Navigation between quantum states by quantum mirrors

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We introduce a technique that allows one to connect any two arbitrary (pure or mixed) superposition states of an N-state quantum system. The proposed solution to this inverse quantum mechanical problem is analytical, exact, and very compact. The technique uses standard and generalized quantum Householder reflections (QHRs), which require external pulses of precise areas and frequencies. We show that any two pure states can be linked by just a single generalized QHR. The transfer between any two mixed states with the same dynamic invariants (e.g., the same density matrix eigenvalues) requires in general N QHRs. Moreover, we propose recipes for synthesis of arbitrary preselected mixed states using a combination of QHRs and incoherent processes (pure dephasing or spontaneous emission).

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I. INTRODUCTION

Quantum-state engineering in atoms and molecules traditionally uses three basic techniques for transfer of population, complete or partial, from one bound energy state to another, single or superposition state: resonant pulses of precise areas (e.g., π pulses in a two-state system or generalized π pulses for multiple states) [1], adiabatic passage using one or more level crossings [2], or stimulated Raman adiabatic passage (STIRAP) and its extensions [3]. All these techniques require the system to be initially in a single energy state; such a state can be easily prepared experimentally, e.g., by optical pumping. Some of these techniques are "tuned" to a specific initial condition: for example, STIRAP requires a counterintuitive pulse sequence to transfer population from state 1 to 3 in a 1-2-3 linkage, but it is largely irrelevant if the system starts in states 2 or 3 (with some exceptions for state 3) [3]. In other words, STIRAP is (very) useful in producing only one column (the first) of the propagator. Similar conclusions apply, to a large extent, also to the other two techniques using pulse areas and level crossings.

These traditional techniques resolve only a small (although important) part of the general problem of quantum-state engineering: given the initial and final states of an N-state system, find a physical set of operations that connect them. This problem requires the construction of the entire propagator, not just a single column or row.

In this paper we introduce a technique for full quantum-state engineering, which produces, in a systematic manner, a propagator that can connect any two preselected superposition states of an N-state quantum system, representing a *qunit* in quantum-information terms [4]. The two states can be pure as well as mixed, and the latter may have the same or different sets of dynamic invariants (constants of motion). The solution consists of two steps: first, find a propagator that connects the two states, and second, find a physical realization of this propagator.

The first part is the mathematical solution of this inverse problem in quantum mechanics, and the solution is different for three types of problems: (i) pure-to-pure states; (ii) mixed-to-mixed states with the same invariants; (iii) mixed-to-mixed states with different invariants. The case (iii), for instance, contains the important problem of engineering an arbitrary preselected mixed state and we pay special attention to it. In this latter respect our exact analytic results are alternative to the (approximate) numeric optimization procedure proposed by Karpati *et al.* [5]; moreover, our approach allows one to engineer any preselected mixed state, whereas the method of Karpati *et al.* [5] can only produce a class of mixed states.

The second part of the solution is the physical realization of the respective propagator. For this we use the recently introduced physical implementation of the quantum Householder reflection (QHR) [6,7] and we show that the QHR is a very powerful tool for quantum state engineering. Remarkably, in case (i) only a single QHR is needed to connect two pure states. In case (ii), a general U(N) propagator is necessary in the general case, which requires N QHRs. In case (iii), some sort of incoherent process is required in order to equalize the different dynamic invariants of the initial and final mixed states, and the remaining coherent U(N) part is realized by QHRs. We describe the use of two such incoherent processes: pure dephasing and spontaneous emission.

The Householder reflection [8] is a powerful and numerically very robust unitary transformation, which has many applications in classical data analysis, e.g., in solving systems of linear algebraic equations, finding eigenvalues of high-dimensional matrices, least-squares optimization, QR decomposition, etc. [9]. In its quantum-mechanical implementation [6,7] it consists of a single interaction step involving N simultaneous pulsed fields of precise areas and detunings in an N-pod linkage pattern, wherein the N states of our system are coupled to each other via an ancillary excited state, as displayed in Fig. 1. We use two types of QHRs: standard and generalized; the latter involves an additional phase factor. The standard QHR can operate on and off resonance, whereas the generalized QHR only off resonance. Any unitary matrix can be decomposed into (and therefore synthesized by) $N-1$ standard QHRs and a phase gate, or N generalized QHRs; hence only N physical operations are needed, which allows one to greatly reduce the number of physical steps, from $O(N^2)$ in existing U(2) realizations [10] to only $O(N)$ with QHRs.
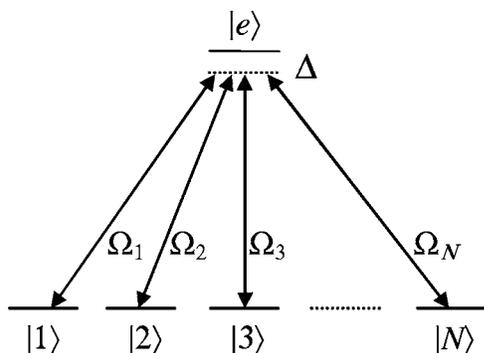
FIG. 1. Physical realization of the quantum Householder reflection: N degenerate [in the rotating-wave approximation (RWA) sense] ground states, forming the *qunit*, coherently coupled via a common excited state by pulsed external fields of the same time dependence and the same detuning, but different amplitudes and phases.

This paper is organized as follows. In Sec. II we review the standard and generalized QHR gates and their physical implementations. In Sec. III we show how two pure states can be connected by means of standard and generalized QHRs. In Sec. IV we construct the propagator connecting two arbitrary mixed states with the same dynamic invariants. Engineering of an arbitrary preselected mixed qunit state is presented in Sec. V. The conclusions are summarized in Sec. VI.

