J. Phys. B: At. Mol. Opt. Phys. 48 (2015) 135502 (5pp)

# Fault-tolerant composite Householder reflection

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Received 31 March 2015 Accepted for publication 8 April 2015 Published 13 May 2015



## Abstract

We propose a fault-tolerant implementation of the quantum Householder reflection, which is a key operation in various quantum algorithms, quantum-state engineering, generation of arbitrary unitaries, and entanglement characterization. We construct this operation using the modular approach of composite pulses and a relation between the Householder reflection and the quantum phase gate. The proposed implementation is highly insensitive to variations in the experimental parameters, which makes it suitable for high-fidelity quantum information processing.

Keywords: composite pulses, Householder transformation, quantum control

(Some figures may appear in colour only in the online journal)

# 1. Introduction

The Householder reflection (HR) [1] is a very powerful tool for a large variety of problems in data analysis: QR decomposition, least-square optimization, finding eigenvalues of large matrices, etc. The decomposition of matrices by HR has been listed as one of the ten greatest discoveries in computational mathematics of the 20th century by the editors of SIAM [2].

Recently, it has been shown that HR has important applications in quantum physics and quantum information too, for instance in quantum algorithms [3, 4], for synthesis of unitary matrices [5], in quantum state engineering [6], as an entanglement witness [7], etc. Furthermore, it has been found [5, 8] that HR is produced naturally by a particular quantum system: under certain conditions the propagator of an *N*-pod quantum system, consisting of *N* degenerate states coupled simultaneously to another state, is given exactly by a HR.

To this end, the necessary conditions in the *N*-pod implementation are of resonant type (specific values of the interaction duration, the couplings and the detuning) and therefore, the thereby generated HR is prone to parameter errors, similarly to qubit addressing by resonant pulses of precise area.

In this paper we propose a fault-tolerant modular implementation of the HR operator by using the technique of composite pulses (CPs). The latter is a highly accurate and robust tool for quantum control, traditionally used in nuclear magnetic resonance (NMR) [9–12], quantum optics [13–15] and quantum computation [16–20]. Ideas similar to composite pulses have been also used for dynamical decoupling [21], as well as outside quantum physics, e.g. in polarization optics [22] and frequency conversion [23]. A composite pulse is a sequence of pulses with well defined relative phases, which are used as control parameters and determined from the condition to produce a desired excitation profile. Of special interest to the present problem are the broadband composite pulses, which produce high-fidelity excitation profiles, which are robust to variations in one or more experimental parameters around certain values of these parameters. The construction of composite HR is based on a relation between the HR and the quantum phase gate, and uses the composite phase gates introduced recently [24].

This paper is organized as follows. In section 2 we briefly sketch the theory behind composite pulses and introduce the HR. In section 3 we discuss how to combine these in order to

obtain a robust composite HR. Section 4 presents the conclusions.

## 2. Composite pulses and Householder reflections

In this section we briefly review the theory of composite pulses, we show how they can be used to produce an errorresilient phase gate, and we introduce the Householder transformation.

#### 2.1. Composite pulses

To explain the idea of CPs, let us consider a simple two-state quantum system, coherently driven by an external field. Such a system is described by the time-dependent Schrödinger equation

$$i\hbar\partial_t \mathbf{c}(t) = \mathbf{H}(t)\mathbf{c}(t),\tag{1}$$

where  $\mathbf{c}(t) = [c_1(t), c_2(t)]^T$  is a column vector containing the probability amplitudes of the two states  $|\psi_1\rangle$  and  $|\psi_2\rangle$ , and the Hamiltonian is

$$\mathbf{H}(t) = (\hbar/2)\Omega(t)e^{-\mathrm{i}\delta(t)} \left|\psi_1\right\rangle \left\langle\psi_2\right| + \mathrm{h.c.}$$
(2)

