Probe readout and quantum-limited measurements

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We consider the readout process on a probe made of N qubits (two-level systems) in a quantum single-parameter estimation scheme. The parameter-dependent evolution of the probe as well as the measurements that are done for readout are assumed to be fixed. We find the optimal initial states of the probe that will saturate the quantum Cramér-Rao bound under these conditions. The relation between the optimal state of the N-qubit probe and that of the one-qubit probe is obtained for both entangling and nonentangling dynamics for the probe qubits. We study the limitations placed on the optimal initial state of the probe and on the achievable measurement uncertainty by the restrictions on the readout procedure.

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I. INTRODUCTION

In modeling quantum limited measurements, in particular single-parameter estimation, a quantum system that acts as the probe interacts with the measured system in a way that depends on the value of the parameter of interest [1–5]. Knowing the change in the state of the probe that is generated by a parameter-dependent Hamiltonian, an estimate of the value of the parameter is obtained. However, there is scope to fall into an infinite regression at this step in the modeling of the measurement because, after all, knowing the state of the probe means a measurement of the parameters that describe the state of the probe. So the question of what or who measures the probe, and how, is immediately brought up. Part of the answer lies in the observation that complete knowledge about the state of the quantum probe is not required to obtain the value of the measured parameter. Furthermore a wide variety of quantum limited measurement schemes can be mapped on to one in which the quantum probe is assembled by putting together a large number of elementary quantum systems with low-dimensional Hilbert spaces [6]. For instance, without loss of generality, one can assume that the probe is made up of N two-level quantum systems or qubits [1]. The results of von Neumann-type projective measurements [7] on to the small, countable, set of basis states of the individual probe units are sufficient to estimate the possibly irrational value of the parameter of interest to any degree of accuracy. The accuracy is dependent on the nature of the quantum probe, the number of elementary units in it, and the number of times the probe is applied. To avoid confusion with the measurement of the parameter, we will refer to the measurements on the probe itself as a readout of the probe.

The readout process is not fully understood either. This is evidenced by several decades of discussions and literature on topics ranging from the collapse of the wave function to decoherence and pointer states [8,9]. However, there is not much debate as to whether such readouts can be performed in the laboratory or not, since it indeed is routinely done. Even more sophisticated readouts that include positive operator valued measures (POVMs) can be done in the laboratory, and they ultimately boil down to making a larger number of projective measurements on the probe [10,11].

The motivation for this paper is the observation that not many types of readouts are possible given the available technology in the design of a quantum limited metrology experiment. For instance, in precision measurements using interferometers and light, the readout of the state of the light at the output ports is often limited to photon counting [1,12–17]. There are several ways of using photon counting to accomplish readouts of parameters, other than photon number, associated with the state of the light in an interferometer, such as relative phase, by combining known transformations of the state with photo counts [18–20]. In particle-based metrology protocols like Ramsey interferometry as well, the output state of the spins or atoms is subject to either Stern-Gerlach-type or fluorescence-type readouts [21,22].

Given the restrictions on the types of readouts that are possible, we find the optimal input state of a quantum probe made of many qubits for a fixed readout procedure and for different choices for the parameter-dependent evolution of the probe. In the next section we review the quantum Cramér-Rao bound that forms the basis for the formulation of the problem. In Sec. III the optimal input state for a nonentangling evolution is found. The optimal input state for an entangling evolution is discussed in Sec. IV followed by a discussion of our results in Sec. V.

II. SATURATING THE QUANTUM CRAMÉR-RAO BOUND

The quantum Cramér-Rao bound [23–26] gives the theoretical lower bound on the measurement uncertainty in the estimate of a single-parameter X as

$$\delta X \geqslant \frac{1}{\sqrt{\mathcal{F}(X)}} \geqslant \frac{1}{\sqrt{\langle \mathcal{L}^2 \rangle}}, \tag{1}$$

where $\mathcal{F}$ is the quantum Fisher information. The symmetric logarithmic derivative operator $\mathcal{L}$ is defined implicitly by the equation

$$\frac{1}{2}(\mathcal{L}\rho_X + \rho_X \mathcal{L}) = \frac{d\rho_X}{dX} \equiv \rho'_X. \tag{2}$$

The measurement uncertainty δX is quantified using the units corrected, root-mean-squared deviation of the estimate of X

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from its true value:

$$\delta X = \frac{X_{\rm est}}{|d\langle X_{\rm est}\rangle_X/dX|} - X.$$

Let a general readout on the probe be described by a POVM with a one-parameter family of elements $E(\xi)$ such that

$$\int d\xi\, E(\xi) = \mathbb{1}.$$

Let $p(\xi|X) = {\rm tr}[E(\xi)\rho_X]$ be the measured probabilities for various outcomes of the POVM when the true value of the measured parameter is X. As shown in Ref. [23], the quantum Fisher information is given by

$$\mathcal{F} = \max_{\{E(\xi)\}} F, \tag{3}$$

where F is the classical Fisher information computed from the probability distribution for the measurement outcomes as

$$F = \int d\xi\; p(\xi|X)\left[\frac{d\ln p(\xi|X)}{dX}\right]^2 = \int d\xi\; \frac{1}{p(\xi|X)}\left[\frac{dp(\xi|X)}{dX}\right]^2.$$

The maximization in the Eq. (3) is over all possible readout procedures (POVMs) on the probe. Such a maximization is indeed a daunting task and even if it can be done, implementing the POVM that maximizes the Fisher information, thereby minimizing the measurement uncertainty, may, in all likelihood, be impossible to implement in the laboratory. The second inequality in (1) circumvents the maximization problem by placing an upper bound on $\mathcal{F}$ in terms of the expectation value of the square of the symmetric logarithmic derivative operator $\mathcal{L}$. This expectation value can be computed directly from the initial state of the probe and its parameter-dependent dynamics, independent of the readout procedure. In the context of the current paper it is worth reprising the sequence of steps detailed in Ref. [23] that lead to this upper bound. We have

$$\begin{aligned} F &= \int d\xi \frac{1}{{\rm tr}[E(\xi)\rho_X]}\left[\frac{d}{dX}{\rm tr}[E(\xi)\rho_X]\right]^2, \\ &= \int d\xi \frac{1}{{\rm tr}[E(\xi)\rho_X]}\{{\rm tr}[E(\xi)\rho_X']\}^2, \\ &= \int d\xi \frac{1}{{\rm tr}[E(\xi)\rho_X]}\left[\frac{1}{2}{\rm tr}\big[E(\xi)\mathcal{L}\rho_X + E(\xi)\rho_X\mathcal{L}\big]\right]^2, \\ &= \int d\xi \frac{1}{{\rm tr}[E(\xi)\rho_X]}({\rm Re}\{{\rm tr}[\rho_X E(\xi)\mathcal{L}]\})^2, \end{aligned} \tag{4}$$

where we have used Eq. (2), the cyclic nature of the trace and the hermiticity of $\mathcal{L}$ and $E(\xi)$ to obtain the last equality in the equation above. Our focus is on the case where the second inequality in (1) is saturated. When

$${\rm Im}\{{\rm tr}[\rho_X E(\xi)\mathcal{L}]\} = 0, \tag{5}$$

we have

$$\begin{aligned} F &= \int d\xi \frac{1}{{\rm tr}[E(\xi)\rho_X]}|{\rm tr}[\rho_X E(\xi)\mathcal{L}]|^2 \\ &= \int d\xi \left|{\rm tr}\left[\frac{\sqrt{\rho_X E(\xi)}}{\sqrt{{\rm tr}[E(\xi)\rho_X]}}\sqrt{E(\xi)}\mathcal{L}\sqrt{\rho_X}\right]\right|^2. \end{aligned} \tag{6}$$

