Hypothesis testing with open quantum systems

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Using a quantum circuit model we derive the maximal ability to distinguish which of several candidate Hamiltonians describe an open quantum system. This theory, in particular, provides the maximum information retrievable from continuous quantum measurement records, available when a smaller open quantum system is perturbatively coupled to a broadband quantized environment.

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Two quantum states $\psi_0$ and $\psi_1$ can be distinguished unambiguously if they are orthogonal and, hence, eigenstates with different eigenvalues of a physical observable. If non-orthogonal states $\psi_0$, $\psi_1$ are provided with equal prior probabilities in an experiment, the strategy distinguishing them with the smallest error probability performs a projective measurement on orthogonal states $\psi_0$, $\psi_1$, chosen with largest possible overlap with $\psi_0$ and $\psi_1$, respectively. The state vector overlap $\alpha = \langle \psi_1 | \psi_0 \rangle$ specifies $|\langle \psi_0 | \psi_0 \rangle|^2 = \frac{1}{2}(1 + \sqrt{1 - |\alpha|^2})$, $\theta = 0, 1$, and the optimal guess that the prepared state was $\psi_0$ if one measures $\psi_0$, has an error probability of

$$P_e = \frac{1}{2}(1 - \sqrt{1 - |\alpha|^2}).$$ (1)

In this Letter, discrimination of quantum states is related to hypothesis testing [1] and parameter estimation [2]. To determine if the evolution of a quantum system is governed by one or another Hamiltonian, one must perform measurements on the system and use their outcome to infer which is the most likely assumption. We study the situation of an open quantum system, $S$, whose interaction with a broadband environment, $E$, permits the Born-Markov approximation, such that the average system behavior is described by a Lindblad master equation. Following Tsang [1], we will allow continuous monitoring of the environment as depicted in Fig. 1a. In [1] it was shown how to discriminate different hypotheses optimally from a given measurement record by solution of a conditional master equations, and, e.g., [3–10] have investigated strategies to obtain precise estimates of physical parameters and time-dependent excitation waveforms from detection signals.

Photon counting and field quadrature measurements represent different ways to probe an optical field with correspondingly different stochastic master equations [11–13]. Rather than addressing particular measurement schemes, we present a method to evaluate the optimal discrimination allowed by any detection protocol which involves monitoring of the environment of the system (the emitted radiation) and the final state of the system itself. Such an analysis is possible because, under the validity of the Born-Markov approximation, a sequence of measurements on the environment do not alter relaxation properties of system (no Zeno-effect), and they may be deferred to a final joint measurement of appropriate environment degrees of freedom. The temporal sequence of detector clicks associated with counting of photons emitted by an atom during time $[0, t]$, is for example equivalent to the counting at time $t$ of photons in volume elements at corresponding distances from the atom.

The information retrieved by measurement records is upper bounded by our ability to discriminate between unprobed states $\psi_0^{SE}(t)$ and $\psi_1^{SE}(t)$ of the system and environment which, according to (1), is given by their scalar product, $\alpha_{SE} = \langle \psi_1^{SE}(t) | \psi_0^{SE}(t) \rangle$. Evaluation of the joint quantum state of the system and environment is prohibitively complicated as it requires inclusion of a vast number of photon number states distributed in an entangled manner over a continuum of field modes. As shown in the following, the state vector overlap can be obtained without recourse to calculation of the states.

The principle behind our derivation is illustrated in Fig. 1. In part (a) of the figure we sketch the quantum system and its environment subject to the Hamil-
tonian $H_0$ and, possibly, to continuous probing of the radiation emitted into the environment. In part (b) of the figure, we introduce the ancilla $A$ and the ancilla qubit-controlled Hamiltonian $H_{ASE} = (|0\rangle\langle 0|)A \otimes H_0(t) + (|1\rangle\langle 1|)A \otimes H_1(t)$ which represents two different candidate Hamiltonians $H_0(t)$ or $H_1(t)$. Such inclusion of ancilla qubit degrees of freedom has been proposed for a variety of tasks, including quantum computing on mixed state quantum systems with one pure qubit [14], estimation of entanglement [15] and thermodynamical [16] properties. Similar, higher dimensional ancillary degrees of freedom are used in particle filter theory with stochastic master equations [5, 7]. For our aim, the ancillary qubit is a theoretical construction to represent alternative hypotheses or parameters in a convenient manner; our theory is not stochastic and it does not apply to any particular measurement protocol.