II. QUANTUM HOUSEHOLDER REFLECTION

A. Definition

The standard QHR is defined as

$$\mathbf{M}(v) = \mathbf{I} - 2|v\rangle\langle v|, \tag{1}$$

where $\mathbf{I}$ is the identity operator and $|v\rangle$ is an N-dimensional normalized complex column vector. The QHR (1) is both Hermitian and unitary, $\mathbf{M} = \mathbf{M}^\dagger = \mathbf{M}^{-1}$, which means that $\mathbf{M}$ is involutary, $\mathbf{M}^2 = \mathbf{I}$. In addition, $\det \mathbf{M} = -1$. For real $|v\rangle$ the Householder transformation (1) has a simple geometric interpretation: reflection with respect to an $(N-1)$-dimensional plane with a normal vector $|v\rangle$. In general, the vector $|v\rangle$ is complex and it is characterized by $2N-2$ real parameters (with the normalization condition and the unimportant global phase accounted for).

The generalized QHR is defined as

$$\mathbf{M}(v;\varphi) = \mathbf{I} + (e^{i\varphi} - 1)|v\rangle\langle v|, \tag{2}$$

where φ is an arbitrary phase. The standard QHR (1) is a special case of the generalized QHR (2) for $\varphi = \pi$: $\mathbf{M}(v;\pi) \equiv \mathbf{M}(v)$. The generalized QHR is unitary, $\mathbf{M}(v;\varphi)^{-1} = \mathbf{M}(v;\varphi)^\dagger = \mathbf{M}(v;-\varphi)$, and its determinant is $\det \mathbf{M} = e^{i\varphi}$.

B. Physical implementation

We have shown recently [6,7] that the standard and generalized QHR operators can be realized physically in a coherently coupled N-pod system shown in Fig. 1. The N de-

generate [in the rotating-wave approximation (RWA) sense [1]] ground states $|n\rangle$ $(n=1,2,\ldots,N)$, which represent the *qunit*, are coupled coherently by N external fields to an ancillary, excited state $|e\rangle \equiv |N+1\rangle$ [6]. The excited state $|e\rangle$ can generally be off resonance by a detuning $\Delta(t)$ [6], which must be the same for all fields. The Rabi frequencies $\Omega_1(t),\ldots,\Omega_N(t)$ of the couplings between the ground states and the excited state have the same pulse-shaped time dependence $f(t)$, but possibly different phases β_n and amplitudes χ_n,

$$\Omega_n(t) = \chi_n f(t) e^{i\beta_n} \quad (n=1,2,\ldots,N). \tag{3}$$

The full qunit+ancilla RWA Hamiltonian reads

$$\mathbf{H}(t) = \frac{\hbar}{2}\begin{bmatrix} 0 & 0 & \cdots & 0 & \Omega_1(t) \\ 0 & 0 & \cdots & 0 & \Omega_2(t) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \Omega_N(t) \\ \Omega_1^*(t) & \Omega_2^*(t) & \cdots & \Omega_N^*(t) & 2\Delta(t) \end{bmatrix}. \tag{4}$$

The exact solution to the Schrödinger equation for the propagator $\mathbf{U}(t)$,

$$i\hbar\frac{d}{dt}\mathbf{U}(t) = \mathbf{H}(t)\mathbf{U}(t), \tag{5}$$

can be found in [6].

The standard QHR $\mathbf{M}(v)$ is realized on exact resonance ($\Delta=0$), for any pulse shape $f(t)$, and for root-mean-square (rms) pulse area

$$A = 2(2k+1)\pi \quad (k=0,1,2,\ldots), \tag{6}$$

where

$$A = \int_{-\infty}^{\infty} \Omega(t)dt, \tag{7}$$

with $\Omega(t) = [\sum_{n=1}^{N}|\Omega_n(t)|^2]^{1/2}$. Then the transition probabilities to the ancilla state vanish and the propagator within the qunit space is given exactly by the standard QHR $\mathbf{M}(v)$ (1). The components of the N-dimensional normalized complex vector $|v\rangle$ are the Rabi frequencies, with the accompanying phases [7]

$$|v\rangle = \frac{1}{\chi}[\chi_1 e^{i\beta_1}, \chi_2 e^{i\beta_2}, \ldots, \chi_N e^{i\beta_N}]^T, \tag{8}$$

where $\chi = (\sum_{n=1}^{N}\chi_n^2)^{1/2}$. Hence the qunit propagator represents a physical realization of the standard QHR in a single interaction step. Any QHR vector (8) can be produced on demand by appropriately selecting the peak couplings χ_n and the phases β_n of the external fields.

The generalized QHR $\mathbf{M}(v;\varphi)$ can be realized in the same N-pod system, but for specific detunings off resonance. Again the transition probabilities to the ancilla state must vanish; the corresponding rms pulse areas (7) in general depend on the pulse shape and differ from the resonance values (6). The propagator within the qunit space is the generalized QHR (2), wherein the phase φ depends on the interaction

parameters. Although the parameters (i.e., the rms area and the detuning) of any needed generalized QHR can be found numerically for essentially any pulse shape, it is very convenient to use a hyperbolic-secant pulse shape, for which there is a simple exact analytic solution: the Rosen-Zener model [11],

$$f(t) = \operatorname{sech}(t/T), \tag{9a}$$

$$\Delta(t) = \Delta_0. \tag{9b}$$

For this pulse shape, the rms area (7) is $A = \pi\chi T$. A generalized QHR transformation $\mathbf{M}(v;\varphi)$ (2) is realized when the interactions satisfy again Eq. (8), and the pulse area and the detuning obey [6,7]

$$A = 2\pi l \quad (l = 1, 2, \dots), \tag{10a}$$

$$\varphi = 2 \arg \prod_{k=0}^{l-1} [\Delta_0 T + i(2k+1)]. \tag{10b}$$

For any given φ, there are l values of Δ_0 that satisfy Eq. (10b) [6]. This is also the case for $\varphi = \pi$, i.e., for the standard QHR, for which one of the solutions is $\Delta_0 = 0$. Hence the standard QHR $\mathbf{M}(v)$ can be realized both on and off resonance, whereas the generalized QHR $\mathbf{M}(v;\varphi)$ can only be realized for nonzero Δ_0. The advantage of tuning off resonance is the lower transient population in the ancilla excited state, which would reduce the population losses if the lifetime of this state is short compared to the interaction duration.

