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Quantum state transformation by optimal projective measurements

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Abstract This paper explores the optimal control of quantum state transformations in finite-dimensional quantum systems by a sequence of non-selective projective measurements. In our schemes, the projectors of each measurement are represented by a unitary matrix. Through variational analysis of the objective function over the unitary group, the necessary condition for a measurement sequence to be a critical point of the underlying state transformation objective is found to be a highly symmetric form as a chain of equalities. Since these equality relations are generally difficult to solve analytically, we focus on the fundamental case employing a single measurement, in which analytical solutions for maximizing the state transformation probability are found between pure states, or between mixed and pure states, or between orthogonal mixed states under two typical type of measurements. These results suggest a new way of designing optimal quantum dynamics control strategies by quantum measurements.

Keywords Quantum control · Quantum measurement · Projective measurement · Optimal control

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1 Introduction

The control of quantum processes is a thriving area of research, both theoretically [1–5] and experimentally [6,7]. So far, most studies have been concerned with coherent manipulation of quantum dynamics, but recently other incoherent driving forces, such as laser noise, decoherence from the environment, and quantum observations, have drawn attention. In contrast to the natural expectation that the influence of incoherent forces will be deleterious toward achieving desired control [8], recent studies [9,10] have shown that controlled quantum dynamics can survive intense field noise and decoherence, and can even cooperate with them under special circumstances [11]. With these observations, it is possible to enhance the target goal more effectively with the help of laser noise and environmental decoherence.

It is well-known that both the outcome and back-action of quantum measurements can be employed to control quantum processes. In the standard closed-loop optimal control experiments [12], the quantum system is non-selectively measured at the end of the controlled quantum evolution trials, and the recorded outcome is processed by a learning algorithm to further optimize the laser pulse. Quantum measurements were also applied to map an unknown mixed state to some target pure state [13] by exploiting the resultant back action based on which coherent control can be selectively performed [14], and shown to be necessary in some laser control [15], dephasing decoherence control [16] and incoherent control problems [17]. One can also achieve quantum control using continuous measurements, e.g., the control of the population branching ratio between two degenerate states [18]. In [19,20], the effect of non optimized measurements upon control by lasers was investigated.

Numerical simulations have been carried out to investigate the ability of manipulating quantum dynamics by quantum measurements [21]. Optimal coherent control fields were shown to be capable of cooperating or fighting with quantum measurements to achieve a good yield, and the performance may be optimized so as to more effectively control the quantum dynamics. Quantum measurements can also increase the controllability of a quantum system by breaking dynamical symmetries, e.g., the quantum Zeno and anti-Zeno effects. In the absence of an active coherent control, instantaneous projective measurements were shown to be capable of driving population transfer in a two-level system, and a scheme for maximal population transfer was found under an arbitrary finite number of measurements, where the quantum anti-Zeno effect can be recovered in the limit of continuous measurements [22,23].

This paper will explore measurement induced quantum state control in more general finite-dimensional quantum systems, in which the problem is more complex and has richer features. The paper is organized as follows. In Sect. 2, we introduce some basic concepts and notation about non-selective measurements and formulate the target function. In Sect. 3, we parametrize a class of equivalent measurements by a unitary matrix, for which a variational analysis can be done over the unitary group. Section 4 analyzes some physically interesting examples with a single projective measurement, including the maximal transformation probability between two pure states, between a pure state and a mixed state, and between two orthogonal mixed states. Concluding remarks are presented in Sect. 5.

2 Quantum control by projective measurements

Consider a general N-level quantum system, with ρ being the density operator of the system, and A is some physical observable to be measured. As A is a Hermitian operator on the Hilbert space, we can express the self adjoint operator A as

$$A = \sum_{i=1}^{n} a_i P_i, \tag{1}$$

where each P_i is a projection operator onto the eigenspace corresponding to the eigenvalue a_i. The projection operators satisfy

$$P_i P_j = \delta_{ij} P_i \tag{2a}$$

$$\sum_{i=1}^{n} P_i = 1 \tag{2b}$$

The result a_i of a selective projective measurement of A is obtained with probability $p_i = \mathrm{Tr} P_i \rho_0$, where ρ_0 is the state of the system before the measurement. The state of the system collapses to $P_i \rho_0 P_i / p_i$ after the selective measurement, if the result reads a_i. If the measurement result is discarded, then the measurement becomes a non-selective one, and the system state after the measurement is the average of all possible outcomes