The combined ancilla, system and environment is initially prepared in a pure state $\frac{1}{\sqrt{2}}(|0\rangle_A + |1\rangle_A) \otimes |\psi^{SE}(t = 0)\rangle$, and it evolves into the state

$$\psi(t) = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |\psi_0^{SE}(t)\rangle + |1\rangle_A \otimes |\psi_1^{SE}(t)\rangle). \quad (2)$$

Note that the desired wave function overlap $\alpha_{SE} = \langle \psi_1^{SE}(t) | \psi_0^{SE}(t) \rangle$ can be formally evaluated as twice the expectation value of the raising operator, $\sigma_A^+ = (|1\rangle\langle 0|)_A$, of the ancilla qubit:

$$\langle \psi_1^{SE}(t) | \psi_0^{SE}(t) \rangle = 2 \sigma_A^+. \quad (3)$$

At this point we use our assumption that the Born-Markov approximation applies for the system-environment interaction, such that the environment degrees of freedom can be eliminated, and the reduced density matrix $\rho_{AS}$ of the system and the ancilla obeys a master equation.

We write the density matrix of the ancilla and the system as the following $2 \times 2$ matrix of matrices

$$\rho_{AS} = \frac{1}{2} \left( \begin{array}{cc} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{array} \right), \quad (4)$$

where $\rho_{00}$, acting on the system state space, are initially identical, $\rho_{00}(0) = \rho_0(0) = |\psi_S(0)\rangle\langle \psi_S(0)|$.

The rows and columns in (4) correspond to the different ancilla states which cause the evolution of the system and the environment under different Hamiltonians. If the hypotheses concern only the unitary part of the system evolution, we apply the ancilla and system Hamiltonian

$$H_{AS} = \left( \begin{array}{cc} H_{0}^S(t) & 0 \\ 0 & H_{1}^S(t) \end{array} \right), \quad (5)$$

while, to represent different environment couplings (e.g., different strengths or different system relaxation operators, the ancilla and the system are subject to Lindblad relaxation terms, $\dot{\rho}_{AS} = \sum_m \mathcal{D}[\hat{c}_m \rho_{AS} \hat{c}_m^\dagger]$, where $\mathcal{D}[\hat{c}]\rho \equiv \hat{c}^\dagger \rho \hat{c} - \frac{1}{2}(\hat{c}^\dagger \hat{c} \rho + \rho \hat{c}^\dagger \hat{c})$, and where $\hat{c}_m^{AS}$ is of the form:

$$\hat{c}_m^{AS} = \left( \begin{array}{cc} c_{m0}^0 & 0 \\ 0 & c_{m1}^1 \end{array} \right). \quad (6)$$

It follows from (3,4) that the desired overlap is given by the trace $\alpha_{SE} = Tr_S(\rho_{01})$. The matrix $\rho_{01}$ is subject to the combined action of the candidate Hamiltonians and relaxation terms, and solves the equation,

$$\dot{\rho}_{01} = \frac{1}{i\hbar}(H_{0}^S \rho_{01} - \rho_{01} H_{1}^S) + \sum_m (\hat{c}_{m0}^0 \rho_{01} \hat{c}_{m1}^1 - \frac{1}{2} (\hat{c}_{m0}^0)^\dagger \hat{c}_{m1}^1 \rho_{01} + \rho_{01} (\hat{c}_{m1}^1)^\dagger \hat{c}_{m0}^0). \quad (7)$$

This equation is structured like the Lindblad master equation, but all operators multiplying $\rho_{01}$ from the left (right) pertain to hypothesis 0 (1). Unlike the usual master equation which conserves the trace of the density matrix, the left and right multiplication with different Hamiltonian and Lindblad operators breaks this invariance and causes the non-trivial time evolution of $\alpha_{SE}$. In [17–19] quantum measurement theory was applied in an alternative derivation of Eq.(7). The present derivation is more straightforward and it allows generalization to a wider range of problems.

For illustration, consider a two-level atom with a ground state $|g\rangle$ and excited state $|e\rangle$ driven on resonance with a Rabi-frequency $\Omega_0 = 0$ or $\Omega_1 = 4\kappa$ while the excited state decays by fluorescence emission with a rate $\kappa$. The atom is initialized in its ground state at $t = 0$. It is straightforward to solve Eq.(7) with $H_{0}^S = \frac{\Omega_0}{2}(|e\rangle\langle g| + |g\rangle\langle e|)$ and identical Lindblad damping operators $\hat{c}_{e}^0 = \sqrt{\kappa}|g\rangle\langle e|$, and in Fig. 2, we show with the fat solid curve the error probability according to (1) with $|\alpha_{SE}|^2 = |\text{Tr}(\rho_{01}(t))|^2$. This curve yields the ultimate limit to our ability to discriminate among Rabi frequencies $\Omega_0$ and $\Omega_1$.

