lower bound.

b. Shell-state method. When the bright state $|d\rangle$ is localized, $\hat{H}|d\rangle$ is supported only on nearest neighbors of $|d\rangle$. We call those nodes the “first shell.” Similarly, $\hat{H}^2|d\rangle$ is a bright state supported on the next-nearest neighbors, the second shell, as well as $|d\rangle$ itself. Since the s th shell is only connected to the $(s \pm 1)$ th shells, we can construct a useful bright state $|\tilde{\beta}_\xi\rangle$ by the following strategy: we start with the zeroth and first shell states $|\tilde{\beta}_0\rangle := |d\rangle$ and $|\tilde{\beta}_1\rangle := \hat{H}|d\rangle$. Each subsequent state $|\tilde{\beta}_s\rangle$ is obtained from orthogonalizing $\hat{H}|\tilde{\beta}_{s-1}\rangle$ to $|\tilde{\beta}_s\rangle$ and $|\tilde{\beta}_{s-1}\rangle$. The procedure is terminated when $s = \xi$ and yields a state with large overlap in the ξ th shell. A lower bound is obtained from $P_{\text{det}} \geq P_{\text{det}}^{\text{shell}} := |\langle \tilde{\beta}_\xi | \psi_{\text{in}} \rangle|^2$. For our nearest-

neighbor hopping $\hat{H}$ on the hypercube, $|\tilde{\beta}_\xi\rangle = \sum_{r_\xi} |r_\xi\rangle / \sqrt{\nu}$, where $\nu = \binom{B}{\xi}$. This is the relevant AUS for r_ξ . Hence lower and upper bound coincide: $P_{\text{det}}^{\text{shell}} = 1/\nu \leq P_{\text{det}} \leq 1/\nu = P_{\text{det}}^{\text{sym}}$.

We also successfully applied the shell-state method to a system with two loops and to one with nonuniform coupling constants [61]. In many situations, the shell-state method gives the exact, simply computed result (e.g., those starred in Fig. 2). As a rule of thumb, $P_{\text{det}}^{\text{shell}}$ is exact, when $|d\rangle$ sits in a symmetry center of the system. More precisely, it is exact when the sequence $\{|\tilde{\beta}_s\rangle\}$ turns out to be fully orthogonalized. We will elaborate on this in [60]. Even when it is not exact, it gives a bound from $2\xi - 1$ orthogonalization operations. This is a huge advantage compared to the minimally necessary $\xi(\xi + 1)/2$ operations in a full Gram-Schmidt procedure [16].

c. Disordered systems. Symmetries lead to tight, possibly exact bounds and remove the necessity of diagonalizing $\hat{H}$. In their absence, when irregularity has broken all degeneracy, Eq. (13) provides the value for P_{det} . Provided the system's spectrum is nondegenerate and $|d\rangle$ has overlap with all eigenstates, the exact result predicts classical behavior: $P_{\text{det}} = 1$. Thus the bounds are not necessary and their performance of rather academic interest. Generically, one obtains $\nu = 1$ giving $P_{\text{det}} = P_{\text{det}}^{\text{sym}} = 1$ from Eqs. (11) and (13). Assuming the eigenstates are extended and span the whole system, one expects that the uncertainty bound behaves like $P_{\text{det}}^{\text{unc}} \sim 1/D$. In the SM, this is demonstrated for random Hamiltonians from the Gaussian unitary ensemble [61]. We also show numerically that the shell-state bound performs polynomially better $P_{\text{det}}^{\text{shell}} \sim D^{-0.75}$.

To conclude, we have used symmetry and an uncertainty principle to find upper and lower bounds on the detection probability. These bounds show a symmetry-induced restriction to well-posed quantum search which requires $P_{\text{det}} = 1$. We showed that P_{det} is surprisingly almost independent of τ . Our results also apply to discrete-time quantum walks as the symmetries and spectral properties can equivalently be obtained from the evolution operator.² Furthermore, they are relevant to non-Hermitian models [7,16,42,55]. We presented the shell-state method, which improves on the uncertainty principle. Our methods perform well in systems with a certain degree of symmetry; exactly those from which one expects a significant quantum computational speedup. The symmetry and uncertainty bounds often allow one to avoid the Hamiltonian's diagonalization and provide a physical interpretation to the value of P_{det} . For very irregular, nondegenerate systems, the answer is immediately provided by the exact formula, making diagonalization again obsolete.

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²Then lower bounds must be computed from states of the form $\hat{U}^s|d\rangle$, where $\hat{U}$ is the walk's unitary step operator.

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