$$\mathcal{M}(\rho) = \sum_{i=1}^{n} P_i \rho_0 P_i. \tag{3}$$

As we can see from the formalism, an important effect of the quantum measurement is that it generally changes the quantum state. This is usually taken as an inevitable disturbance of the system. However, the measurement can also be employed to actively control the quantum system dynamics. Suppose that we can perform m projective measurements within some time interval, and represent the k-th measurement by $\mathcal{M}^{(k)}$ characterized by n_k projectors $\{P_{i_k}^{(k)}\}$, $i_k = 1, \ldots, n_k$, which satisfy

$$P_{i_k}^{(k)} P_{j_k}^{(k)} = \delta_{i_k j_k} P_{i_k}^{(k)} \tag{4a}$$

$$\sum_{i_k=1}^{n_k} P_{i_k}^{(k)} = I. \tag{4b}$$

If the measurement $\mathcal{M}^{(k)}$ is nonselective, then the quantum state changes from ρ_0 to $\mathcal{M}^{(k)}(\rho_0) = \sum_{i_k=1}^{n_k} P_{i_k}^{(k)} \rho_0 P_{i_k}^{(k)}$. After successively performing the measurements $\mathcal{M}^{(1)}, \mathcal{M}^{(2)}, \ldots, \mathcal{M}^{(m)}$, the final resultant ρ_f becomes:

$$\rho_f = \mathcal{M}^{(m)}\mathcal{M}^{(m-1)}\ldots\mathcal{M}^{(1)}(\rho_0)$$
$$= \sum_{i_m=1}^{n_m}\cdots\sum_{i_1=1}^{n_1} P_{i_m}^{(m)}\ldots . P_{i_1}^{(1)}\rho_0 P_{i_1}^{(1)}\ldots P_{i_m}^{(m)} \tag{5}$$

Consider the objective of driving the system from some initial state ρ_0 to a final state θ, or maximing the expectation value of some desired quantum observable θ, where we set our goal as choosing the proper sequenced operators $P_{i_k}^{(k)}, i_k = 1, \ldots, n_k, k = 1, \ldots, m$ to maximize the target function

$$J\left[P_1^{(1)}, \ldots, P_{n_1}^{(1)}, \ldots, P_1^{(m)}, \ldots, P_{n_m}^{(m)}\right]$$
$$= \mathrm{Tr}\left[\theta \sum_{i_m=1}^{n_m}\cdots\sum_{i_1=1}^{n_1} P_{i_m}^{(m)}\ldots P_{i_1}^{(1)}\rho_0 P_{i_1}^{(1)}\ldots P_{i_m}^{(m)}\right]. \tag{6}$$

The general case could include a coherent external field for additional control. We also neglect the free evolution between measurements, which is easy to include via a transformation between the Schrdinger picture and interaction picture, as discussed before [23]. For simple 2-level quantum systems, with the help of Pauli matrices, a complete analytical solution is found including explicit expressions for the optimal measured observables and for the maximal objective value given any expected system state, any initial system density matrix, and any number of measurements [22]. However, for general N-level quantum systems, $N > 2$, the analysis is much more difficult, and further study is necessary.

3 Necessary condition for optimal projective measurements

In an N-dimensional Hilbert space, the n projectors $\{P_i\}$, $i = 1, \ldots, n$, which characterize a single measurement $\mathcal{M}$, are orthogonal and commutable,

$$P_i P_j = P_j P_i = 0, \quad \text{for } i \neq j. \tag{7}$$

so there exists a unitary matrix U which can diagonize all the projectors simultaneously,

$$P_i = U I_i U^\dagger, \quad i = 1, \ldots, n. \tag{8}$$

Here $\{I_1, \ldots, I_n\}$ are diagonal matrices whose diagonal elements are either 1 or 0, and the summation of all I_i is the identity operator in the N-dimensional space,

$$\sum_{i=1}^{n} I_i = U^\dagger\left(\sum_{i=1}^{n} P_i\right)U = I, \tag{9}$$

because the projectors $\{P_i\}$, $i = 1, \ldots, n$, are complete (Eq. 2b). Consequently, quantum measurements could be classified by the set of diagonal matrices $\{I_1, \ldots, I_n\}$. In the same class, the corresponding projectors are equivalent up to multiplication by a unitary matrix. Hence, a measurement $\mathcal{M}^{(k)}$ in a class can be characterized by a unitary matrix U_k,

$$\begin{aligned}\rho_k = \mathcal{M}(U_k)\rho_0 &= \sum_{i_k=1}^{n_k} P_{i_k}^{(k)} \rho_0 P_{i_k}^{(k)} \\ &= \sum_{i_k=1}^{n_k} U_k I_{i_k}^{(k)} U_k^\dagger \rho_0 U_k I_{i_k}^{(k)} U_k^\dagger \end{aligned} \tag{10}$$

which is more convenient than the n_k projectors $\{P_{i_k}^{(k)}\}$, $i_k = 1, \ldots, n_k$. Therefore, the target yield after being measured for m times can be written as a function of the unitary matrices

$$J[U_1, \ldots, U_m] = \mathrm{Tr}\,[\theta \mathcal{M}(U_m) \ldots \mathcal{M}(U_1)\rho_0]. \tag{11}$$