The detection of just a single photon is incompatible with $\Omega = 0$, while if no photon is detected our best guess among the two choices is that $\Omega = 0$. If $\Omega = \Omega_1$, the probability of detecting no photons until time $t$ can be obtained by propagating the so-called no-jump wave function of the system, $|\psi_{S,J}(t)\rangle = a(t)|g\rangle + b(t)|e\rangle$, according to a non-hermitian system Hamiltonian [11, 12], $H_{NJ} = \frac{\Omega_1}{2}(|e\rangle\langle g| + |g\rangle\langle e|) - \frac{\kappa}{2} |e\rangle\langle e|$, and the probability of observing no photon detection event is given by $P_{NJ} = |a(t)|^2 + |b(t)|^2$. The probability that $\Omega = \Omega_1$ is wrongly associated with $\Omega = 0$ is thus $\frac{1}{2}(|a(t)|^2 - |b(t)|^2)$, shown as the thin solid curve in Fig. 2. From an initial value of $\frac{1}{2}$ the error probability decreases, as it becomes less and less likely that no photon has been detected from the laser driven atom.

Had we instead considered the case, where only a measurement on the atom is allowed at the end of the interaction time $t$, such a measurement should distinguish between the two density matrices, $\rho_0$ and $\rho_1$, respectively.
evolved by the Lindblad master equations with the different Hamiltonians. The minimal probability of making an assignment error is here provided by Helstrom [20],

\[ P_e^t = \frac{1}{2} + \sum_{\gamma_j \leq 0} \gamma_j, \]

where the sum is over the negative eigenvalues of the operator \( \frac{1}{2}(\rho_1 - \rho_0) \). In Fig. 2, \( P_e^t \) is shown as the dotted green curve for the case of \( \Omega_0 = 0 \) and \( \Omega_1 = 4\kappa \). Since the system evolves into steady states with only partially distinguishable density matrices, the error probability by atomic detection does not approach zero in the long time limit.

The quantity \(|a(t)|^2\) derived above for the unnormalized no-jump wave function is the probability that, despite the non-vanishing \( \Omega = \Omega_1 \), no photon has been detected and the atom is in its ground state at time \( t \). Using a combination of photon counting and detection of the final atomic excitation thus yields the erroneous assignment (of a vanishing Rabi-frequency when \( \Omega = \Omega_1 \)) with a probability \(|a|^2/2\), shown as the dashed red curve in Fig. 2. We observe that at particular finite probing times, we can distinguish the hypotheses with certainty. These are the times where the no-jump wavefunction has no ground state population, and a non-vanishing Rabi frequency results in a photonic or atomic excitation with certainty.

The probability \(|a(t)|^2\) for observing no photon and no atomic excitation equals the population of the system and environment quantum state component with no excitations. This is precisely the state \( |\psi_{0E}^\theta(t)\rangle \) obtained for \( \Omega_0 = 0 \) and, hence the overlap between the candidate system and environment states is given by, \( |\alpha_{SE}|^2 = |a(t)|^2 \). The photon counting analysis thus allows calculation of the minimal error probability (1) which is, however, not reached by counting but by projecting on the orthogonal, highly entangled superposition states \( \{\psi_\theta^{SE}\} \) of the atom and the quantized radiation field.

Two non-vanishing Rabi frequencies both permit excitation of the system and emission of radiation, and our no-jump analysis does not suffice to determine the overlap \( \alpha_{SE} \). Eq.(7) is readily solved for any sets of hypotheses about Rabi frequencies, and we find that, for a vanishing detuning, our ability to distinguish two real Rabi frequencies depends only on their difference \( \Omega_1 - \Omega_0 \). Despite the striking fact that the pair of candidate values \( \Omega_0 = -2\kappa \), \( \Omega_1 = 2\kappa \), yield completely equivalent photon count signals and final atomic excited state populations, according to Eq.(7) they are equally well distinguished as \( \Omega_0 = 0 \), \( \Omega_1 = 4\kappa \). To reveal the sign of the Rabi frequency, the measurement must be sensitive to the phase of the emitted field and the excited state amplitude in the atom. The dependence on only \( \Omega_1 - \Omega_0 \) occurs because addition of an extra driving Hamiltonian which commutes with all the other Hamiltonian terms causes a common unitary rotation and hence no change of the overlap of the system and environment states, \( \psi_\theta^{SE} \). Extra Rabi frequency terms do not, however, commute with detuning terms in the Hamiltonian, and we obtain different results when the system is probed off resonance.

Figure 2: (Color online) Time dependent probability for erroneously assigning whether an atom with decay rate \( \kappa \) is excited resonantly with a Rabi frequency of \( \Omega_0 = 0 \) or \( \Omega_1 = 4\kappa \). The error probability is shown for a purely atomic measurement (green, dotted curve), photon counting (blue, thin solid curve), photon counting and a measurement of the final atomic excitation (red, dashed curve). The black, fat solid curve shows the minimal error achievable by any measurement on the system and the radiation field.
ically from the scalar products among states $\psi(\theta), \psi(\theta + \Delta\theta_1), \psi(\theta + \Delta\theta_2)$ or by a perturbative expansion of the master equation [17, 19]. The measurements saturating the Cramér-Rao bound may, however, be hard to find in practice. As shown in [17] photon counting is for example excellent for some parameters, but superseded by homodyne detection for others.