Using the Schwarz inequality, $|\langle x,y\rangle|^2 \leqslant \langle x,x\rangle\langle y,y\rangle$ for the trace norm, we can write an upper bound on the classical Fisher information as

$$F \leqslant \int d\xi\; {\rm tr}\left\{\frac{E(\xi)\rho_X}{{\rm tr}[E(\xi)\rho_X]}\right\}{\rm tr}[E(\xi)\mathcal{L}^2\rho_X]. \tag{7}$$

The Schwarz inequality is saturated when

$$\sqrt{E(\xi)\rho_X} = \lambda_\xi\sqrt{E(\xi)}\mathcal{L}\sqrt{\rho_X}, \tag{8}$$

for all ξ, where λ_ξ are constants [see Eq. (11)] that depend only on ξ. Assuming Eq. (8) holds, we get

$$\mathcal{F} = \int d\xi\; {\rm tr}[E(\xi)\mathcal{L}^2\rho_X] = {\rm tr}(\mathcal{L}^2\rho_X) = \langle\mathcal{L}^2\rangle, \tag{9}$$

and the second inequality in (1) is saturated. Equations (5) and (8) furnish the conditions on the the readout procedure (POVM) such that a quantum probe in the initial state ρ_X that undergoes the parameter-dependent evolution implicitly contained in $\mathcal{L}$ will attain the quantum Cramér-Rao bound. Multiplying Eq. (8) by $\sqrt{E(\xi)}$ from the left and $\sqrt{\rho_X}$ from the right we obtain

$$E(\xi)\left(\mathcal{L} - \frac{1}{\lambda_\xi}\mathbb{1}\right)\rho_X = 0, \tag{10}$$

for any ρ_X. The above equation is satisfied if the readout is taken to be a set of orthogonal projectors, $E(\xi)$, on to the complete set of orthonormal eigenstates of $\mathcal{L}$. The constants λ_ξ are therefore inverses of the eigenvalues of $\mathcal{L}$ with

$$\frac{1}{\lambda_\xi} = \frac{{\rm tr}[E(\xi)\mathcal{L}\rho_X]}{{\rm tr}[E(\xi)\rho_X]}. \tag{11}$$

Condition (5) implies that λ_ξ are real.

In situations where the readout procedure is fixed due to practical reasons or otherwise, one can now formulate the problem of finding the optimal initial state of the probe ρ_X as follows. We limit ourselves to the rather common case where the readout is a complete set of orthogonal projective measurements. Even if the readout is realized by a more general POVM, we assume that a suitable Neumark extension [10,11] has been used to reduce it to complete set of orthonormal projectors. Given this complete set of orthogonal projectors denoted as $\{|\xi\rangle\}$, we can construct the symmetric logarithmic derivative operator corresponding to this readout procedure as

$$\mathcal{L} = \sum_\xi \frac{1}{\lambda_\xi}|\xi\rangle\langle\xi|.$$

The optimal initial state of the probe ρ_X for this readout satisfies the equation

$$\tfrac{1}{2}(\mathcal{L}\rho_X + \rho_X\mathcal{L}) = \rho' = -i[H,\rho_X], \tag{12}$$

assuming that the parameter-dependent evolution of the probe is generated by the Hamiltonian

$$H_{\rm probe} = XH. \tag{13}$$

In the following we will investigate the solutions of Eq. (12) for two choices of H, one that entangles the probe qubits and one that does not. The number of probe qubits N is the resource against which the performance of the measurement scheme is calibrated. The discussion here is quite general and can be applied to the case where the number of probe units itself is not the most important resource. For instance, in interferometry with light the circulating power in the interferometer and not the number of photons is the crucial, limited resource [12]. In other words, in our discussion, N is essentially a place holder for the relevant resource for each measurement scheme, and a mapping between the real resource and N can be found quite easily for most quantum limited metrology schemes.

III. NONENTANGLING EVOLUTION OF THE PROBE QUBITS

Let the parameter-independent part of the Hamiltonian in (13) that governs the time evolution of the N-qubit probe have the form

$$H = \sum_{j=1}^{N} h^{(j)}, \tag{14}$$

where $h^{(j)}$ is an operator that acts only on the jth qubit. By construction the time evolution generated by this Hamiltonian will not lead to entanglement between the probe qubits. Without loss of generality, using the freedom to define a basis independently for the two-dimensional Hilbert spaces of each of the individual qubits, we choose all the single-qubit operators to be identical and equal to

$$h^{(j)} = \tfrac{1}{2}\sigma_3^{(j)}.$$

Once we choose to define the basis for the Hilbert space of each qubit so that the evolution Hamiltonian is as given above, we make the assumption that the readout procedure is limited due to practical considerations or otherwise to projective measurements along the states $|+\rangle$ and $|-\rangle$ for each qubit where

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle). \tag{15}$$

The symmetric logarithmic derivative operator for which this readout procedure saturates the quantum Cramér-Rao bound is then

$$\mathcal{L} = \sum_{j_1,j_2\ldots j_N} \frac{1}{\lambda_{j_1 j_2 \ldots j_N}} |j_1 j_2 \ldots j_N\rangle\langle j_1 j_2 \ldots j_N|,$$

where $j_l = \{+,-\}$. The optimal state of the N-qubit probe corresponding to this dynamics and readout can now be found by solving Eq. (12).

