Generalized Limits for Single-Parameter Quantum Estimation

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We develop generalized bounds for quantum single-parameter estimation problems for which the coupling to the parameter is described by intrinsic multisystem interactions. For a Hamiltonian with k-system parameter-sensitive terms, the quantum limit scales as $1/N^k$, where N is the number of systems. These quantum limits remain valid when the Hamiltonian is augmented by any parameter-independent interaction among the systems and when adaptive measurements via parameter-independent coupling to ancillas are allowed.

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Many problems that lie at the interface between physics and information science can be addressed using techniques from parameter estimation theory. Precision metrology, timekeeping, and communication offer prominent examples; the parameter of interest might be the strength of an external field, the evolved phase of a clock, or a communication symbol. Fundamentally, single-parameter estimation is a quantum-mechanical problem: one must infer the value of a coupling constant γ in the Hamiltonian $H_\gamma = \hbar\gamma h_0$ of a probe system by observing the evolution of the probe due to H_γ [1–5]. We take γ to have units of frequency, thus making h_0 a dimensionless coupling Hamiltonian.

Quantum mechanics places limits on the precision with which γ can be determined. It is now well established, via the quantum Cramér-Rao bound [1–4], that the optimal uncertainty in any single-parameter quantum estimation procedure is $\delta\gamma \sim 1/\sqrt{\nu}t\Delta h_0$, where ν is the number of independent probes used, t is the evolution time of each probe, and Δh_0 is the standard deviation (uncertainty) of h_0 [3,4]. The $1/\sqrt{\nu}$ dependence is the standard statistical improvement with the number of trials; generally, for non-Gaussian statistics, the sensitivity $1/\sqrt{\nu}t\Delta h_0$ can only be attained asymptotically for large ν. But besides increasing the number of trials, there are two other obvious ways to improve the sensitivity: (i) the probe can be allowed to evolve under H_γ for a longer time t; (ii) the quantum state of the probe can be chosen to maximize the deviation Δh_0. In all practical settings, decoherence or other noise and temporal fluctuations in γ limit the useful interaction time. For a given parameter estimation problem, h_0 is fixed, as is its maximum deviation.

Quantum mechanics does, however, provide another opportunity: gathering N probe systems into a single probe, which is prepared in an appropriate entangled state; if Δh_0 for the entangled state increases faster than $\sqrt{N}$, the sensitivity improves, provided there is still a sufficient number of probes to reach the asymptotic regime in the number of trials. This Letter focuses on how $\delta\gamma$ scales with N, the number of systems in a probe. Thus we work throughout with bounds on the sensitivity of a single probe, remembering that the bounds can be achieved only by averaging over many probes, but preferring not to muddy the discussion by carrying along the $1/\sqrt{\nu}$ dependence on the number of probes.

For the N systems in a probe, it has been traditional to consider Hamiltonians of the form

$$H_\gamma = \hbar\gamma h_0, \qquad h_0 = \sum_{j=1}^{N} h_j, \tag{1}$$

where h_0 is the collective dimensionless Hamiltonian that results from summing over identical single-system couplings h_j for the individual probe constituents. Restriction to Hamiltonians that are separable and invariant under particle exchange, as in Eq. (1), is physically motivated: in metrology it is desirable to make the coupling to the parameter homogeneous, and in many physical implementations, even the measurements performed on the probe are unable to distinguish between individual constituent systems.

To determine how the optimal parameter uncertainty scales with N, one maximizes the deviation Δh_0 over joint states of the probe systems. If entanglement is not allowed, the probe systems can themselves be regarded as independent probes; in this case, Δh_0 scales as $\sqrt{N}$, producing the so-called shot-noise limit found in precision magnetometry, gravimetry, and timekeeping [6]. When entanglement is allowed, however, one can choose the initial probe state to be the "cat state,"

$$\frac{1}{\sqrt{2}}(|\lambda_M, \ldots, \lambda_M\rangle + |\lambda_m, \ldots, \lambda_m\rangle), \tag{2}$$

where for system j, $|\lambda_M\rangle$ ($|\lambda_m\rangle$) is the eigenstate of h_j with maximum (minimum) eigenvalue λ_M (λ_m). This yields a deviation $\Delta h_0 = N(\lambda_M - \lambda_m)/2$ that scales linearly in N [3,5], a scaling known as the Heisenberg limit. Evolution under H_γ for time t introduces a relative phase $e^{i\phi(t)}$ into the cat state, with $\phi(t) = \gamma tN(\lambda_M - \lambda_m)$, and leaves Δh_0 unchanged; the Heisenberg limit can be attained (asymp-

totically for many trials) by measuring on each probe system an observable two of whose eigenvectors are $|\pm\rangle = (|\lambda_M\rangle \pm |\lambda_m\rangle)/\sqrt{2}$.