This implementation is particularly suited for a qutrit ($N = 3$) formed of the magnetic sublevels of an atomic level with angular momentum $J = 1$; then the ancilla state should be a $J = 0$ state. The three pulsed fields can be delivered from the same laser by using beam splitters and polarizers, which would automatically ensure that all of them have the same detuning and pulse shape. Moreover, with femtosecond pulses it would be possible to use pulse shapers [12], which can easily deliver pulses with the desired areas. Of course, the use of femtosecond pulses offers another advantage: decoherence is irrelevant on such time scales.

C. Householder decomposition of a U(N) propagator

The standard QHR $\mathbf{M}(v)$ and the generalized QHR $\mathbf{M}(v;\varphi)$ can be used for $\mathrm{U}(N)$ decomposition [7]. Any N-dimensional unitary matrix $\mathbf{U}$ ($\mathbf{U}^{-1} = \mathbf{U}^\dagger$) can be expressed as a product of $N-1$ standard QHRs $\mathbf{M}(v_n)$ ($n = 1, 2, \dots, N-1$) and a phase gate,

$$\mathbf{\Phi}(\phi_1, \dots, \phi_N) = \sum_{n=1}^{N} e^{i\phi_n} |n\rangle\langle n| = \operatorname{diag}\{e^{i\phi_1}, \dots, e^{i\phi_N}\}, \tag{11}$$

as

$$\mathbf{U} = \mathbf{M}(v_1)\mathbf{M}(v_2) \cdots \mathbf{M}(v_{N-1})\mathbf{\Phi}(\phi_1, \phi_2, \dots, \phi_N), \tag{12}$$

or as a product of N generalized QHRs,

$$\mathbf{U} = \mathbf{M}(v_1;\varphi_1)\mathbf{M}(v_2;\varphi_2) \cdots \mathbf{M}(v_N;\varphi_N). \tag{13}$$

These QHR decompositions of a general $\mathrm{U}(N)$ transformation make it possible to solve the important quantum-mechanical problem of transferring an N-state quantum system from one arbitrary preselected initial superposition state to another such state, i.e., the inverse problem of quantum-state engineering. The cases of pure and mixed states require separate analyses.

III. TRANSITION BETWEEN PURE STATES

A. Transition by standard QHRs

A pure qunit state is described by a state vector $|\Psi\rangle = \sum_{n=1}^{N} c_n |n\rangle$, where the vectors $|n\rangle$ represent the qunit basis states, and c_n is the complex-valued probability amplitude of state $|n\rangle$. Given the preselected initial state $|\Psi_i\rangle$ and the final state $|\Psi_f\rangle$ of the qunit, we wish to find a propagator $\mathbf{U}$, such that

$$|\Psi_f\rangle = \mathbf{U}|\Psi_i\rangle. \tag{14}$$

We shall show that one of the possible solutions of Eq. (14) reads

$$\mathbf{U} = \mathbf{M}(v_f)\mathbf{D}\mathbf{M}(v_i), \tag{15}$$

where $\mathbf{M}(v_i)$ and $\mathbf{M}(v_f)$ are standard QHRs. Here $\mathbf{D}$ is an N-dimensional unitary matrix, which, when acting upon a single-qunit basis state $|n\rangle$, only shifts its phase,

$$\mathbf{D}|n\rangle = e^{i\phi_n}|n\rangle. \tag{16}$$

For example, $\mathbf{D}$ can be an arbitrary N-dimensional phase gate (11). Alternatively, $\mathbf{D}$ can be an arbitrary N-dimensional generalized QHR $\mathbf{M}(v;\varphi)$ with vector $|v\rangle$ orthogonal to the qunit state $|n\rangle$, $\langle v|n\rangle = 0$. Finally $\mathbf{D}$ can be the identity $\mathbf{D} = \mathbf{I}$.

In order to prove Eq. (15) we first define the vector

$$|v_{\alpha n}\rangle = \frac{|\Psi_\alpha\rangle - e^{i\varphi_{\alpha n}}|n\rangle}{\sqrt{2(1 - |\langle\Psi_\alpha|n\rangle|)}}, \tag{17}$$

where $|n\rangle$ is an arbitrarily chosen basis qunit state, $\varphi_{\alpha n} = \arg\langle n|\Psi_\alpha\rangle$, and $\alpha = i$ or f. The QHR $\mathbf{M}(v_{in})$ acting upon $|\Psi_i\rangle$ reflects it onto the single-qunit state $|n\rangle$,

$$\mathbf{M}(v_{in})|\Psi_i\rangle = e^{i\varphi_{in}}|n\rangle. \tag{18}$$

The action of $\mathbf{D}$ upon $|n\rangle$ only shifts its phase [see Eq. (16)]. The action of $\mathbf{M}(v_{fn})$ upon $|n\rangle$ reflects this vector onto the final state,

$$\mathbf{M}(v_{fn})|n\rangle = e^{-i\varphi_{fn}}|\Psi_f\rangle. \tag{19}$$

Equations (18), (16), and (19) imply that

$$\mathbf{M}(v_{fn})\mathbf{D}\mathbf{M}(v_{in})|\Psi_i\rangle = e^{i(\varphi_{in} - \varphi_{fn} + \phi_n)}|\Psi_f\rangle, \tag{20}$$

which, up to an unimportant phase, proves Eq. (15).

The arbitrariness in the choice of the unitary matrix $\mathbf{D}$, and the intermediate basis state $|n\rangle$, means that the solution (15) for $\mathbf{U}$ is not unique. However, what is important is that it always exists. In fact the availability of multiple solutions offers some flexibility for a physical implementation. In par-

ticular we can always choose $\mathbf{D}=\mathbf{I}$; then the physical realization of the propagator $\mathbf{U}$ requires only two standard QHRs.

In several important special cases only a single standard QHR is needed for a pure-to-pure transition.