We first look at the case where the probe is made of a single qubit, i.e., $N = 1$. In this case

$$\mathcal{L} = \frac{1}{\lambda_+}|+\rangle\langle+| + \frac{1}{\lambda_-}|-\rangle\langle-|.$$

We write an arbitrary state of the probe as

$$\rho_X = \tfrac{1}{2}(\mathbb{1} + a_i\sigma_i),$$

where σ_i, $i = 1,2,3$ are the Pauli matrices and the dependence of the state on X is hidden in the dependence of the coefficients a_i on the estimated parameter. Using

$$|+\rangle\langle+| = \tfrac{1}{2}(\mathbb{1} + \sigma_1) \quad \text{and} \quad |-\rangle\langle-| = \tfrac{1}{2}(\mathbb{1} - \sigma_1),$$

and the anticommutation relations of the Pauli matrices we have

$$\begin{aligned}\frac{1}{2}\{\mathcal{L},\rho_X\} &= \frac{1}{4}\bigg[\left(\frac{1+a_1}{\lambda_+} + \frac{1-a_1}{\lambda_-}\right)\mathbb{1} + \left(\frac{1+a_1}{\lambda_+} - \frac{1-a_1}{\lambda_-}\right)\sigma_1 \\ &\quad + \left(\frac{1}{\lambda_+} + \frac{1}{\lambda_+}\right)a_2\sigma_2 + \left(\frac{1}{\lambda_+} + \frac{1}{\lambda_+}\right)a_3\sigma_3\bigg]\end{aligned} \tag{16}$$

and

$$-i[H,\rho_X] = -\tfrac{1}{2}(a_2\sigma_1 - a_1\sigma_2). \tag{17}$$

Inserting Eqs. (16) and (17) into Eq. (2) we find a solution as

$$\frac{1}{\lambda_+} = -\frac{1}{\lambda_-} = -a_2, \quad \text{with} \quad a_1 = 0. \tag{18}$$

Since a_3 does not appear in the right side of the equation, we are free to choose its value depending on the available state preparation procedure for the probe qubit. Using Eq. (18) we have

$$\mathcal{L} = -a_2|+\rangle\langle+| + a_2|-\rangle\langle-| = -a_2\sigma_1.$$

The quantum Fisher information is therefore

$$\mathcal{F} = \langle\mathcal{L}^2\rangle = \mathrm{tr}\big(a_2^2\mathbb{1}\rho\big) = a_2^2.$$

The choice, $a_2 = \pm 1$ maximizes $\mathcal{F}$ and positivity of the state of the probe qubit now requires that $a_3 = 0$. So we find two possible optimal states of the one-qubit probe for the given dynamics and readout as

$$\tilde{\rho}_X = \tfrac{1}{2}(\mathbb{1} \pm \sigma_2). \tag{19}$$

The results obtained so far are not anything new or unexpected. In Ramsey interferometers [22,27] using atoms with two effective states in play forming qubits, the effective evolution of the probe units is modeled as rotations about the σ_3 axis in the Bloch sphere while the qubits themselves are initialized along the σ_1 or σ_2 directions. The optimal readout is then measurements on the individual probe qubits along σ_2 or σ_1 directions, respectively. The point of the preceding discussion is primarily to illustrate the means of obtaining the optimal state of the probe given that the readout is fixed.

For dynamics generated by a nonentangling Hamiltonian of the form given in Eq. (14), it is known that the Heisenberg limited scaling of $1/N$ is obtained for a "Schrödinger cat" state that is highly entangled [3–5]. However, this assumes the ability to do a phase kick-back operation after the parameter-dependent evolution of the probe followed by projective measurements in order to implement, in effect, a readout on to a basis of entangled states. If we restrict the readout on each probe qubit to be along the basis given in (15), then we have to again use the approach discussed above to find the optimal initial state of a multiqubit quantum probe.

We briefly discuss the $N = 2$ case first. We have

$$\mathcal{L} = \frac{1}{\lambda_{++}}|++\rangle\langle++| + \frac{1}{\lambda_{+-}}|+-\rangle\langle+-| + \frac{1}{\lambda_{-+}}|-+\rangle\langle-+| + \frac{1}{\lambda_{--}}|--\rangle\langle--|$$

and

$$H^{(2)} = \tfrac{1}{2}(\sigma_3 \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_3).$$

Using the commutators and anticommutators for tensor products of Pauli operators given in [28], and assuming that the initial state of the two qubits, $\rho_X^{(2)}$ has the generic form

$$\rho_X^{(2)} = \tfrac{1}{4}(\mathbb{1} \otimes \mathbb{1} + a_i\sigma_i \otimes \mathbb{1} + b_j \mathbb{1} \otimes \sigma_j + c_{ij}\sigma_i \otimes \sigma_j),$$

we obtain 16 algebraic equations (see Appendix A for details) from Eq. (12) by equating coefficients of corresponding operators. It is worth noting that the Schrödinger cat states,

$$|\Phi_\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle),$$

with the corresponding density matrices

$$\rho_\pm^{(2)} = \tfrac{1}{4}(\mathbb{1} \otimes \mathbb{1} + \sigma_1 \otimes \sigma_1 \pm \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3),$$

are not solutions of the equations we obtain. This again is symptomatic of the restriction on the readout procedure we have imposed. On the other hand it is straightforward to verify, as is done in Appendix A, that

$$\tilde{\rho}_X^{(2)} = \tilde{\rho}_X \otimes \tilde{\rho}_X$$

is a solution, where $\tilde{\rho}_X$ is the optimal state of the single-qubit probe obtained in Eq. (19). We find that

$$\mathcal{L} = -2|++\rangle\langle++| + 2|--\rangle\langle--| = -\sigma_1 \otimes \mathbb{1} - \mathbb{1} \otimes \sigma_1,$$

so that

$$\mathcal{F} = \langle \mathcal{L}^2 \rangle = 2\langle \mathbb{1} \otimes \mathbb{1} + \sigma_1 \otimes \sigma_1 \rangle = 2 = 4\langle \Delta^2 H^{(2)} \rangle.$$

Generalizing to N qubits we again find that

$$\tilde{\rho}_X^{(N)} = \tilde{\rho}_X^{\otimes N}$$

is a solution of Eq. (12) with

$$\frac{1}{\lambda_{j_1 j_2 \cdots j_N}} = \frac{1}{\lambda_{j_1}} + \frac{1}{\lambda_{j_2}} + \cdots + \frac{1}{\lambda_{j_N}}, \quad j_l = \{+,-\}.$$

Detailed proofs of these results are given in Appendices A 1 and A 2. Significantly, we see that $\langle \mathcal{L}^2 \rangle$ scales as N rather than as N^2. So one does not reach the Heisenberg limited scaling of $1/N$ for the linear, nonentangling, parameter-dependent dynamics of the quantum probe.

The main point of the preceding discussion on a particular example of nonentangling dynamics is to highlight the fact that with a restricted readout procedure, it might not be possible to go beyond the shot-noise-limited scaling of $1/\sqrt{N}$ for the measurement uncertainty even if the ability to initialize the quantum probe in arbitrary entangled quantum states is available. In other words, for implementing quantum limited measurements that beat the shot noise limit, we see that devising ways of doing possibly complicated readouts can be as important as control over the initial state of the quantum probe and its dynamics.

IV. ENTANGLING DYNAMICS

Now let us consider entangling dynamics for the probe qubits generated by

$$H^{(N)} = \tfrac{1}{2}\sigma_3^{\otimes N}. \tag{20}$$

Note that this Hamiltonian does not belong to the family of nonlinear Hamiltonians discussed in Refs. [29,30] that leads to measurement schemes in which the uncertainty scales as $1/N^k$ or $1/N^{k-1/2}$ with respect to N depending on whether the initial state of the probe is entangled or not.