It should be pointed out that the target yield also depends on $\{r_{i_k}^{(k)}\}$, the set of ranks of projectors $\{I_{1,} \cdots, I_n\}$

$$r_{i_k}^{(k)} \equiv \mathrm{rank}\left(I_{i_k}^{(k)}\right) = \mathrm{rank}\left(P_{i_k}^{(k)}\right). \tag{12}$$

which has not been optimized in this paper.

Suppose that J achieves the maximum value at $\mathcal{U} = \{U_1, \ldots, U_m\}$, we can parametrize its neighborhood by $\{e^{i\delta A_1} U_1, \ldots, e^{i\delta A_m} U_m\}$, where $\{\delta A_k\}$ are arbitrary infinitesimal Hermitian matrices, with which we can conveniently calculate the variation of $\{U_k\}$ by taking first-order term in the Taylor expansion, and hence that of $P_{i_k}^k$ as below

$$\begin{aligned}\delta P_{i_k}^{(k)} &= \delta U_k I_{i_k}^{(k)} U_k^\dagger + U_k I_{i_k}^{(k)} \delta U_k^\dagger \\ &= i\delta A_k U_k I_{i_k}^{(k)} U_k^\dagger - i U_k I_{i_k}^{(k)} U_k^\dagger \delta A_k \\ &= i[\delta A_k, P_{i_k}^{(k)}]. \end{aligned} \tag{13}$$

Then, substituting $\delta P_{i_k}^{(k)}$ into δJ gives

$$\begin{aligned}\delta J &= \delta \mathrm{Tr}\,[\theta \mathcal{M}(U_m) \ldots \mathcal{M}(U_1)\rho_0] \\ &= i \sum_{k=1}^{m} \sum_{i_m=1}^{n_m} \ldots \sum_{i_1=1}^{n_1} \mathrm{Tr}\{P_{i_m}^{(m)} \ldots P_{i_{k+1}}^{(k+1)} \left[\delta A_k, P_{i_k}^{(k)}\right] P_{i_{k-1}}^{(k-1)} \ldots P_{i_1}^{(1)} \rho_0 P_{i_1}^{(1)} \ldots \\ &\quad \times P_{i_m}^{(m)} \theta + P_{i_m}^{(m)} \ldots P_{i_1}^{(1)} \rho P_{i_1}^{(1)} \ldots P_{i_{k-1}}^{(k-1)} [\delta A_k, P_{i_k}^{(k)}] P_{i_{k+1}}^{(k+1)} \ldots P_{i_m}^{(m)} \theta\} \end{aligned}$$

$$= i \sum_{k=1}^{m} \sum_{i_k=1}^{n_k} \mathrm{Tr}\{\left[\delta A_k, P_{i_k}^{(k)}\right] (\mathcal{M}(U_{k-1}) \ldots \mathcal{M}(U_1) \rho_0 P_{i_k}^{(k)} \mathcal{M}(U_{k+1}) \ldots \mathcal{M}(U_m) \theta$$
$$+ \mathcal{M}(U_{k+1}) \ldots \mathcal{M}(U_m) \theta P_{i_k}^{(k)} \mathcal{M}(U_{k-1}) \ldots \mathcal{M}(U_1) \rho_0)\}, \tag{14}$$

which leads to the condition for the critical points

$$\delta J = i \mathrm{Tr} \sum_{k=1}^{m} \delta A_k \{[\mathcal{M}(U_k) \ldots \mathcal{M}(U_1)\rho_0, \mathcal{M}(U_{k+1}) \ldots \mathcal{M}(U_m)\theta]$$
$$- [\mathcal{M}(U_{k-1}) \ldots \mathcal{M}(U_1)\rho_0, \mathcal{M}(U_k) \ldots \mathcal{M}(U_m)\theta]\} \equiv 0 \tag{15}$$