(1) If the qunit is in a single initial basis state $|\Psi_i\rangle=|n\rangle$ then, as follows from Eq. (19), only a single QHR $\mathbf{M}(v_{fn})$ is sufficient to transfer it into an arbitrary superposition state $|\Psi_f\rangle$, with $|v_{fn}\rangle$ given by Eq. (17).

(2) Likewise, an arbitrary initial superposition state $|\Psi_i\rangle$ can be linked to any single final state $|\Psi_f\rangle=|n\rangle$ by only a single QHR $\mathbf{M}(v_{in})$, with $|v_{in}\rangle$ given by Eq. (17).

(3) If $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are orthogonal ($\langle\Psi_f|\Psi_i\rangle=0$), then again only a single standard QHR $\mathbf{M}(v)$, with $|v\rangle=(1/\sqrt{2})(|\Psi_f\rangle-|\Psi_i\rangle)$, is sufficient to connect them.

(4) If $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are superpositions with *real* coefficients, then again a single QHR $\mathbf{M}(v)$ links them, with $|v\rangle=(|\Psi_f\rangle-|\Psi_i\rangle)/\sqrt{2(1-\langle\Psi_f|\Psi_i\rangle)}$.

B. Transition by a generalized QHR

A generalized QHR is ideally suited for a pure-to-pure transition because, as is easily seen, only one generalized QHR is sufficient to reflect state $|\Psi_i\rangle$ onto $|\Psi_f\rangle$,

$$\mathbf{U}=\mathbf{M}(v;\varphi), \tag{21}$$

where

$$|v\rangle=\frac{|\Psi_f\rangle-|\Psi_i\rangle}{\sqrt{2(1-\mathrm{Re}\langle\Psi_f|\Psi_i\rangle)}}, \tag{22a}$$

$$\varphi=2\arg(1-\langle\Psi_i|\Psi_f\rangle)+\pi. \tag{22b}$$

In comparison with (15) the solution (21) is unique; there is no arbitrariness in the choice of the QHR vector $|v\rangle$ (up to an unimportant global phase) and the phase φ.

C. Examples

As a first example, we consider a qutrit ($N=3$), for which the QHR implementation is particularly suitable. The single-to-superposition transition

$$|\Psi_i\rangle=|1\rangle\rightarrow\frac{|1\rangle+|2\rangle+|3\rangle}{\sqrt{3}}=|\Psi_f\rangle \tag{23}$$

is performed by a single QHR $\mathbf{M}(v)$, with

$$|v\rangle=\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{3}}}[\sqrt{3}-1,-1,-1]^T. \tag{24}$$

Figure 2 shows the corresponding time evolutions of the populations and the state mismatch, (not to be confused with the arbitrary diagonal matrix $\mathbf{D}$)

$$D(t)=\frac{\sum_{mn}|\rho_{mn}(t)-\rho_{mn}^f|}{\sum_{mn}|\rho_{mn}^i-\rho_{mn}^f|}, \tag{25}$$

where ρ_{mn} are the elements of the qutrit density matrix ρ. This definition of D applies to pure and mixed states as well.
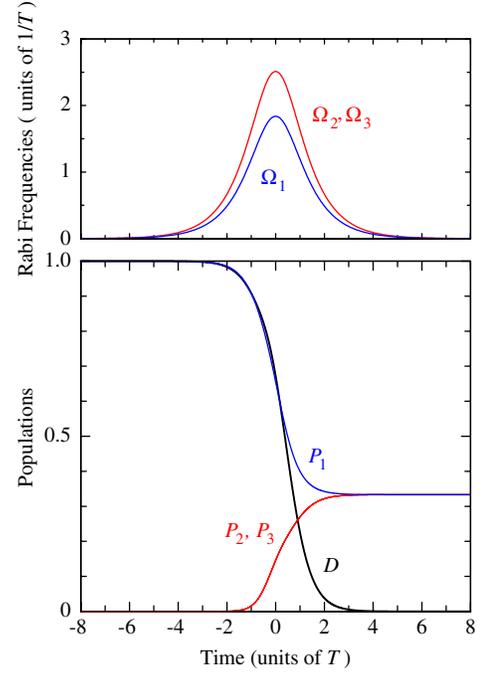
FIG. 2. (Color online) Time evolution of the pulsed fields (top) and the populations and the state mismatch D (bottom) for the transition (23) in a qutrit. We have assumed sech pulses, $f(t)=\mathrm{sech}(t/T)$, and rms pulse area $A=4\pi$ ($\chi T=4$). The individual couplings χ_n ($n=1,2,3$) are given by the components of the QHR vector (24), each multiplied by χ. The detuning is $\Delta_0 T=1.732$ (which gives $\varphi=\pi$).

The behavior of D allows us to verify that both the populations and the phases of the probability amplitudes of the target state $|\Psi_f\rangle$ are produced by the QHR. Indeed, as time progresses, D approaches zero, which implies that $|\Psi(t)\rangle$ aligns with $|\Psi_f\rangle$.

In another example, we transfer a two-state superposition to a three-state superposition,

$$\frac{|1\rangle+|3\rangle}{\sqrt{2}}\rightarrow\frac{|1\rangle+e^{i\pi/3}|2\rangle+e^{i\pi/7}|3\rangle}{\sqrt{3}}, \tag{26}$$

by two standard QHRs, $\mathbf{U}=\mathbf{M}(v_f)\mathbf{M}(v_i)$, with

$$|v_i\rangle=[-0.383,0,0.924]^T, \tag{27a}$$

$$|v_f\rangle=[-0.460,0.628e^{i\pi/3},0.628e^{i\pi/7}]^T, \tag{27b}$$

or by one generalized QHR $\mathbf{U}=\mathbf{M}(v;\varphi)$, with

$$|v\rangle=[0.194e^{0.213\pi i},0.863e^{-0.454\pi i},0.467e^{-0.083\pi i}]^T, \tag{28}$$

and $\varphi=0.574\pi$. Figure 3 shows the time evolution of the populations and the state mismatch (25) for a standard QHR implementation, and Fig. 4 for generalized QHR. In both cases, the mismatch D vanishes, indicating the creation of the desired superposition (26). The generalized QHR implementation is clearly superior because it creates the target state in a single step.