The readout procedure in this case is also the same as before with independent measurements of the individual qubits along the $|\pm\rangle$ axis. However, despite this restriction $\tilde{\rho}_X^{\otimes N}$ is not, in general, a solution to Eq. (12). In fact, for the entangling Hamiltonian in Eq. (20) one can show that (see Appendix B) if $\tilde{\rho}_X^{(2d)}$ for $d = 1,2,\ldots$ is not a solution of the same equation giving the optimal state of a quantum probe made of $2d$ (even number of) qubits.

For $N = 2$, it is still worthwhile to find the optimal state even if it cannot be $\tilde{\rho}_X \otimes \tilde{\rho}_X$. One possible solution for Eq. (12) is the state

$$\tilde{\rho}_X^{(2)} = \tfrac{1}{4}(\mathbb{1} \otimes \mathbb{1} + c_{11}\sigma_1 \otimes \sigma_1 + c_{23}\sigma_2 \otimes \sigma_3 + c_{32}\sigma_3 \otimes \sigma_2). \tag{21}$$

This state is pure when $c_{11} = c_{23} = c_{32} = 1$. However, for this state $\langle \mathcal{L}^2 \rangle = 1$, indicating that it does not attain the $1/N$ scaling for the measurement uncertainty expected for the N-qubit probe. In fact the restriction that the qubits are measured independently means that even with two qubits, the measurement uncertainty is not improved compared to the single-qubit probe. The solution to Eq. (12) obtained in (21) is not unique either. For instance, another solution is obtained immediately from the state above by changing the signs of c_{23} and c_{32} which in turn swaps $1/\lambda_{++}$ and $1/\lambda_{--}$. For larger N one can solve the system of algebraic equations generated from Eq. (12) by equating the coefficients of corresponding operators to find one or more optimal initial states of the probe that saturate the quantum Cramér-Rao bound for the entangling dynamics.

Rather than solving for the optimal state on a case-by-case basis, it is more useful to pursue solutions of the form $\tilde{\rho}_X^{\otimes N}$ even though we have ruled out such solutions for even N. For odd N we can show that $\tilde{\rho}_X^{\otimes N}$ is a solution of Eq. (12) with the λ given by

$$\frac{1}{\lambda_{j_1 j_2 \ldots j_N}} = \frac{i^{N+3}}{\lambda_{j_1}\lambda_{j_2}\cdots\lambda_{j_N}},$$

where $1/\lambda_{j_l}$ are the eigenvalues of $\mathcal{L}$ for the $N = 1$ case. The proof of this result is rather technical and long and is given in Appendix C. This is not a very useful result because $1/\lambda_{j_l}$ have values ± 1 and so $1/\lambda_{j_1,j_2\ldots j_N} = \pm 1$ for odd N. A simple computation shows that then $\mathcal{L}^2 = \mathbb{1}$ and so $\langle \mathcal{L}^2 \rangle = 1$. In other words, no advantage is obtained in having N qubits in the probe rather than one if the N are initialized in the state $\tilde{\rho}_X^{\otimes N}$. Even with the entangling evolution, in a real experiment, if the ability to initialize and readout the probe in states that are not simple tensor products is not available, then the reduction in measurement uncertainty promised by quantum limited metrology is wiped out.

V. CONCLUSION

A general quantum limited measurement for estimating a single parameter can be thought of having three stages. There is a preparation stage in which the quantum system that is acting as the probe of the measured parameter is initialized in a particular quantum state. The second stage is the parameter-dependent evolution of the quantum probe, and the last stage is the readout of the probe. The advantages of using specific, often entangled, initial states of the quantum probe was explored extensively during the initial phase of the development of the theory and implementation of quantum limited measurement schemes [4,5,31–34]. How the dynamics influences the measurement uncertainty was explored more recently [3,29,30,35].

This paper is focused on the third stage of a quantum metrology scheme when considerations, practical or otherwise, limit the types of readout that can be done on the quantum probe. This analysis is done in the limited context of qubit-based metrology schemes. Extensions to other quantum limited measurement schemes including interferometry with squeezed states, NOON states, for example, may also be considered. We see that arbitrary state preparations and dynamics might not be particularly useful in delivering an improved measurement uncertainty if there are limitations on the readout. For instance, in the case of the N-qubit probe evolving under a nonentangling Hamiltonian, the Schrödinger cat state turns out not to be the optimal state because of the restriction that the readout is limited to independent measurements on each of the N qubits. In the case of the entangling dynamics we see that when the initial state of the probe is a product state then with the same restriction as before on the readout, the performance of the measurement scheme is no better than what can be done with a single-qubit probe.

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APPENDIX A: NONENTANGLING HAMILTONIAN

For two qubits, Eq. (12) leads to 16 equations connecting λ_{++}, λ_{+-}, λ_{-+} and λ_{--} to the 15 coefficients a_i, b_j, and c_{ij} defining the state of the probe. These are obtained by equating the coefficients of operators of the form $\sigma_\alpha \otimes \sigma_\beta$, $\alpha,\beta = 0,\ldots,4$ with $\sigma_0 \equiv \mathbb{1}$. Using the notation

$$\kappa_{\pm\pm\pm} = \left(\frac{1}{\lambda_{++}} \pm \frac{1}{\lambda_{+-}} \pm \frac{1}{\lambda_{-+}} \pm \frac{1}{\lambda_{--}}\right),$$

the equations we get are

$$\begin{aligned}
K_{+++} + K_{+--}a_1 + K_{-+-}b_1 + K_{--+}c_{11} &= 0,\\
K_{-+-} + K_{--+}a_1 + K_{+++}b_1 + K_{+--}c_{11} &= -4b_2,\\
K_{+--} + K_{+++}a_1 + K_{--+}b_1 + K_{-+-}c_{11} &= -4a_2,\\
K_{--+} + K_{-+-}a_1 + K_{+--}b_1 + K_{+++}c_{11} &= -4c_{12} - 4c_{21},\\
K_{+++}b_2 + K_{+--}c_{12} &= 4b_1,\\
K_{+--}b_2 + K_{+++}c_{12} &= 4c_{11} - 4c_{22},\\
K_{+++}a_2 + K_{-+-}c_{21} &= 4a_1,\\
K_{-+-}a_2 + K_{+++}c_{21} &= 4c_{11} - 4c_{22},\\
K_{+++}a_3 + K_{-+-}c_{31} &= 0,\\
K_{-+-}a_3 + K_{+++}c_{31} &= -4c_{32},\\
K_{+++}b_3 + K_{+--}c_{13} &= 0,\\
K_{+--}b_3 + K_{+++}c_{13} &= -4c_{23},\\
K_{+++}c_{22} - K_{--+}c_{33} &= 4c_{12} + 4c_{21},\\
K_{+++}c_{23} + K_{--+}c_{32} &= 4c_{13},\\
K_{--+}c_{23} + K_{+++}c_{32} &= 4c_{31},\\
K_{+++}c_{33} - K_{--+}c_{22} &= 0.
\end{aligned} \tag{A1}$$