For arbitrary Hermitian matrices $\{\delta A_k\}$, $k = 1, \ldots, m$, this implies that

$$[\mathcal{M}(U_k) \ldots \mathcal{M}(U_1)\rho_0,\ \mathcal{M}(U_{k+1}) \ldots \mathcal{M}(U_m)\theta]$$
$$= [\mathcal{M}(U_{k-1}) \ldots \mathcal{M}(U_1)\rho_0,\ \mathcal{M}(U_k) \ldots \mathcal{M}(U_m)\theta], \tag{16}$$

for all $k = 1, \ldots, m$, which are a chain of equalities:

$$\begin{aligned}
&[\rho_0, \mathcal{M}(U_1) \ldots \mathcal{M}(U_m)\theta] \\
&= \ldots \\
&= [\mathcal{M}(U_k) \ldots \mathcal{M}(U_1)\rho_0, \mathcal{M}(U_{k+1}) \ldots \mathcal{M}(U_m)\theta] \\
&= \ldots \\
&= [\mathcal{M}(U_m) \ldots \mathcal{M}(U_1)\rho_0, \theta].
\end{aligned} \tag{17}$$

These equalities form the necessary condition for optimal measurements to yield a maximal outcome. Any measurements satisfying these equations can be a maximum, minimum or a saddle point of the target function.

4 Optimal state transformation by a single quantum measurement

There are many numerical algorithms to optimize the state transformation probability [24], but more insight can be obtained from analytical solutions, which will be discussed in this section. The optimal solutions with an arbitrary number of measurements have been obtained analytically for the transformation between two arbitrary states in simple two-level quantum systems [22]. However, the extension to general N-level quantum systems is not trivial. In principle, from the chain of Eq. (16), each equality has the form of a single measurement case,

$$[\mathcal{M}(U_k)\rho_{k-1}, \theta_{m-k}] = [\rho_{k-1}, \mathcal{M}(U_k)\theta_{m-k}] \tag{18}$$

for the following initial and final states

$$\rho_{k-1} = \mathcal{M}(U_{k-1}) \ldots \mathcal{M}(U_1)\rho_0, \tag{19a}$$
$$\theta_{m-k} = \mathcal{M}(U_{k+1}) \ldots \mathcal{M}(U_m)\theta. \tag{19b}$$

This suggests that the problem for multiple measurements is equivalent to the problem with a single measurement but between two arbitrary mixed states, even if both the intial and final states are pure states. However, even the latter equations are not easy to solve for general N-level quantum systems. To illuminate the nature of the measurement induced control, we restrict ourselves to several physically interesting and important cases to which analytical solutions are available.

4.1 Transformation between pure states

Consider the transformation between two pure states $|\alpha\rangle$ and $|\beta\rangle$ induced by one measurement represented by N 1-rank projectors. Then Eq. (16) for a single measurement can be reduced to:

$$[\mathcal{M}(U)\rho, \theta] = [\rho, \mathcal{M}(U)\theta] \tag{20}$$

in which $\rho = |\alpha\rangle\langle\alpha|$ $\theta = |\beta\rangle\langle\beta|$. The target function J is:

$$\begin{aligned} J &= \sum_{i=1}^{N} \langle i| U^{\dagger} |\alpha\rangle \langle\alpha| U |i\rangle \langle i| U^{\dagger} |\beta\rangle \langle\beta| U |i\rangle \\ &= \sum_{i=1}^{N} |\alpha_i|^2 |\beta_i|^2 \end{aligned} \tag{21}$$

where $\alpha_i = \langle i|U^{\dagger}|\alpha\rangle$, $\beta_i = \langle i|U^{\dagger}|\beta\rangle$ and $\langle\alpha|\beta\rangle = \sum_{i=1}^{D} \alpha_i^* \beta_i \equiv \gamma$.

Calculating the matrix elements of Eq. (20) separately, we can see that:

$$\left(\alpha_p^*\alpha_p - \alpha_q^*\alpha_q\right) \beta_p^*\beta_q + \left(\beta_p^*\beta_p - \beta_q^*\beta_q\right) \alpha_p^*\alpha_q = 0, \quad 1 \le p, q \le N. \tag{22}$$

If some $\alpha_p = 0$, then we have $\alpha_q^*\alpha_q\beta_p^*\beta_q = 0$, for any other $q \neq p$. If further $\beta_p = 0$, then these equations pose no constraints on the remaining α_q and β_q. Otherwise, $\alpha_q^*\alpha_q\beta_q = 0$, which implies that either $\alpha_q = 0$ or $\beta_q = 0$. This indicates for any subscript p, $\alpha_p\beta_p = 0$ and the corresponding target function J is also 0.