In conclusion of this section, we have shown that any two pure superposition qunit states can be connected by just a
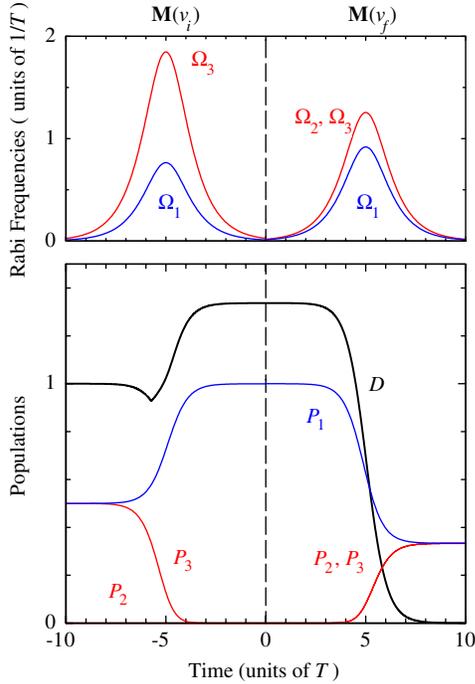
FIG. 3. (Color online) Time evolution of the pulsed fields (top) and the populations and the state mismatch D (bottom) for the qutrit transition (26). We have assumed sech pulse shapes with rms pulse area $A = 2\pi$ ($\chi T = 2$) and detuning $\Delta = 0$. The individual couplings χ_n ($n = 1, 2, 3$) are given by the components of the standard QHR vectors (27), each multiplied by χ.

single generalized QHR, or by two standard QHRs. This suggests that the QHR, and particularly the generalized version, is a very convenient and efficient tool for pure-to-pure state navigation in Hilbert space.

We now turn our attention to mixed states.

IV. COHERENT NAVIGATION BETWEEN MIXED STATES

A mixed qunit state can be described by its density matrix ρ, whose spectral decomposition reads

$$\rho = \sum_{n=1}^{N} r_n |\psi_n\rangle\langle\psi_n|. \qquad (29)$$

The eigenvalues r_n of ρ satisfy $\sum_{n=1}^{N} r_n = 1$, and $|\psi_n\rangle$ are the orthonormalized ($\langle\psi_k|\psi_n\rangle = \delta_{kn}$) complex eigenvectors of ρ. The density matrix is Hermitian; hence it can be parametrized by $N^2 - 1$ real parameters.

A Hermitian Hamiltonian induces unitary evolution between an initial mixed state ρ_i and a final state ρ_f,

$$\rho_f = \mathbf{U}\rho_i\mathbf{U}^\dagger. \qquad (30)$$

A unitary evolution does not change the eigenvalues $\{r_n\}_{n=1}^{N}$, which are therefore dynamic invariants, as is easily seen from Eq. (30) (as an equivalent set of dynamic invariants one can take the set $\{\mathrm{Tr}\rho^n\}_{n=1}^{N}$). Therefore, a unitary propagator $\mathbf{U}$ can only connect mixed states with the same set of invariants $\{r_n\}_{n=1}^{N}$. In order to connect mixed states with different invari-
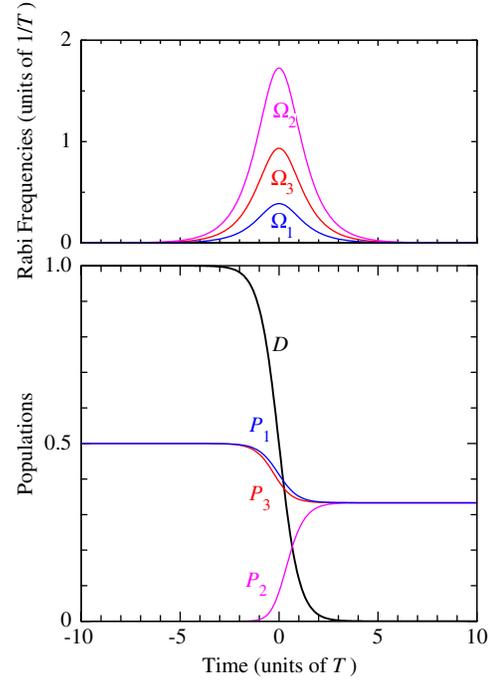
FIG. 4. (Color online) Time evolution of the pulsed fields (top) and the populations and the state mismatch D (bottom) for the qutrit transition (26). We have assumed sech pulse shapes with rms pulse area $A = 2\pi$ ($\chi T = 2$). The individual couplings χ_n ($n = 1, 2, 3$) are given by the components of the generalized QHR vector (28), each multiplied by χ. The detuning is $\Delta T = 0.791$, which produces the desired phase $\varphi = 0.574\pi$.

ants we need an incoherent process; we shall return to this problem in the next section. Here we shall find the solution to the problem of linking two mixed states with the same invariants.