We argue that symmetric linear coupling to collective probe operators, the assumption that underlies Eq. (1) and many $1/N$ scaling derivations based on collective uncertainty relations [6–8], should not be considered fundamental to metrology. For example, some condensed and even quantum-optical systems exhibit nonlinear collective effects due to multibody or tensor-field interactions [9–11]. In such systems, multibody terms in the Hamiltonian can couple to metrologically relevant parameters. In this Letter we generalize single-parameter quantum estimation to intrinsic many-body interactions and obtain parameter uncertainty scalings that outperform $1/N$. Our work is largely inspired by a recent paper by Roy and Braunstein [12], which claimed an exponential scaling for a collection of N qubits with a particular Hamiltonian. Using our results, we argue below that their proposed exponential scaling is unphysical.

We turn now to showing that Hamiltonians with intrinsic k-body terms generate a family of parameter estimation problems, characterized by k, where the quantum limit scales as $1/N^k$. For this purpose, we consider Hamiltonians of the form

$$H_\gamma(t) = \hbar\gamma h_0 + \tilde{H}(t), \qquad h_0 = \sum_{\{j_1,\ldots,j_k\}} h^{(k)}_{j_1,\ldots,j_k}, \tag{3}$$

where h_0 is the dimensionless Hamiltonian that describes coupling to the parameter. The auxiliary Hamiltonian $\tilde{H}(t)$ is discussed below. In h_0, k denotes the degree of multibody coupling, with the sum running over all subsets of k systems. We could also include couplings of different degrees up to a maximum degree, but since the maximum degree dominates the sensitivity scaling, we stick with a single degree k in the following. We assume that the k-body coupling $h^{(k)}$ is symmetric under exchange of probe systems. Moreover, we assume that k and $h^{(k)}$ are independent of the number of probe systems. We make this latter assumption, that h_0 is an intensive property of the probe, because we want to consider a particular kind of coupling to the parameter which remains unchanged as N changes. For real physical systems, the symmetry and intensive assumptions will hold only approximately and only over some range of values of N.

The auxiliary Hamiltonian $\tilde{H}(t)$ includes all parameter-independent contributions to H_γ. For example, it includes the free Hamiltonians of the probe systems and any parameter-independent interactions among them. In addition, we can introduce an undetermined number of ancillas and let $\tilde{H}$ include the couplings of the ancillas to the probe systems and any couplings among the ancillas. Measurements on the ancillas can be included as part of an overall final measurement on the probe-ancilla system; since the Cramér-Rao bound that underlies our analysis holds for all possible measurements and ways of estimating γ from the measurement results, the bounds we derive hold for arbitrary measurements on the ancillas. This conclusion applies even to measurements on the ancillas that are carried out during the evolution time and whose results are used to condition measurements on other ancillas or to control the coupling of other ancillas to the probe. By the principle of deferred measurement [13], which is illustrated in Fig. 1, all such measurements can be shuffled to the end of the evolution time by making appropriate adjustments to $\tilde{H}$.