For the particular case in which

$$\rho_X^{(2)} = \tilde{\rho}_X \otimes \tilde{\rho}_X = \tfrac{1}{4}(\mathbb{1}\otimes\mathbb{1} + \sigma_2\otimes\mathbb{1} + \mathbb{1}\otimes\sigma_2 + \sigma_2\otimes\sigma_2),$$

the nontrivial equations among Eqs. (A1) are

$$K_{+++} = K_{--+} = 0, \quad K_{-+-} = K_{+--} = -4.$$

From these equations we get

$$\frac{1}{\lambda_{++}} = -\frac{1}{\lambda_{--}} = -2$$

and

$$\frac{1}{\lambda_{+-}} = -\frac{1}{\lambda_{-+}} = 0$$

as a possible solution. Note that in this case,

$$\frac{1}{\lambda_{jk}} = \frac{1}{\lambda_j} + \frac{1}{\lambda_k}, \quad j,k = \{+,-\}.$$

1. *N* qubits

In Ref. [23], an alternate expression for the symmetric logarithmic derivative operator is obtained as

$$\mathcal{L}(O) = \sum_{p_j+p_k\neq 0} \frac{2}{p_j+p_k} O_{jk}|j\rangle\langle k|; \quad O_{jk} = \langle j|O|k\rangle,$$

where O is the operator on which $\mathcal{L}$ acts. We write the optimal single-qubit state as

$$\tilde{\rho}_X = \sum_j p_j |j\rangle\langle j|.$$

In our particular example the basis in which $\tilde{\rho}_X$ is diagonal is given by the vectors, $|i\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$ and $|\bar{i}\rangle = (|0\rangle - i|1\rangle)/\sqrt{2}$. In the remainder we want to use the result $\mathcal{F} = \langle \mathcal{L}^2(\rho')\rangle$, also obtained in Ref. [23]. For the single-qubit probe with evolution generated by $H = \sigma_3/2$ we have

$$\rho'_{jk} = -i\langle j|[H,\tilde{\rho}_X]|k\rangle = -\frac{i}{2}(p_k - p_j)\langle j|\sigma_3|k\rangle$$

and

$$\mathcal{L}(\rho') = -i\sum_{jk}\frac{p_k - p_j}{p_j + p_k}\langle j|\sigma_3|k\rangle |j\rangle\langle k|,$$

with the sum extending over all j,k such that $p_j + p_k \neq 0$. If the readout procedure corresponds to projective measurements with elements

$$E_n = |\theta_n\rangle\langle\theta_n|,$$

we have

$$\mathrm{tr}[\rho E_n \mathcal{L}(\rho')] = -i\sum_{jk} p_k \frac{p_k - p_j}{p_k + p_j}\langle j|\sigma_3|k\rangle\langle k|\theta_n\rangle\langle\theta_n|j\rangle$$

and

$$\mathrm{tr}[\rho E_n] = \sum_j p_j |\langle j|\theta_n\rangle|^2.$$

This gives us

$$\frac{1}{\lambda_n} = -i\frac{\sum_{jk} p_k \frac{p_k - p_j}{p_k + p_j}\langle j|\sigma_3|k\rangle\langle k|\theta_n\rangle\langle\theta_n|j\rangle}{\sum_l p_l |\langle l|\theta_n\rangle|^2}.$$

The N-qubit state tensor product state can be written as

$$\rho_X^{(N)} = \sum_{j_1,j_2\ldots j_N} p_{j_1}p_{j_2}\cdots p_{j_N}|j_1 j_2\cdots j_N\rangle\langle j_1 j_2\cdots j_N|,$$

while the Hamiltonian corresponding to nonentangling evolution on the N qubits is

$$H = \tfrac{1}{2}(\sigma_3 \otimes \mathbb{1}^{\otimes(N-1)} + \cdots + \mathbb{1}^{\otimes(N-1)} \otimes \sigma_3).$$

From $\rho' = -i[H,\rho]$, and denoting the string $j_1 j_2 \ldots j_N$ as $\vec{j}$, we have

$$\begin{aligned}
\rho'_{\vec{j}\vec{k}} &= -i\langle\vec{j}|[H,\rho]|\vec{k}\rangle \\
&= -\frac{i}{2}\sum_{l=1}^{N} p_{j_1}p_{j_2}\ldots p_{k_l}\ldots p_{j_N}\langle j_l|\sigma_3|k_l\rangle\prod_{n\neq l}\delta_{j_n k_n} \\
&\quad + \frac{i}{2}\sum_{l=1}^{N} p_{j_1}p_{j_2}\ldots p_{j_l}\ldots p_{j_N}\langle j_l|\sigma_3|k_l\rangle\prod_{n\neq l}\delta_{j_n k_n} \\
&= -\frac{i}{2}\sum_{l=1}^{N}(p_{k_l} - p_{j_l})\langle j_l|\sigma_3|k_l\rangle\prod_{m\neq l}p_{j_m}\delta_{j_m k_m};
\end{aligned}$$

using the above, we obtain

$$\begin{aligned}
\mathcal{L}(\rho') = -i\sum_{l=1}^{N}\sum_{j_1,\ldots,j_l,\ldots j_N,k_l}\frac{p_{k_l} - p_{j_l}}{p_{j_l} + p_{k_l}}\langle j_l|\sigma_3|k_l\rangle \\
\times |j_1,\ldots j_l,\ldots j_N\rangle\langle j_1,\ldots k_l,\ldots j_N|.
\end{aligned}$$

Assuming that the readout procedure consists of projective measurements corresponding to the operators,

$$E_{\vec{n}} = |\theta_{n_1}\theta_{n_2}\cdots\theta_{n_N}\rangle\langle\theta_{n_1}\theta_{n_2}\cdots\theta_{n_N}|,$$

we have

$$\begin{aligned}
&\mathrm{tr}[\rho E_{\vec{n}}\mathcal{L}(\rho')] \\
&= -i\sum_{l=1}^{N}\sum_{j_1,\ldots,j_l,\ldots j_N,k_l} p_{j_l}\frac{p_{j_l} - p_{k_l}}{p_{j_l} + p_{k_l}}\langle j_l|\sigma_3|k_l\rangle\langle j_l|\theta_{n_l}\rangle \\
&\quad \langle\theta_{n_l}|k_l\rangle\prod_{m\neq l}p_{j_m}|\langle j_m|\theta_{n_m}\rangle|^2 \\
&= -i\sum_{l=1}^{N}\left(\sum_{\{j_m\}_{m\neq l}}\prod_{m\neq l}p_{j_m}|\langle j_m|\theta_{n_m}\rangle|^2\right) \\
&\quad \times\left(\sum_{j_l k_l}p_{j_l}\frac{p_{j_l} - p_{k_l}}{p_{j_l} + p_{k_l}}\langle j_l|\sigma_3|k_l\rangle\langle j_l|\theta_{n_l}\rangle\langle\theta_{n_l}|k_l\rangle\right),
\end{aligned}$$

where $\{j_m\}_{m\neq l}$ stands for $j_1,\ldots,j_{l-1},j_{l+1},\ldots,j_N$. Similarly we have

$$\begin{aligned}
&\mathrm{tr}(E_{\vec{n}}\rho) \\
&= \sum_{j_1\ldots j_N}\prod_m p_{j_m}|\langle j_m|\theta_{n_m}\rangle|^2 \\
&= \left(\sum_{\{j_m\}_{m\neq l}}\prod_{m\neq l}p_{j_m}|\langle j_m|\theta_{n_m}\rangle|^2\right)\left(\sum_{j_l}p_{j_l}|\langle j_l|\theta_{n_l}\rangle|^2\right).
\end{aligned}$$