Because the eigenvalues $\{r_n\}_{n=1}^{N}$ of ρ_i and ρ_f are the same, we have the equality

$$\mathbf{R}_i^\dagger \rho_i \mathbf{R}_i = \mathbf{R}_f^\dagger \rho_f \mathbf{R}_f = \rho_0, \qquad (31)$$

where the unitary matrices $\mathbf{R}_i$ and $\mathbf{R}_f$ diagonalize, respectively, ρ_i and ρ_f, and $\rho_0 = \mathrm{diag}\{r_1, r_2, \ldots, r_N\}$. By replacing Eq. (31) into Eq. (30) we find

$$\rho_0 = \mathbf{D}\rho_0\mathbf{D}^\dagger, \qquad (32a)$$

$$\mathbf{D} = \mathbf{R}_f^\dagger \mathbf{U} \mathbf{R}_i. \qquad (32b)$$

Because $\mathbf{D}$ is a unitary matrix we find $\rho_0 \mathbf{D} = \mathbf{D}\rho_0$. Since ρ_0 is diagonal, $\mathbf{D}$ must be diagonal too. There are no other restrictions on $\mathbf{D}$; hence $\mathbf{D}$ can be an arbitrary diagonal matrix; for example, we can always choose $\mathbf{D} = \mathbf{I}$. It follows from Eq. (32b) that the solution for $\mathbf{U}$ is

$$\mathbf{U} = \mathbf{R}_f \mathbf{D} \mathbf{R}_i^\dagger. \qquad (33)$$

Hence, the transfer between two mixed states requires a general $\mathrm{U}(N)$ propagator. The latter can be expressed as a product of $N-1$ standard QHRs $\mathbf{M}(v_n)$ ($n = 1, 2, \ldots, N-1$) and a phase gate $\mathbf{\Phi}(\phi_1, \phi_2, \ldots, \phi_N)$, Eq. (12), or by N generalized QHRs $\mathbf{M}(v_n; \varphi_n)$ ($n = 1, 2, \ldots, N$), Eq. (13) [7].

We take as an example a qutrit, with the arbitrarily chosen initial and final density matrices

$$\rho_i = \begin{bmatrix} 0.490 & 0.115e^{-0.789\pi i} & 0.158e^{0.107\pi i} \\ 0.115e^{0.789\pi i} & 0.336 & 0.018e^{-0.675\pi i} \\ 0.158e^{-0.107\pi i} & 0.018e^{0.675\pi i} & 0.175 \end{bmatrix},$$

(34a)

$$\rho_f = \begin{bmatrix} 0.298 & 0.022e^{0.689\pi i} & 0.033e^{0.319\pi i} \\ 0.022e^{-0.689\pi i} & 0.180 & 0.177e^{0.909\pi i} \\ 0.033e^{-0.319\pi i} & 0.177e^{-0.909\pi i} & 0.523 \end{bmatrix},$$

(34b)

which have the same eigenvalues $r_1 = 0.6$, $r_2 = 0.3$, $r_3 = 0.1$. These density matrices can be connected by the unitary propagator (33) with $\mathbf{D} = \mathbf{I}$: $\mathbf{U} = \mathbf{R}_f \mathbf{R}_i^\dagger$. The latter can be expressed as a product of two standard QHRs and one phase gate $\mathbf{U} = \mathbf{M}(v_1)\mathbf{M}(v_2)\mathbf{\Phi}$, with

$$|v_1\rangle = [0.612e^{0.532\pi i}, 0.091e^{0.211\pi i}, 0.785e^{0.690\pi i}]^T,$$

(35a)

$$|v_2\rangle = [0, 0.533e^{-0.181\pi i}, 0.846e^{0.859\pi i}]^T,$$

(35b)

$$\mathbf{\Phi} = \mathrm{diag}\{e^{-0.468\pi i}, e^{0.819\pi i}, e^{-0.350\pi i}\},$$

(35c)

or by three generalized QHRs, $\mathbf{U} = \mathbf{M}(v_1;\varphi_1)\mathbf{M}(v_2;\varphi_2)\mathbf{M}(v_3;\varphi_3)$, with

$$|v_1\rangle = [0.721e^{0.659\pi i}, 0.080e^{-0.209\pi i}, 0.689e^{0.270\pi i}]^T,$$

(36a)

$$|v_2\rangle = [0, 0.813e^{0.469\pi i}, 0.582e^{-0.261\pi i}]^T,$$

(36b)

$$|v_3\rangle = [0, 0, 1]^T,$$

(36c)

$$\varphi_1 = -0.841\pi, \quad \varphi_2 = 0.969\pi, \quad \varphi_3 = -0.128\pi.$$

(36d)

Figure 5 shows the respective time evolution of the populations and the state mismatch (25) for the generalized QHR realization. The first QHR $\mathbf{M}(v_3;\varphi_3)$ does not cause population changes because it is in fact a phase gate. As time progresses, the mismatch decreases and the target density matrix (34b) is approached.

V. SYNTHESIS OF ARBITRARY PRESELECTED MIXED STATES

As was shown in the previous sections, by applying one or more QHRs one can connect any two arbitrary pure states, or two arbitrary mixed states with the same dynamic invariants $\{r_n\}_{n=1}^N$. Mixed states with different invariants cannot be connected by coherent Hermitian evolution because these invariants are constants of motion. Hence in order to connect mixed states with different invariants we need a mechanism with non-Hermitian dynamics, which can alter the dynamic invariants.
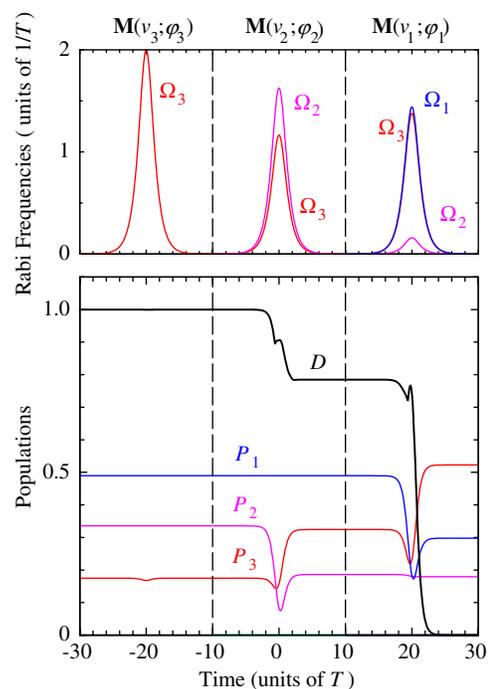
FIG. 5. (Color online) Time evolution of the pulsed fields (top) and the populations and the state mismatch (bottom) for the transition between states (34a) and (34b) in a qutrit. We have assumed sech pulse shapes and rms pulse area $A = 2\pi$ $(\chi T = 2)$. The individual couplings χ_n $(n = 1, 2, 3)$ are given by the components of the generalized QHR vectors (36) each multiplied by χ. The detunings are $\Delta_1 T = -0.255$, $\Delta_2 T = 0.049$, and $\Delta_3 T = -4.918$, which produce the phases (36d).