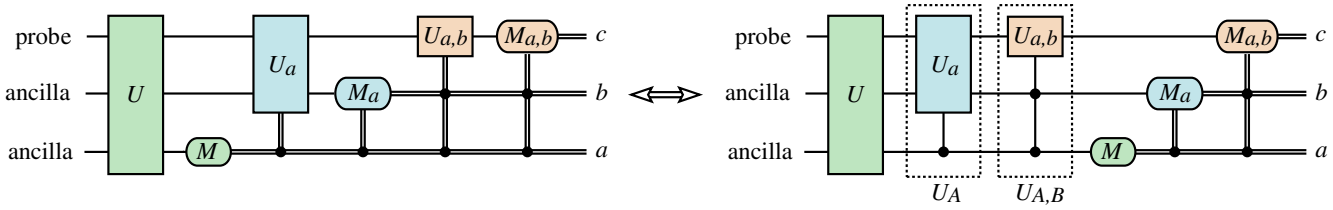

FIG. 1 (color online). Quantum-circuit diagrams illustrating the principle of deferred measurement. In the circuit on the left, a measurement M on the lower ancilla yields result a; this result controls a subsequent unitary U_a, applied to the probe and the upper ancilla, and determines a conditional measurement M_a on the upper ancilla, which has result b. The two measurement results then control a unitary $U_{a,b}$ applied to the probe and a conditional measurement $M_{a,b}$ on the probe. The left-hand circuit is equivalent to the circuit on the right, in which the controls are applied coherently (boxed gates U_A and $U_{A,B}$), and the measurements, deferred to the end of the circuit, tell one which unitary was applied. Without loss of generality, we can assume the measurements are described by orthogonal projectors P_a, $P_{b|a}$, and $P_{c|a,b}$, because any generalized measurement can be modeled by a projection-valued measurement on an extended system. The unitary transformations in the left-hand circuit, U_a and $U_{a,b}$, are evolution operators generated by the Hamiltonians $\hbar\gamma h_0 + \tilde{H}_a(t)$ and $\hbar\gamma h_0 + \tilde{H}_{a,b}(t)$, whereas the corresponding coherent controlled unitaries in the circuit on the right, U_A and $U_{A,B}$, are generated by the Hamiltonians $\hbar\gamma h_0 + \sum_a \tilde{H}_a(t) \otimes P_a$ and $\hbar\gamma h_0 + \sum_{a,b} \tilde{H}_{a,b}(t) \otimes P_{b|a}P_a$. It is easy to verify from the evolution equations that the controlled unitaries in the right-hand circuit are given by $U_A = \sum_a U_a \otimes P_a$ and $U_{A,B} = \sum_{a,b} U_{a,b} \otimes P_{b|a}P_a$. Thus the principle of deferred measurement can be rendered algebraically in the following way: if we use the left-hand circuit, the probability for obtaining results a, b, and c takes the form $\mathrm{tr}(C_{a,b,c}\rho_0 C^\dagger_{a,b,c})$, where ρ_0 is the initial state of the probe and ancillas and $C_{a,b,c} = P_{c|a,b}U_{a,b}P_{b|a}U_aP_aU$; pulling the measurement projectors to the left in $C_{a,b,c}$ changes the unitaries to the corresponding coherent controlled operations, i.e., $C_{a,b,c} = P_{c|a,b}P_{b|a}P_aU_{A,B}U_AU$, which gives the form of the probability obtained from the right-hand circuit.

Now let ρ_0 be the initial state of the probe and any ancillas. After a time t, the state evolves to $\rho_\gamma(t) = U_\gamma(t)\rho_0 U_\gamma^\dagger(t)$, where the evolution operator is generated by the Hamiltonian (3):

$$i\hbar\frac{\partial U_\gamma(t)}{\partial t} = H_\gamma(t)U_\gamma(t). \tag{4}$$

At time t, measurements are made on the probe and ancillas, the results of which are used to make an estimate $\gamma_{\rm est}$ of the parameter. An appropriate statistical measure of the estimate's precision is the units-corrected mean-square deviation of $\gamma_{\rm est}$ from γ [3,4],

$$\delta^2\gamma = \left\langle\left(\frac{\gamma_{\rm est}}{|d\langle\gamma_{\rm est}\rangle/d\gamma|} - \gamma\right)^2\right\rangle, \tag{5}$$

although care must be taken in using this measure for periodic parameters such as a phase [14]. All expectation values are with respect to $\rho_\gamma(t)$.

The quantum Cramér-Rao bound states that [1–4]

$$\delta^2\gamma \geq \frac{1}{\mathcal{I}_\gamma(t)}, \qquad \mathcal{I}_\gamma(t) = \mathrm{tr}(\rho_\gamma(t)\mathcal{Q}_\gamma^2(t)) = \langle\mathcal{Q}_\gamma^2(t)\rangle, \tag{6}$$

where $\mathcal{I}_\gamma(t)$ is the quantum Fisher information. The Hermitian operator $\mathcal{Q}_\gamma(t)$, defined (implicitly) by

$$\frac{1}{2}(\mathcal{Q}_\gamma\rho_\gamma + \rho_\gamma\mathcal{Q}_\gamma) = \frac{\partial\rho_\gamma}{\partial\gamma} = -i[K_\gamma, \rho_\gamma], \tag{7}$$

is called the symmetric logarithmic derivative and

$$K_\gamma(t) = i\frac{\partial U_\gamma(t)}{\partial\gamma}U_\gamma^\dagger(t) \tag{8}$$

is the Hermitian generator of displacements in γ. If there is no auxiliary Hamiltonian, $K_\gamma(t) = th_0$.