So the eigenvalues of $\mathcal{L}(\rho')$ for the N-qubit probe undergoing nonentangling evolution is

$$\begin{aligned}
\frac{1}{\lambda_{\vec{n}}} &= \sum_{l=1}^{N}\frac{\sum_{j_l k_l}p_{j_l}\frac{p_{j_l} - p_{k_l}}{p_{j_l} + p_{k_l}}\langle j_l|\sigma_3|k_l\rangle\langle j_l|\theta_{n_l}\rangle\langle\theta_{n_l}|k_l\rangle}{\sum_{j_l}p_{j_l}|\langle j_l|\theta_{n_l}\rangle|^2} \\
&= \sum_{l=1}^{N}\frac{1}{\lambda_{n_l}}.
\end{aligned} \tag{A2}$$

2. $\mathcal{L}$ for nonentangling dynamics

Using the expression for $1/\lambda_{\vec{n}}$ from Eq. (A2) and the fact that corresponding to the optimal state of the one-qubit probe, the eigenvalues of $\mathcal{L}$ are ∓ 1, we can write the symmetric logarithmic derivative operator on the N-qubit probe as

$$\mathcal{L} = -N|+\cdots+\rangle\langle+\cdots+| + \cdots + N|-\cdots-\rangle\langle-\cdots-|. \tag{A3}$$

Using $|+\rangle\langle+| = (\mathbb{1}+\sigma_1)/2$ and $|-\rangle\langle-| = (\mathbb{1}-\sigma_1)/2$ we get

$$\mathcal{L} = -\frac{1}{2^N}\sum_{r=0}^{N}(N-2r)[\hat{\mathcal{C}}(\mathbb{1}+\sigma_1)^{\otimes(N-r)}\otimes(\mathbb{1}-\sigma_1)^{\otimes r}],$$

where r is the number of $|-\rangle\langle-|$ projectors in each term in Eq. (A3) and $\hat{\mathcal{C}}$ is a shorthand indicating the sum of all terms that are tensor products of $N-r$ factors of $(\mathbb{1}+\sigma_1)$ and r factors of $(\mathbb{1}-\sigma_1)$.

Once the sum is distributed over the tensor product, we get terms with $N-q$ factors that are $\mathbb{1}$ and q σ_1 with

$q=0,1,\ldots,N$. Now consider one such term with fixed positions for $\mathbb{1}$ and σ_1. We first focus on the sign of each one of such terms with fixed locations for $\mathbb{1}$ and σ that come from the various terms in the expression for $\mathcal{L}$. If out of the q factors of σ_1, an odd number s of them come from the r $(\mathbb{1}-\sigma_1)$ factors then the term, as a whole is negative. Now, out of the total q factors of σ_1 we can pick s of them in ${}^qC_s$ ways. Now, out of the $N-q$ factors of $\mathbb{1}$, $r-s$ of them have to come from the $(\mathbb{1}-\sigma_1)$ terms. These $r-s$ factors can be picked in ${}^{N-q}C_{r-s}$ ways. The remaining $\mathbb{1}$ and σ_1 come from the $(\mathbb{1}+\sigma_1)$ terms. The number of terms with $N-q$ $\mathbb{1}$ and q σ_1 at fixed locations is ${}^NC_r$. From this we have to subtract twice the number of such terms with negative signs to obtain the total number of terms of this kind as

$$ {}^NC_r - 2\sum_{s=1,3,\cdots}^{\min(r,q)} {}^{N-q}C_{r-s}\,{}^qC_s. $$

We have for all $q \geqslant 0$

$$ -\sum_{r=0}^{N}(N-2r)\,{}^NC_r = -N2^N + 2N\sum_{r=0}^{N-1} {}^{N-1}C_r = 0. $$

Hence

$$ \mathcal{L} = \frac{2}{2^N}\sum_{q=1}^{N}\sum_{r=0}^{N}\sum_{s=1,3,\cdots}^{\min(r,q)}(N-2r)\,{}^{N-q}C_{r-s}\,{}^qC_s \times\{\hat{\mathcal{C}}\mathbb{1}^{\otimes(N-q)}\otimes\sigma_1^{\otimes q}\}. $$

For $q=1$ the summation in the $\mathcal{L}$ reduces to

$$ 2\sum_{r=1}^{N}(N-2r)\,{}^{N-1}C_{r-1} = -2^N. $$

Now for any $q>1$, we have

$$ \begin{aligned} &\sum_{r=1}^{N}\sum_{s=1,3,\cdots}^{\min(q,r)}(N-2r)^{N-q}C_{r-s}\,{}^qC_s \\ &= N\sum_{r=1}^{N}\sum_{s=1,3,\cdots}^{\min(q,r)} {}^{N-q}C_{r-s}\,{}^qC_s \\ &\quad -2(N-q)\sum_{r=1}^{N}\sum_{s=1,3,\cdots}^{\min(q,r)} {}^{N-q-1}C_{r-s-1}\,{}^qC_s \\ &\quad -2q\sum_{r=1}^{N}\sum_{s=1,3,\cdots}^{\min(q,r)} {}^{N-q}C_{r-s}\,{}^{q-1}C_{s-1}. \end{aligned} \tag{A4} $$

To compute the sums in the equation above, we use the following results: For $q>1$, $\sum_{i=1,3,\ldots}^{q} {}^qC_i = 2^{q-1}$ and $\sum_{i=0,2,\ldots}^{q-1} {}^{q-1}C_i = 2^{q-2}$. Equation (A4) becomes

$$ \begin{aligned} &\sum_{r=1}^{N}\sum_{s=1,3,\cdots}^{\min(q,r)}(N-2r)\,{}^{N-q}C_{r-s}\,{}^qC_s \\ &= N\sum_{i=1,3,\cdots}^{q} {}^qC_i\sum_{j=0,1,\cdots}^{N-q} {}^{N-q}C_j \\ &\quad -2(N-q)\sum_{i=1,3,\cdots}^{q} {}^qC_i\sum_{j=0,1,\cdots}^{N-q} {}^{N-q}C_j \\ &\quad -2q\sum_{i=0,2,\cdots}^{q-1} {}^{q-1}C_i\sum_{j=0,1,\cdots}^{N-q-1} {}^{N-q-1}C_j = 0. \end{aligned} $$