In this section we shall describe two techniques for engineering an arbitrary mixed state, starting from a single pure state. This is the most interesting special case of the general problem of connecting two arbitrary mixed states, because the initial state can be prepared routinely by optical pumping. Moreover, the general mixed-to-mixed problem can be reduced to the single-to-mixed problem by optically pumping the initial mixed state into a single state.

The two techniques use a combination of coherent and incoherent evolutions. The coherent evolution uses QHRs, whereas the incoherent non-Hermitian evolution is induced either by pure dephasing or spontaneous emission. We shall consider the two techniques separately.

A. Using dephasing

We assume that the qunit is initially in the single qunit state $\rho_i = |i\rangle\langle i|$, and we wish to transform the system to an arbitrary mixed state ρ_f. Let us denote again the eigenvalues of ρ_f by r_n $(n = 1, 2, \ldots, N)$. We proceed as follows.

(1) First, using the prescription from Sec. III, we apply a single QHR to transfer state $|i\rangle$ to a pure superposition state, in which the populations are equal to the eigenvalues of ρ_f: $\rho_{nn} = r_n$ $(n = 1, 2, \ldots, N)$. The phases of this superposition are irrelevant.

(2) In the second step we switch the dephasing on and let all coherences decay to zero. This can be done, for example,
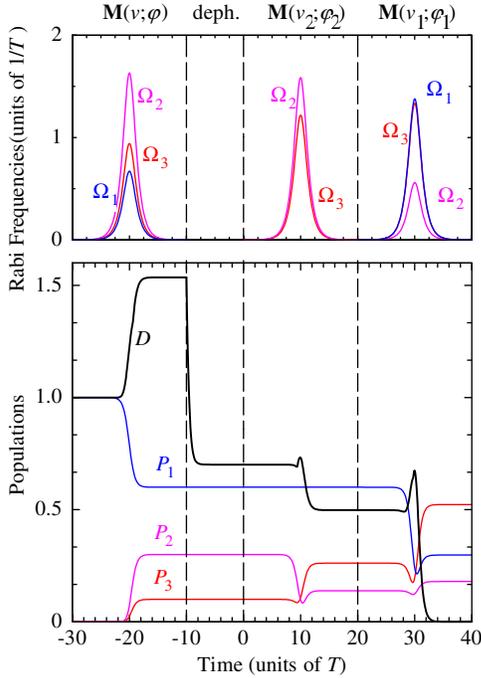
FIG. 6. (Color online) Time evolution of the pulsed fields (top) and the populations and the state mismatch (25) (bottom) for mixed-state engineering in a qutrit. The qutrit starts in state $|1\rangle$ and the target final state is given by Eq. (34b). We have assumed sech pulse shapes and rms pulse area $A=2\pi$ ($\chi T=2$). The individual couplings χ_n ($n=1,2,3$) are given by the components of the generalized QHR vectors (37) and (40), each multiplied by χ. The detunings are $\Delta=0$, $\Delta_1 T=0.072$ and $\Delta_2 T=-0.396$, which produce the desired QHR phases (40c). The dephasing rate is $\Gamma=2/T$.

by using phase-fluctuating far-off-resonance laser pulses. In the end of this process, the density matrix will be diagonal, with the eigenvalues r_n of ρ_f on the diagonal, which implies that it will have the same dynamic invariants as ρ_f.

(3) The third step is to connect this intermediate state to the desired state ρ_f by a sequence of QHRs, as explained in the previous Sec. IV.

In summary, we need *three* steps: a single QHR, a dephasing process, and a sequence of QHRs. Figure 6 shows the evolution of the populations and the state mismatch (25) during the engineering of the mixed state (34b) by the dephasing technique. The first step is the single QHR $\mathbf{M}(v)$, with QHR vector

$$|v\rangle = [-0.336, 0.816, 0.471]^T, \qquad (37)$$

which transfers the single initial state $|1\rangle$ to the pure superposition state

$$\rho_1 = \begin{bmatrix} 0.6 & \sqrt{0.18} & \sqrt{0.06} \\ \sqrt{0.18} & 0.3 & \sqrt{0.03} \\ \sqrt{0.06} & \sqrt{0.03} & 0.1 \end{bmatrix}. \qquad (38)$$

The second step is the pure dephasing process, which nullifies all coherences and leaves the density matrix in a diagonal form,

$$\rho_2 = \begin{bmatrix} 0.6 & 0 & 0 \\ 0 & 0.3 & 0 \\ 0 & 0 & 0.1 \end{bmatrix}. \qquad (39)$$

The third step is a sequence of two generalized QHRs, which transfer ρ_2 into the desired final density matrix ρ_f, Eq. (34b). The QHR components read

$$|v_1\rangle = [0.689e^{0.454\pi i}, 0.280e^{0.436\pi i}, 0.668e^{-0.477\pi i}]^T,$$
$$(40a)$$

$$|v_2\rangle = [0, 0.793e^{0.740\pi i}, 0.609e^{0.025\pi i}]^T, \qquad (40b)$$

$$\varphi_1 = 0.954\pi, \quad \varphi_2 = -0.760\pi. \qquad (40c)$$

B. Using spontaneous emission

In the method, which uses spontaneous emission, we start again in a single-qunit state $\rho_i=|i\rangle\langle i|$, and the target is the arbitrary mixed state ρ_f. The procedure now consists of only two steps: incoherent and coherent. It is particularly well suited for a qutrit, which we shall describe, although it is readily extended to more states. This method requires a closed qunit-ancilla transition; if the ancilla state can decay to other levels then the fidelity will be reduced accordingly.