The only case left now is that $\alpha_p \neq 0 \neq \beta_p$, in which case we can transform Eq. (22) into

$$\frac{\alpha_p}{\alpha_q} - \frac{\alpha_q^*}{\alpha_p^*} + \frac{\beta_p}{\beta_q} - \frac{\beta_q^*}{\beta_p^*} = 0. \tag{23}$$

Suppose that $\alpha_p/\alpha_q = re^{i\phi}$ and $\beta_p/\beta_q = se^{i\psi}$, then

$$\left(s - s^{-1}\right) e^{i\phi} = -\left(r - r^{-1}\right) e^{i\psi}, \tag{24}$$

which leads to two possible relationships between any $p \neq q$:

$$\begin{cases} (i). \ \frac{\alpha_p}{\alpha_q} = \frac{\beta_q^*}{\beta_p^*} \\ (ii). \ \frac{\alpha_p}{\alpha_q} = -\frac{\beta_p}{\beta_q} \end{cases}. \tag{25}$$

Denote the sets of pairs (p, q) which satisfy (i) by $\{S_i\}$, pairs in S_i, S_j $i \neq j$ satisfy (ii). If there are more than two such sets, we will find, for example, $\frac{\alpha_{S_1}}{\alpha_{S_2}} = -\frac{\beta_{S_1}}{\beta_{S_2}}$, $\frac{\alpha_{S_1}}{\alpha_{S_3}} = -\frac{\beta_{S_1}}{\beta_{S_3}}$ consequently $\frac{\alpha_{S_2}}{\alpha_{S_3}} = \frac{\beta_{S_2}}{\beta_{S_3}}$ which contradicts with the assumption $\frac{\alpha_{S_2}}{\alpha_{S_3}} = -\frac{\beta_{S_2}}{\beta_{S_3}}$. Thus, the number of such equivalent sets is at most two.

If there is only one set S_1, then it is easy to see that $\alpha_i^* \beta_i = \gamma/n$, in which n is the number of non-zero pairs in $(\alpha_i, \ \beta_i)$, and the value of the target function J is $\frac{|\gamma|^2}{n}$. If there are two sets S_1 and S_2, we can easily prove that the norms of all α_p are identical, as well as those of all β_p, and the relative phase between each (α_p, β_p) pair is constant within each subset. Therefore, we can write α_i and β_i as:

$$\begin{array}{rl} \alpha = & (r_1 e^{i\phi_1}, \ \ldots \ , r_1 e^{i\phi_{n_1}}, \quad r_2 e^{i\delta_1}, \ \ldots \ , r_2 e^{i\delta_{n_2}}, \quad 0, \ldots, 0) \\ \beta = & \underbrace{(z r_1 e^{i\phi_1}, \ldots, z r_1 e^{i\phi_{n_1}},}_{S_1} \ \underbrace{-z r_2 e^{i\delta_1}, \ldots, -z r_2 e^{i\delta_{n_2}},}_{S_2} \ \underbrace{0, \ldots, 0)}_{\text{zero part}} \end{array} \tag{26}$$

from which we derive the following equations:

$$\begin{cases} n_1 r_1^2 + n_2 r_2^2 & = 1 \\ |z|^2 (n_1 r_1^2 + n_2 r_2^2) & = 1 \\ z(n_1 r_1^2 - n_2 r_2^2) & = \gamma, \end{cases} \tag{27}$$

and thereby specify the corresponding critical values of the target function as follows

$$\begin{aligned} J &= |z|^2 (n_1 r_1^4 + n_2 r_2^4) \\ &= \frac{(1 \pm |\gamma|)^2}{4n_1} + \frac{(1 \mp |\gamma|)^2}{4n_2}. \end{aligned} \tag{28}$$

It is easy to see that the maximal value is $\frac{1+|\gamma|^2}{2}$ when $n_1 = n_2 = 1$. Compared with the case with only one set S_1, whose maximal value occurs when $n = 2$, we can determine that the global maximum value is $\frac{1+|\gamma|^2}{2}$, i.e., the maximum transition probability between two pure states (with overlap amplitude $|\gamma|$) by a single measurement.

In conclusion, the maximal state transition probability between two pure states $|\alpha\rangle$ and $|\beta\rangle$ is

$$J_{\max} = \frac{1 + |\langle\alpha|\beta\rangle|^2}{2}. \tag{29}$$

It is interesting to note that, the maximum of the N-level system is just the same as that of a simple 2-level system spanned by the initial state $|\alpha\rangle$ and the final state $|\beta\rangle$, which has been extensively studied [22,23].