Thus the symmetric logrithmic derivative for an N-qubit probe evolving under a nonentangling Hamiltonian is

$$ \mathcal{L} = -\{\hat{\mathcal{C}}\mathbb{1}^{\otimes(N-1)}\otimes\sigma_1\}. $$

APPENDIX B: ENTANGLING HAMILTONIAN

When the parameter-dependent evolution is generated by the entangling Hamiltonian, $\sigma_3^{\otimes N}/2$, and we consider an initial state of the probe of the form $\tilde{\rho}_X^{\otimes N}$, we have

$$ \rho' = -\frac{i}{2}[(\sigma_3\rho)^{\otimes N} - (\rho\sigma_3)^{\otimes N}]. $$

Now,

$$ \begin{aligned} \rho'_{\vec{j},\vec{k}} &= -\frac{i}{2}\prod_l\langle j_l|\sigma_3\rho|k_l\rangle + \frac{i}{2}\prod_l\langle j_l|\rho\sigma_3|k_l\rangle \\ &= -\frac{i}{2}\prod_l p_{j_l}\langle j_l|\sigma_3|k_l\rangle + \frac{i}{2}\prod_l p_{j_l}\langle j_l|\sigma_3|k_l\rangle, \end{aligned} $$

and using the above, we obtain

$$ \mathcal{L}(\rho') = -i\sum_{\{j_l,k_l\}}\frac{\prod_l p_{k_l} - \prod_l p_{j_l}}{\prod_l p_{k_l} + \prod_l p_{j_l}}\prod_l\langle j_l|\sigma_3|k_l\rangle \times|j_1,j_2,\ldots j_N\rangle\langle k_1,k_2,\ldots k_N| $$

and

$$ \mathrm{tr}[\rho E_{\vec{n}}\mathcal{L}(\rho')] = -i\sum_{\{j_l,k_l\}}\frac{\prod_l p_{k_l}\left(\prod_i p_{k_i} - \prod_i p_{j_i}\right)}{\prod_l p_{k_l} + \prod_l p_{j_l}} \times\prod_l\langle j_l|\sigma_3|k_l\rangle\langle k_l|\theta_{n_l}\rangle\langle\theta_{n_l}|j_l\rangle. \tag{B1} $$

We also have

$$ \mathrm{tr}(E_{\vec{n}}\rho) = \sum_{\{j_l\}}\prod_l p_{j_l}|\langle j_l|\theta_{n_l}\rangle|^2. \tag{B2} $$

We get $1/\lambda_{\vec{n}}$ by dividing the right-hand side of Eq. (B1) by that of Eq. (B2). Note that the denominator in (B2) is real and so is the first part of each term in the double sum in (B1). So the product term $\prod_l\langle j_l|\sigma_3|k_l\rangle\langle k_l|\theta_{n_l}\rangle\langle\theta_{n_l}|j_l\rangle$, has to be pure imaginary for $1/\lambda_{\vec{n}}$ to be real as required for saturating the bound on the Fisher information as discussed in Sec. II. However, each term in this product comes form each qubit in the probe. So if we assume that each qubit in the probe is in the optimal state $\tilde{\rho}_X$ corresponding to the $N=1$ state, then for each qubit $\langle j|\sigma_3|k\rangle\langle k|\theta_n\rangle\langle\theta_n|j\rangle$ has to be pure imaginary so that again, the bound is saturated as assumed. This implies that when N is even, then $\lambda_{\vec{n}}$ are all purely imaginary, and so the tensor product state $\tilde{\rho}_X^{\otimes N}$ is not the optimal state of the probe corresponding to the entangling dynamics and readout procedure that we are considering when N is even.

1. Optimal state of a two-qubit probe

Using the same notation as in Appendix A, Eq. (12) reduces to the following 16 algebraic equations:

$$\begin{aligned}
K_{+++} + K_{+--}a_1 + K_{-+-}b_1 + K_{--+}c_{11} &= 0,\\
K_{--+} + K_{-+-}a_1 + K_{+--}b_1 + K_{+++}c_{11} &= 0,\\
K_{+--} + K_{+++}a_1 + K_{--+}b_1 + K_{-+-}c_{11} &= -4c_{23},\\
K_{-+-} + K_{--+}a_1 + K_{+++}b_1 + K_{+--}c_{11} &= -4c_{32},\\
K_{+++}a_3 + K_{-+-}c_{31} &= 0,\\
K_{+++}c_{22} - K_{--+}c_{33} &= 0,\\
K_{+++}b_2 + K_{+--}c_{12} &= 4c_{31},\\
K_{+++}a_2 + K_{-+-}c_{21} &= 4c_{13},\\
K_{-+-}a_3 + K_{+++}c_{31} &= -4b_2,\\
K_{+++}b_3 + K_{+--}c_{13} &= 0,\\
K_{+--}b_3 + K_{+++}c_{13} &= -4a_2,\\
K_{+++}c_{33} - K_{--+}c_{22} &= 0,\\
K_{+++}c_{21} + K_{-+-}a_2 &= 0,\\
K_{+++}c_{12} + K_{+--}b_2 &= 0,\\
K_{+++}c_{32} + K_{--+}c_{23} &= 4b_1,\\
K_{+++}c_{23} + K_{--+}c_{32} &= 4a_1.
\end{aligned} \qquad \text{(B3)}$$

In this case, as noted earlier it is easy to verify that $\tilde{\rho}_X^{(2)} = \tilde{\rho}_X \otimes \tilde{\rho}_X$ does not give any solution for $1/\lambda_n$. Solving these equations for the variables a_i, b_j, and c_{ij} and applying in the general form of ρ for two qubits we get the optimal initial state for the two-qubit probe. Multiple solutions are allowed, and for maximizing $\langle \mathcal{L}^2 \rangle$ we look for pure state solutions. One pure state solution may be obtained by setting all a_i, b_j, and c_{ij} to zero except for $c_{11} = 1$ and $c_{23} = c_{32} = \pm 1$, which then leads to

$$\frac{1}{\lambda_{++}} = -\frac{1}{\lambda_{--}} = -1 \quad \text{and} \quad \frac{1}{\lambda_{+-}} = \frac{1}{\lambda_{-+}} = c,$$

where c can be any real number, including 0.