For pure states, differentiating $\rho_\gamma = \rho_\gamma^2$ shows that

$$\mathcal{Q}_\gamma(t) = 2\frac{\partial\rho_\gamma(t)}{\partial\gamma} = -2i[K_\gamma(t), \rho_\gamma(t)]. \tag{9}$$

Then the Fisher information reduces to a multiple of the variance of $K_\gamma(t)$:

$$\mathcal{I}_\gamma(t) = 4(\langle K_\gamma^2(t)\rangle - \langle K_\gamma(t)\rangle^2) = 4\Delta^2 K_\gamma(t). \tag{10}$$

For mixed states, the variance provides an upper bound on the Fisher information, instead of equality [4].

We define the operator seminorm $\|H\|$ of a Hermitian operator H as $\|H\| = M_H - m_H$, where M_H (m_H) is the maximum (minimum) eigenvalue of H. This seminorm is invariant under unitary transformations and obeys the triangle inequality, i.e., $\|H + K\| \leq \|H\| + \|K\|$ [15]. The importance of the seminorm is that its square provides an upper bound on the variance, i.e., $\Delta^2 H \leq \|H\|^2/4$ [16]. The maximum variance is achieved by pure states of the form $(|M_H\rangle + e^{i\phi}|m_H\rangle)/\sqrt{2}$.

We can now summarize the chain of inequalities satisfied by the estimation precision,

$$\frac{1}{\delta\gamma} \leq \sqrt{\mathcal{I}_\gamma(t)} \leq 2\Delta K_\gamma(t) \leq \|K_\gamma(t)\|, \tag{11}$$

leaving us with the final task of bounding the seminorm of $K_\gamma(t)$ for the dynamics of Eqs. (3) and (4). To do so, we define a new Hermitian operator,

$$F_\gamma(t) = U_\gamma^\dagger(t)K_\gamma(t)U_\gamma(t) = iU_\gamma^\dagger(t)\frac{\partial U_\gamma(t)}{\partial\gamma}, \tag{12}$$

which satisfies the evolution equation, $\partial F_\gamma(t)/\partial t = U_\gamma^\dagger(t)h_0U_\gamma(t)$, with initial condition $F_\gamma(0) = iU_\gamma^\dagger(0)\times(\partial U_\gamma(0)/\partial\gamma) = 0$, since $U_\gamma(0) = I$. Straightforward integration provides $F_\gamma(t)$, which then yields

$$K_\gamma(t) = \int_0^t ds U_\gamma(t)U_\gamma^\dagger(s)h_0U_\gamma(s)U_\gamma^\dagger(t). \tag{13}$$

The triangle inequality and the unitary invariance of the seminorm imply that

$$\|K_\gamma(t)\| \leq \int_0^t ds\|U_\gamma(t)U_\gamma^\dagger(s)h_0U_\gamma(s)U_\gamma^\dagger(t)\| \leq t\|h_0\|, \tag{14}$$

which gives us the desired bound on the sensitivity [17],

$$\delta\gamma \geq \frac{1}{t\|h_0\|}. \tag{15}$$

This bound on the estimation precision applies for any coupling Hamiltonian h_0. The optimal sensitivity is determined by h_0—indeed, by the range of energies in h_0—and cannot be improved by use of a parameter-independent auxiliary Hamiltonian $\tilde{H}$ or of ancillas not coupled directly to the parameter, although both of these might be used in practice to make the required optimal measurement accessible [8].

We now apply the bound (15) to draw physical conclusions about the sensitivity scaling for the various forms of h_0. For the separable, symmetrically coupled Hamiltonian of Eq. (1), we recover the usual $1/N$ scaling. But for the symmetric k-body coupling of Eq. (3), the triangle inequality applied to the seminorm,

$$\|h_0\| \leq \sum_{\{j_1,\ldots,j_k\}}\|h^{(k)}_{j_1,\ldots,j_k}\| \leq \binom{N}{k}\|h^{(k)}\| \sim \frac{N^k}{k!}\|h^{(k)}\|, \tag{16}$$

gives a sensitivity limit that scales as $1/N^k$. For $k > 1$, the coupling Hamiltonian itself generates entanglement between probe systems, making it more difficult to compare the sensitivities afforded by initially entangled and separable input states. Our objective here is not to make such a comparison, but to state the optimal sensitivity scaling that can be achieved in principle given a k-body coupling Hamiltonian. It is in this sense that we refer to k as generating a family of distinct quantum parameter estimation problems.