4.2 Transformation between mixed and pure states

Here we consider the transformation between a mixed state and a pure state, where the measurement involves only two projectors, $P = |v\rangle\langle v|$ and its complement $Q = I - P$. Thus, the quantum state will be randomly projected onto the state $|v\rangle$ or into its orthogonal subspace after the measurement. Such measurements are interesting for two reasons. Firstly, the measurement procedure produces only two exclusive results, success or failure, e.g. the test of an unknown state whether it has a certain component characterized by a pure state. Many experiments fall into this category [25]. Secondly, the resulting maximization problem can be reduced from being on the unitary group to the Hilbert space, which, as will be seen below, greatly simplifies the derivation.

For this case, Eq. (20) still applies, but here we will present a more direct proof. Suppose that the desired pure desired state is $|1\rangle$ and the initial mixed state is ρ, then after the measurement, the initial state ρ becomes

$$\rho' = P\rho P + (I - P)\rho(I - P), \tag{30}$$

and our goal is to maximize $\mathrm{Tr}(\rho' |1\rangle \langle 1|)$. First, we can simplify this problem by rotating the last $N - 1$ basis vectors by applying the proper unitary transformation

$$U = \begin{bmatrix} 1 & 0 \\ 0 & U' \end{bmatrix} \tag{31}$$

that keeps $|1\rangle \langle 1|$ unchanged and changes ρ into the following form:

$$\tilde{\rho} = \begin{bmatrix} \tilde{\rho}_{11} & \tilde{\rho}_{12} & \tilde{\rho}_{13} & \cdots & \tilde{\rho}_{1N} \\ \tilde{\rho}_{21} & \tilde{\rho}_{22} & 0 & \cdots & 0 \\ \tilde{\rho}_{31} & 0 & \tilde{\rho}_{33} & 0 & \vdots \\ \vdots & \vdots & 0 & \ddots & 0 \\ \tilde{\rho}_{N1} & 0 & \cdots & 0 & \tilde{\rho}_{NN} \end{bmatrix}. \tag{32}$$

Note that this unitary transform will not change the maximum of $\mathrm{Tr}(\rho' |1\rangle \langle 1|)$,

$$\begin{aligned} \mathrm{Tr}(\rho' |1\rangle \langle 1|) &= \mathrm{Tr}(U^\dagger \rho' U U^\dagger |1\rangle \langle 1| U) \\ &= \mathrm{Tr}(U^\dagger (P\rho P + (I - P)\rho(I - P)) U U^\dagger |1\rangle \langle 1| U) \\ &= \mathrm{Tr}((P'\tilde{\rho}P' + (I - P')\tilde{\rho}(I - P')) |1\rangle \langle 1|) \\ &= \mathrm{Tr}(\tilde{\rho}' |1\rangle \langle 1|) \end{aligned} \tag{33}$$

where $\tilde{\rho}' = P'\tilde{\rho}P' + (I - P')\tilde{\rho}(I - P')$, and $P' = U^\dagger P U$. Hence we just need to optimize $\mathrm{Tr}(\tilde{\rho}' |1\rangle \langle 1|)$.

Let $|v\rangle = (x_1, x_2, x_3, \ldots, x_N)$, which generates the projector $P' = |v\rangle\langle v|$, and direct calculation shows

$$\begin{aligned}\mathrm{Tr}(\tilde{\rho}'\,|1\rangle\langle 1|) &= \tilde{\rho}_{11} + 2\,|x_1|^2\left(|x_1|^2\,\tilde{\rho}_{11} + \cdots + |x_N|^2\,\tilde{\rho}_{NN} - \tilde{\rho}_{11}\right)\\ &\quad + \left(2\,|x_1|^2 - 1\right)\left(x_1\left(x_2^*\tilde{\rho}_{21} + \cdots + x_N^*\tilde{\rho}_{N1}\right) + c.c.\right)\\ &= \frac{\tilde{\rho}_{11}}{2} + 2\left(\left(z_1 - \frac{1}{2}\right)^*, z_2^*, \ldots, z_N^*\right)\tilde{\rho}\left(\left(z_1 - \frac{1}{2}\right)^*, z_2^*, \ldots, z_N^*\right)^\dagger\end{aligned} \tag{34}$$

where $z_i = x_1^* x_i$. The function $\mathrm{Tr}(\tilde{\rho}'\,|1\rangle\langle 1|)$ achieves its maximum when $((z_1 - \frac{1}{2})^*, z_2^*, \ldots, z_N^*)^\dagger$, whose modulus is $\frac{1}{2}$, is the eigenvector of $\tilde{\rho}$ corresponded to its largest eigenvalue, and the maximum value is $\frac{\tilde{\rho}_{11}+\mathrm{Max}\{\tilde{\lambda}_i\}}{2}$ in which $\{\tilde{\lambda}_i\}$ are the eigenvalues of $\tilde{\rho}$. The unitary transformation U in Eq. (31) does not change ρ_{11} and the eigenvalues of ρ, so the maximum is just $\dfrac{\rho_{11} + \mathrm{Max}\{\lambda_i\}}{2}$ where$\{\lambda_i\}$ are the eigenvalues of ρ.