It is possible here to apply directly the incoherent step, which produces a density matrix with the desired final dynamic invariants, without the need to prepare first a coherent qunit superposition, as in the dephasing method above. The idea is to use laser-induced spontaneous emission from the ancilla excited state to prepare a completely incoherent superposition of the qunit states with populations ρ_{nn} equal to the eigenvalues r_n of ρ_f,

$$\rho = \sum_{n=1}^{3} r_n |n\rangle\langle n|. \qquad (41)$$

For this we apply a sequence of appropriately chosen laser pulses from the qunit states to the excited state, which decays back to the qunit states and redistributes the population among them.

There are various scenarios possible, which can produce the desired incoherent qunit superposition. Here we describe a scenario which looks particularly simple and easy to implement for the qutrit formed of the magnetic sublevels $M=-1,0,1$ of a $J=1$ level and an ancilla excited level with $J=0$ (this implies also equal spontaneous decay branching ratios from the $J=0$ level to the M sublevels of the qutrit). For definiteness, and without loss of generality, we assume that the eigenvalues of ρ_f are ordered as $r_1 \geq r_2 \geq r_3$. We need three pulses: a short pulse from state $|1\rangle$, a long pulse from state $|3\rangle$, and again a short pulse from state $|1\rangle$ (here short and long are related to the lifetime of the excited state).

The short pulse from the initially populated state $|1\rangle$, with excitation probability p_1, transfers population p_1 to the excited state, 1/3 of which decays back to each of the qutrit states. The ensuing density matrix reads

$$\rho_1 = \text{diag}\left\{ 1 - \frac{2}{3}p_1, \frac{1}{3}p_1, \frac{1}{3}p_1 \right\}. \tag{42}$$

We then apply a sufficiently long pulse from state $|3\rangle$, so that its population is completely depleted and distributed among states $|1\rangle$ and $|2\rangle$. The resulting density matrix is

$$\rho_2 = \text{diag}\left\{ 1 - \frac{1}{2}p_1, \frac{1}{2}p_1, 0 \right\}. \tag{43}$$

We now apply again a short pulse from state $|1\rangle$, with a different probability p_2, and then wait for spontaneous emission from the excited state. The result is

$$\rho_3 = \text{diag}\left\{ \left(1 - \frac{1}{2}p_1\right)\left(1 - \frac{2}{3}p_2\right), \frac{1}{2}p_1 \right.$$
$$\left. + \frac{1}{3}p_2\left(1 - \frac{1}{2}p_1\right), \frac{1}{3}p_2\left(1 - \frac{1}{2}p_1\right) \right\}. \tag{44}$$

It is easy to show that in order to create the mixed state (41) we should have the probabilities

$$p_1 = 2(r_2 - r_3), \tag{45a}$$

$$p_2 = \frac{3r_3}{r_1 + 2r_3}. \tag{45b}$$

Because we assumed that $r_1 \geqq r_2 \geqq r_3$ the probabilities p_1 and p_2 belong to the interval $[0,1]$ and are well defined. Such probabilities can be produced by resonant pulses with appropriate pulse areas. These pulses should be short compared to the lifetime of the excited state in order to avoid spontaneous emission during their action.

Once we have prepared the mixed qutrit state (41), which has the same invariants as ρ_f, we can apply QHRs to transfer this state into the desired final state ρ_f, as described in Sec. IV.

VI. CONCLUSIONS

In this paper we have proposed a technique that allows one to connect any two quantum superposition states, pure or mixed, of an N-state atom. The solution of this inverse problem in quantum mechanics contains two parts: (i) mathematical derivation of the propagator that links the desired initial and final density matrices, and (ii) physical realization of this propagator. In the general case of arbitrary mixed states, the implementations combine coherent Hermitian and incoherent non-Hermitian interactions induced by pulsed laser fields. In general, the propagator is not unique, which reflects the multitude of paths between two qunit states; this also allows for some flexibility in the choice of the most convenient path.

The physical realization uses an N-pod configuration of N lower states, forming the qunit, and an ancillary upper state.

It is particularly convenient for a qutrit, where the $N=3$ states are the magnetic sublevels of a $J=1$ level and the ancilla state is a $J=0$ level. Then only a single tunable laser is needed to provide the necessary polarized laser pulses. Femtosecond pulses look particularly suitable because of the high degree of control of the pulse shapes and areas by pulse shapers, and the absence of any decoherence on these time scales.

The Hermitian part uses a sequence of sets of short coherent laser pulses with appropriate pulse areas and detunings. For each set, the propagator of the N-pod represents a quantum Householder reflection. A sequence of at most N suitably chosen QHRs can synthesize any desired unitary propagator.

We have shown that any two arbitrary preselected pure superposition states can be connected by a single QHR only, because the respective propagator has exactly the QHR symmetry. Two mixed states, with the same set of dynamic invariants, require a general U(N) transformation, which can be realized by at most N QHRs. This is a significant improvement over the existing setups involving $O(N^2)$ operations, which can be crucial in making quantum-state engineering and qunit operations experimentally feasible.

The most general case of two arbitrary mixed states with different dynamic invariants requires an incoherent step, which equalizes the invariants of the initial density matrix to those of the final density matrix. We have demonstrated how this can be done by using pure dephasing or spontaneous decay of the ancillary upper state. Once the invariants are equalized, the problem is reduced to the one of connecting two mixed states with the same invariants, which, as explained above, can be done by at most N QHRs. This method has been described for a qutrit, but it is easily generalized to an arbitrary qunit.

The present results can have important applications in the storage of quantum information. For example, a qubit can encode two continuous parameters: the population ratio of the two qubit states and the relative phase of their amplitudes. A qunit in a pure state can encode $2(N-1)$ parameters ($N-1$ populations and $N-1$ relative phases), i.e., by using qunits information can be encoded in significantly fewer particles than with qubits. Moreover, a mixed qunit state can encode as many as N^2-1 real parameters. This may be particularly interesting if the number of particles that can be used is restricted, e.g., due to decoherence [4].

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