An important special case occurs when $\tilde{H}(t) = 0$, so that $K_\gamma(t) = th_0$, the k-body coupling terms in h_0 are products

of single-system operators, i.e., $h^{(k)}_{j_1,\ldots,j_k} = h_{j_1} \cdots h_{j_k}$, and the single-system operators have nonnegative eigenvalues. Then the inequalities in Eqs. (14) and (16) become equalities, and an initial cat state (2) attains the maximum deviation, i.e.,

$$\Delta K_\gamma(t) = \frac{1}{2}\|K_\gamma(t)\| = \frac{t}{2}\|h_0\| = \frac{t}{2}\binom{N}{k}(\lambda_M^k - \lambda_m^k). \tag{17}$$

The brief discussion (for $k = 1$) following Eq. (2) can be applied directly to achieving the sensitivity limit for arbitrary k, except that the relative phase generalizes to

$$\phi(t) = \gamma t\binom{N}{k}(\lambda_M^k - \lambda_m^k).$$

Our result can be used to analyze the recent paper by Roy and Braunstein (RB) [12], which inspired the work we report here. In our notation, RB consider a system of N qubits with a dimensionless coupling Hamiltonian

$$h_0 = \frac{1}{2}(\Sigma_+ + \Sigma_-), \qquad \Sigma_\pm = \prod_{j=1}^{N}(X_j \pm iY_j), \tag{18}$$

where X_j and Y_j are Pauli operators for the jth qubit. When the products are multiplied out, h_0 becomes a sum of 2^{N-1} commuting Pauli products; it has maximum deviation $\Delta h_0 = \|h_0\|/2 = 2^{N-1}$, which gives a quantum limit that scales exponentially in N. RB suggest that their Hamiltonian describes the atomic transitions of N atoms associated in a molecule, but the fundamental coupling in this case is a separable sum, as in Eq. (1), describing separate transitions for each atom. The RB coupling could arise as an effective Nth-order process, but it would not be justified to neglect processes of other orders. To achieve the RB Hamiltonian as a fundamental interaction would require coupling the atoms to a rank-N tensor field, but in this case, every value of N would involve a different fundamental coupling. One could scarcely claim to be estimating the same coupling constant as N changes if the fundamental interaction is changing.

The most realistic possibility for taking advantage of multibody couplings in parameter estimation will be for pairwise couplings ($k = 2$). Hamiltonians with symmetrically parametrized two-body terms arise naturally in field-theoretic systems, such as quantum degenerate gases, superconductors, and atomic ensembles coupled to a common electromagnetic field mode. Atom-atom interactions in a Bose-Einstein condensate [18] might offer a physically realistic approach to surpassing the conventional Heisenberg limit, possibly even achieving $1/N^2$ scaling. We envisage situations where an external field modulates the strength of the two-body scattering term in the second-quantized condensate Hamiltonian. Such a modulation occurs for both a magnetically tuned Feshbach resonance and density variations due to gravitational gradients.

While exponential sensitivity improvements appear unphysical, more modest quadratic or other polynomial improvements beyond the Heisenberg limit could be essential for achieving the sensitivities required in the most demanding precision measurements.

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[15] Letting $|M_L\rangle$ be the eigenvector of $L = H + K$ with maximum eigenvalue M_L, we have $M_L = \langle M_L|L|M_L\rangle = \langle M_L|H|M_L\rangle + \langle M_L|K|M_L\rangle \leq M_H + M_K$, and similarly for $|m_L\rangle$. The triangle inequality follows.
[16] Maximization of $\Delta^2 H$ can be carried out in two steps. First, maximize $\Delta^2 H$ for fixed $\langle H\rangle = \mu M_H + (1-\mu)m_H$ to give $\Delta^2 H = \mu(1-\mu)(M_H - m_H)^2$, corresponding to probabilities $p_M = \mu$ and $p_m = 1-\mu$ for the maximum and minimum eigenvalues. Maximization over μ then gives the maximum variance $(M_H - m_H)^2/4$ at $\mu = 1/2$.
[17] The result underlying the bound (15) was obtained by Giovannetti *et al.* [5] for the case of discrete operations, as opposed to continuous time evolution, and was used there to show that multiround protocols with single-system probes (and allowing for ancillas and adaptive measurements) have the same optimal sensitivity as single-round protocols with multisystem entangled probes. We use the bound in a different way, and our derivation shows directly that the ultimate sensitivity cannot be improved when the auxiliary Hamiltonian $\tilde{H}$ acts simultaneously with the coupling Hamiltonian h_0.
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