In conclusion, the maximal transformation probability between the mixed state ρ and the pure state $|\beta\rangle$ induced by the measurement is

$$J_{\max} = \frac{\rho_{\max} + \langle\beta|\rho|\beta\rangle}{2}, \tag{35}$$

and the vector generating the optimal projector $P = |v\rangle\langle v|$ is

$$|v\rangle = \frac{|\rho_{\max}\rangle + |\beta\rangle}{\||\rho_{\max}\rangle + |\beta\rangle\|}, \tag{36}$$

where $|\rho_{\max}\rangle$ is the eigenvector of ρ with the largest eigenvalue $\rho_{\max}$, and the phase of $|\rho_{\max}\rangle$ is fixed by $\langle\rho_{\max}|\beta\rangle$ being real. The maximum yield (i.e., the state transformation probability) only depends on $\rho_{\max}$ and the overlap of the pure state and the mixed state. In particular, the value of the maximal yield between two pure states is same as that produced by N independent projectors, Eq. (29) in Sect. 4.1. However, numerical simulations show that this might not be true when one of the states is mixed [26].

4.3 Transformation between orthogonal mixed states

Although the measurement-induced transformation between two arbitrary mixed states is hard to analyze, the special case of the transformation between two orthogonal mixed states ρ and θ (i.e., $tr(\rho\theta) = 0$) can be treated. Under the same two-projector measurements, without loss of generality, we assume that the initial state ρ is diagonalized, so that

$$0 = \mathrm{Tr}\rho\theta = \sum_{k=1}^{N} \rho_{kk}\theta_{kk}, \tag{37}$$

where ρ_{kk} and θ_{kk} are all non-negative diagonal elements. As ρ_{kk} is positive, then θ_{kk} must be zero, and consequently all θ_{kj}, $j = 1, \ldots, N$ have to vanish [27]. Hence, the initial and desired states can be decomposed into

$$\rho = \rho_1 I_{k_1} \oplus \cdots \oplus \rho_r I_{k_r} \oplus 0 \cdot I_{\sum l_i} \oplus 0 \cdot I_{H_0} \tag{38a}$$
$$\theta = 0 \cdot I_{\sum k_i} \oplus \theta_1 I_{\ell_1} \oplus \cdots \oplus \theta_s I_{\ell_s} \oplus 0 \cdot I_{H_0} \tag{38b}$$

where the nonzero eigenvalues $\rho_1, \ldots, \rho_r, \theta_1, \ldots, \theta_s$ correspond to eigenspaces $H_1^\rho, \ldots, H_r^\rho, H_1^\theta, \ldots, H_s^\theta$, and $\{I_{k_i}, I_{l_j}\}$ are identity matrices on these eigenspaces (k_i and l_j are the degeneracy of the eigenvalues). In addition, their common zero eigenspace is denoted by H_0. Again, let the projector be $P = |v\rangle\langle v|$, the target function is

$$\begin{aligned} J(v) &= \mathrm{Tr}[(P\rho P + (I - P)\rho(I - P))\theta] \\ &= 2\langle v|\rho|v\rangle\langle v|\theta|v\rangle \end{aligned} \tag{39}$$

By introducing a Lagrange multiplier, we have the expanded target function

$$J(v, \lambda) = \langle v|\rho|v\rangle\langle v|\theta|v\rangle - \lambda(\langle v|v\rangle - 1). \tag{40}$$

Denote $\rho(v) = \langle v|\rho|v\rangle$ and $\theta(v) = \langle v|\theta|v\rangle$, then differentiating J with respect to v produces

$$(\rho(v)\theta + \theta(v)\rho - \lambda I_D)|v\rangle = 0. \tag{41}$$

which implies that each critical point $|v\rangle$ must be an eigenvector of the matrix $M(v) = \rho(v)\theta + \theta(v)\rho$ corresponding to some eigenvalue λ. Obviously, the eigenvalue can be $\lambda = 0$ or some special values of $\rho_i\theta(v)$ and $\theta_j\rho(v)$. Now we can classify the critical points into the following cases:

(i) The critical point is the eigenvector of $\lambda = 0$. If in this case $\rho(v) = 0$, then the corresponding eigenspace of $\lambda = 0$ is $H_0 \oplus H_1^\theta \oplus \cdots \oplus H_s^\theta$, and any unit vector in this subspace is a critical point corresponding to $J = 0$. Similarly, any unit vector in $H_0 \oplus H_1^\rho \oplus \cdots \oplus H_r^\rho$ is an eigenvector of $\lambda = 0$ when $\theta(v) = 0$, and in this case $J = 0$. If both $\rho(v)$ and $\theta(v)$ are nonzero, then $v \in H_0$, in which case we also have $J = 0$.