One may readily imagine strategies to improve experiments and obtain better discrimination or parameter estimation. Our theory constitutes an excellent starting point for such an optimization effort, where, e.g., the initial state and an available control Hamiltonian on the system added to both $H_0$ and $H_1$ in (7) can be varied with the aim to minimize $|\text{Tr}(\rho_{01}(t))|^2$. Further system measurements are described by the action of completely positive maps which may either attain a continuous Lindblad form or they may apply discrete transformations $\rho_{01} \rightarrow \sum_n K_n \rho_{01} K_n^\dagger$ with $\sum_n K_n^\dagger K_n = I$. The information gain from such measurements is assessed by the value of $|\text{Tr}(\rho_{01}(t))|^2$, which may, in turn, be minimized by variation of the measurement operators.

As an example of such optimization, we have considered the ability to distinguish whether a two level system is driven on resonance or with a given detuning $\delta$ (caused, e.g., by dispersive coupling to an external influence). After a fast transient, the error probability for this assignment decays exponentially with time, and since Eq.(7) is a linear set of equations, we can find the characteristic time scale of this decay from the eigenvalue of the corresponding $4 \times 4$ matrix with the smallest (negative) real part. We expect that there exists an optimum Rabi-frequency since very weak probing yields no signal while very strong probing causes power broadening of the transition. In Fig. 3, we show the flow of the relevant complex eigenvalue $\lambda$ under variation of the Rabi frequency between 0 and $2\kappa$. The curves represent different detunings, $\delta = 0.5\kappa, ..., 2.5\kappa$, that we want to distinguish from zero, and they all approach a vanishing real part for $\Omega \rightarrow 0$, while the largest negative real part, and hence the fastest convergence of $\alpha_{SF}$, is found for intermediate values of $\Omega \sim 0.75\kappa$, except for the smallest detuning which is ideally distinguished with a weaker probe field, $\Omega = 0.62\kappa$.

Our introduction of an ancilla to encode different hypotheses allows us to regard the quantity $\langle \sigma_+^A \rangle$ as the expectation value of a real physical observable. This implies that we may evaluate this quantity by a host of standard methods in quantum theory: evolution in the Heisenberg picture, input-output theory, phase space distribution functions, ... . In some problems, continuous variable states may be restricted to Gaussian Wigner functions, which can be represented efficiently by their first and second moments only [9, 23] (this also applies in some hybrid systems with mixed continuous and discrete variables, cf, e.g., [24]). Rather than solving a master equation exactly, we may also use perturbative or variational methods to evaluate the desired expectation values with sufficient precision. Many-body systems may thus be well described by effective approximations, such as Hartree or Hartree-Fock mean fields, multi-orbital mean-field theory [21], and matrix product states [22], to mention a few. Also, the Monte Carlo Wave Function method [11, 12] yields correct mean values via wave functions that evolve due to simulated measurements on the environment of a quantum system. Notably, even though the measurements simulated may not distinguish the hypotheses (such as photon counting does not distinguish Rabi frequencies of opposite signs), we can simulate the time-evolution of (4) and thus determine $\langle \sigma_+^A \rangle$ which yields the achievements of the optimal detection scheme.

In conclusion, we have used a circuit model with a qubit ancilla to address hypothesis testing and parameter estimation. We have identified a simple reduced system state operator and an associated effective master equation that yield the scalar product between pure quantum states of the system and the environment. This scalar product sets the limit to how well the states, and hence the evolution hypotheses, may be distinguished by any measurement scheme. Optimal distinguishability is achieved by projection on entangled states of the system and the environment suggests, which may be approximated by adaptive schemes applying feedback on the system or choosing among measurements according to earlier detection outcomes [9, 25, 26]. The effective evaluation of the theory makes it a good starting point for optimization and for studies of the role of finite detection efficiency and unobserved dissipation channels [6, 10]. It may also provide crucial insights into the consequence of, e.g., measurement feedback, phase transitions and large deviation behaviour [9, 27–29] for hypothesis testing and

![Figure 3: Complex eigenvalues (with the smallest negative real part) of Eq.(7) for the distinction of the detuning $\delta$ from zero, shown for different discrete values of $\delta$, and for Rabi frequencies $\Omega$ varied continuously between 0 (lower endpoint of each curve) and 2$\kappa$. The leftmost point of each curve reveals the largest negative value attained and thus the optimal rate of convergence of the assignment error.](image-url)
parameter estimation.

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