APPENDIX C: $1/\lambda$ FOR ODD N

Starting from Eq. (B1) by that of Eq. (B2) we find the eigenvalues of $\mathcal{L}(\rho')$ for an N-qubit probe undergoing entangling evolution as

$$\frac{1}{\lambda_{\vec{n}}} = \frac{-i \sum_{\{j_l,k_l\}} \frac{\prod_l p_{k_l}(\prod_i p_{k_l} - \prod_i p_{j_l})}{\prod_l p_{k_l} + \prod_l p_{j_l}}}{\sum_{\{j_l\}} \prod_l p_{j_l} |\langle j_l|\theta_{n_l}\rangle|^2} \times \prod_l \langle j_l|\sigma_3|k_l\rangle\langle k_l|\theta_{n_l}\rangle\langle\theta_{n_l}|j_l\rangle. \qquad \text{(C1)}$$

The optimal single-qubit state $\tilde{\rho}_X$ is diagonal in the eigenbasis $\{|i\rangle, |\bar{i}\rangle\}$ of the σ_2 operator, and so we can write it as

$$\tilde{\rho}_X = p_i|i\rangle\langle i| + p_{\bar{i}}|\bar{i}\rangle\langle\bar{i}|,$$

so that $|j_l\rangle, |k_l\rangle = \{|i\rangle, |\bar{i}\rangle\}$. As before the readout operators, $|\theta_{n_l}\rangle\langle\theta_{n_l}|$ are given by $|+\rangle\langle+|$ and $|-\rangle\langle-|$. Using the inner products, $\langle i|\pm\rangle = (1 \mp i)/2$, $\langle\bar{i}|\pm\rangle = (1 \pm i)/2$, $\langle i|+\rangle\langle+|\bar{i}\rangle = -i/2$, and $\langle i|-\rangle\langle-|\bar{i}\rangle = i/2$ we get for any choice of θ_n,

$$\sum_{\{j_l\}} \prod_l p_{j_l} |\langle j_l|\theta_{n_l}\rangle|^2 = \frac{1}{2^N}(p_i + p_{\bar{i}})^N. \qquad \text{(C2)}$$

Since $\langle i|\sigma_3|i\rangle = \langle\bar{i}|\sigma_3|\bar{i}\rangle = 0$ and $\langle i|\sigma_3|\bar{i}\rangle = 1$, only terms with $\vec{j} = \vec{\bar{k}}$ contribute to the expression for $\rho'_{\vec{j}\vec{k}}$ and hence to $\mathcal{L}(\rho')$ and $1/\lambda_n$ as well. Consider a single term in the double sum over $\{j_l, k_l\}$ in the numerator of Eq. (C1), where

$$|\vec{j}\rangle = |i, i, \ldots, i, \bar{i}\rangle \quad \text{and} \quad |\vec{k}\rangle = |\bar{i}, \bar{i}, \ldots, \bar{i}, i\rangle.$$

In this term we have the factor

$$\begin{aligned}
\prod_l \langle j_l|\theta_{n_l}\rangle\langle\theta_{n_l}|k_l\rangle &= \mp\frac{i}{2} \cdot \mp\frac{i}{2} \cdots \mp\frac{i}{2} \cdot \pm\frac{i}{2}\\
&= \frac{i^N}{2^N}(\mp \cdot \mp \cdots \mp \cdot \pm).
\end{aligned}$$

In the double sum over $\{j_l, k_l\}$ in Eq. (C1), there will be ${}^N C_1$ terms each having $N-1$ $(\mp)$ terms and one $(\pm)$ term. In general, there will be ${}^N C_r$ terms each having $N-r$ $(\mp)$ terms and r $(\pm)$ terms. When $E_{\vec{n}}$ and hence θ_{n_l} is fixed, then every term with $N-r$ $\mp$ terms and r $\pm$ terms has the same sign, and so they can all be grouped together. We represent these terms that are grouped together as $\{\underbrace{\mp\cdots\mp}_{N-r}\underbrace{\pm\cdots\pm}_{r}\}$, since the group is labeled by r. Using this notation and Eq. (C2), we have

$$\begin{aligned}
\frac{1}{\lambda_{\vec{n}}} = {}& Q\frac{p_N^0 - p_0^N}{p_N^0 + p_0^N}\, {}^N C_0 p_N^0\{\mp\mp\cdots\mp\}\\
&+ Q\frac{p_{N-1}^1 - p_1^{N-1}}{p_{N-1}^1 + p_1^{N-1}}\, {}^N C_1 p_{N-1}^1\{\mp\mp\cdots\mp\pm\}\\
&+ \cdots\\
&+ Q\frac{p_{N-r}^r - p_r^{N-r}}{p_{N-r}^r + p_r^{N-r}}\, {}^N C_r p_{N-r}^r\{\mp\cdots\mp\pm\cdots\pm\}\\
&+ \cdots\\
&- Q\frac{p_{N-r}^r - p_r^{N-r}}{p_{N-r}^r + p_r^{N-r}}\, {}^N C_{N-r} p_r^{N-r}\{\pm\cdots\pm\mp\cdots\mp\}\\
&- \cdots\\
&- Q\frac{p_{N-1}^1 - p_1^{N-1}}{p_{N-1}^1 + p_1^{N-1}}\, {}^N C_{N-1} p_1^{N-1}\{\pm\pm\cdots\pm\mp\}\\
&- Q\frac{p_N^0 - p_0^N}{p_N^0 + p_0^N}\, {}^N C_N p_0^N\{\pm\pm\cdots\pm\},
\end{aligned}$$

where $Q = \frac{-i^{N+1}}{(p_i + p_{\bar{i}})^N}$ and $p_{N-r}^r = (p_i)^{N-r}(p_{\bar{i}})^r$. Now consider the first and last terms of the sum as a pair:

$$\begin{aligned}
A_1 = {}& Q\frac{p_N^0 - p_0^N}{p_N^0 + p_0^N}\, {}^N C_0 p_N^0\{\mp\mp\cdots\mp\}\\
&- Q\frac{p_N^0 - p_0^N}{p_N^0 + p_0^N}\, {}^N C_N p_0^N\{\pm\pm\cdots\pm\}.
\end{aligned} \qquad \text{(C3)}$$

Since N is odd, for a given choice of $E_{\vec{n}}$, $\{\mp\mp\cdots\mp\}$ and $\{\pm\pm\cdots\pm\}$ have opposite signs. Hence, Eq. (C3) reduces to

$$A_1 = \pm Q\left({}^N C_0 p_N^0 - {}^N C_N p_0^N\right).$$

Similarly, we can pair up the remaining terms. Since for even and odd r

$$Q\frac{p_{N-r}^r - p_r^{N-r}}{p_{N-r}^r + p_r^{N-r}}\,{}^N C_r\, p_{N-r}^r\{\mp\cdots\mp\pm\cdots\pm\}$$

for any $E_{\vec{n}}$ has opposite signs, we get

$$\frac{1}{\lambda_{\vec{n}}} = \pm\frac{i^{N+3}(p_i - p_{\bar{i}})^N}{(p_i + p_{\bar{i}})^N}.$$

The sign of $\lambda_{\vec{n}}$ depends on the choice of $E_{\vec{n}}$s. Using $1/\lambda_{n_l} = \pm(p_i - p_{\bar{i}})/(p_i + p_{\bar{i}})$, we see that for any odd N,

$$\frac{1}{\lambda_{\vec{n}}} = \frac{i^{N+3}}{\lambda_{n1}\lambda_{n_2}\cdots\lambda_{n_N}}.$$

Generalizing the above result, the best initial state for any $2^n(2m+1)$ number of qubits can be obtained as $\rho = \rho_{2^n}^{\otimes(2m+1)}$, where $m,n = 0, 1, 2, \ldots$ and ρ_{2^n} is the best initial state of 2^n qubits.

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