(ii) The critical point is an eigenvector of some nonzero eigenvalue, and all nonzero eigenvalues of $M(v)$, i.e., $\rho_i\theta(v)$ and $\theta_j\rho(v)$, are mutually different. In this case, we can see that $v \in H_i^\rho$ ($v \in H_j^\theta$) when $\lambda = \rho_i\theta(v)$ ($\lambda = \theta_j\rho(v)$) and correspondingly $\theta(v) = 0$ ($\rho(v) = 0$) and hence $J = 0$.

(iii) The critical point is an eigenvector of some nonzero eigenvalue $\rho_i\theta(v) = \theta_j\rho(v)$, whose eigenspace is the direct sum of H_i^ρ and H_j^θ. Suppose that $v = v_\rho + v_\theta$ where $v_\rho \in H_i^\rho$ and $v_\theta \in H_j^\theta$, then the equation $\rho_i\theta(v) = \theta_j\rho(v)$ implies that $\|v_\rho\|^2 = \|v_\theta\|^2 = 1/2$. Correspondingly, $J = \frac{1}{2}\rho_i\theta_j$ and there are generally rs possible critical values for different ρ_i and θ_j. The degeneracy of the eigenvalues of $\rho(v)$ or $\theta(v)$ will reduce the number of the critical values but not the critical values themselves.

In conclusion, the maximum transformation probability between two orthogonal mixed states ρ and θ induced by the measurement is

$$J\text{max} = \frac{1}{2}\rho_{\text{max}}\theta_{\text{max}}, \tag{42}$$

when the vector $|v\rangle$ in the projector $P = |v\rangle\langle v|$ is

$$|v\rangle = \frac{1}{\sqrt{2}}(|\rho_{\text{max}}\rangle + |\theta_{\text{max}}\rangle). \tag{43}$$

Here $|\rho_{\text{max}}\rangle$ and $|\theta_{\text{max}}\rangle$ are the eigenvectors of ρ and θ corresponding to the largest eigenvalues, ρ_{max} and θ_{max}, respectively. The maximum transformation probability is determined only by ρ_{max} and θ_{max}. In particular, if the initial and final states are both pure states, the resulting maximal yield is $1/2$, which conforms to the results obtained in Sect. 4.1.

5 Conclusions and discussion

We have shown that quantum measurements can be effectively applied to control quantum dynamics. In the case that a finite number of measurements are employed, we have derived a necessary condition for critical points of the optimal state transition. This condition is utilized to find the maximal state transformation probability between two pure states of an N-level quantum system under a single measurement with N independent projective operators. Moreover, studies on the control with a two-projector single measurement provide analytical solutions for the maximal state transition problems between more general states, including from a mixed state to a pure state, and between two orthogonal mixed states. These studies are based on the first-order necessary conditions via the variations of the target function. Further second-order analysis on the corresponding Hessian form will provide more information about the critical points, and hence a deeper understanding of the complexity of quantum control by optimized measurements.

In this paper, we are concerned with optimizing the projectors (or corresponding unitary matrices) within a certain class of measurements to maximize the transformation probabilities. In addition, numerical simulations have shown that the ranks of the projectors that classifies the different equivalent classes of measurements are also essential, on which further studies are needed. Moreover, towards the optimization with multiple measurements, we need to find a way to analytically solve optimal state transformation between two arbitrary non-orthogonal mixed states.

Finally, it should be noted that the complexity of the results to some extent originates from the restrictions on the available measurements (in this paper we consider only projective measurements). If we can apply arbitrary generalized POVM measurements [28] defined as $M(\rho) = \sum K_i \rho K_i^\dagger$, where the measurement is represented by the set of Kraus operators that satisfy $\sum K_i^\dagger K_i = I$, then according to previous studies, i.e., perfect transformation between two arbitrary states is possible [29]. Moreover, the search for such global optimal measurements will not be hindered by any locally maximal suboptimal solutions [30].

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