Here  $\Omega(t)$  is the Rabi frequency and  $\delta(t) = \int_0^t \Delta(t') dt'$ , where  $\Delta = \omega_0 - \omega$  is the detuning between the field frequency  $\omega$  and the Bohr transition frequency  $\omega_0$ . (Time dependence may be present in  $\Delta$  due to time-dependent (chirped) field frequency or dynamic Stark or Zeeman shift in  $\omega_0$ .) The propagator of the system, which is an operator that connects the initial and final amplitudes,  $\mathbf{c}(t_f) = \mathbf{U}\mathbf{c}(t_i)$ , can be parameterized by using the two complex Cayley–Klein parameters a and b,

$$\mathbf{U} = \begin{bmatrix} a & b \\ -b^* & a^* \end{bmatrix}.$$
 (3)

A constant phase shift in the Rabi frequency  $\Omega(t) \rightarrow \Omega(t)e^{i\phi}$ is imprinted onto the off-diagonal elements of the propagator,

$$\mathbf{U}_{\phi} = \begin{bmatrix} a & b \mathrm{e}^{\mathrm{i}\phi} \\ -b^* \mathrm{e}^{-\mathrm{i}\phi} & a^* \end{bmatrix}.$$
(4)

A composite pulse is by definition a sequence of pulses with different phases. The propagator of a composite pulse, for a sequence of n pulses, is

$$\mathbf{U}^{(n)} = \mathbf{U}(\phi_n) \cdots \mathbf{U}(\phi_2) \mathbf{U}(\phi_1).$$
 (5)

If the phases  $\phi_k$  are chosen appropriately, the propagator  $U^{(n)}$  can be made much more robust to variations in the experimental parameters than the single-pulse propagator U. This is the basic idea behind CPs and in such a way one can produce a huge variety of broadband (BB), narrowband (NB), and passband (PB) CPs with respect to variations in essentially any experimental parameter [13]. It is of particular relevance to us how CPs can be used to construct a quantum phase gate.

#### 2.2. Composite phase gate

A single-qubit phase gate is defined as the  $2 \times 2$  matrix

$$\Phi = \begin{bmatrix} e^{i\alpha/2} & 0\\ 0 & e^{-i\alpha/2} \end{bmatrix},$$
 (6)

where  $\alpha$  is the phase difference between the two states of the qubit, accumulated due to the gate operation. It was recently demonstrated [24] that the propagator of a sequence of two CPs can be made equal to  $\Phi$ . Explicitly, we have

$$\boldsymbol{\Phi} = \mathbf{U}_{\mathrm{CP}_2} \mathbf{U}_{\mathrm{CP}_1},\tag{7}$$

 $\mathbf{U}_{\mathrm{CP}_{1}} = \mathbf{U}(\phi_{n}) \cdots \mathbf{U}(\phi_{2})\mathbf{U}(\phi_{1}), \qquad (8a)$ 

$$\mathbf{U}_{\mathrm{CP}_2} = \mathbf{U}(\xi_n) \cdots \mathbf{U}(\xi_2) \mathbf{U}(\xi_1), \tag{8b}$$

and

where

$$\xi_k = \phi_k + \pi + \alpha/2. \tag{9}$$

The phases  $\phi_k$  and  $\xi_k$  are just the phases of the CPs and are chosen depending on which type of error-resilient CP we want to construct. A detailed description of the composite phase gate is presented elsewhere [24].

#### 2.3. Householder reflection

The standard HR is defined as

$$\mathbf{M}(v) = \mathbf{I} - 2 |v\rangle \langle v|, \tag{10}$$

where **I** is the identity operator and  $|\nu\rangle$  is an *N*-dimensional normalized complex column-vector. The HR (10) is both Hermitian and unitary,  $\mathbf{M} = \mathbf{M}^{\dagger} = \mathbf{M}^{-1}$ , which means that **M** is involutary,  $\mathbf{M}^2 = \mathbf{I}$ . In addition, det  $\mathbf{M} = -1$ . For real  $|\nu\rangle$ the Householder transformation (10) has a simple geometric interpretation: reflection with respect to an (N - 1)-dimensional plane with a normal vector  $|\nu\rangle$ . In general, the vector  $|\nu\rangle$ is complex and it is characterized by 2N - 2 real parameters (two parameters are discounted due to the normalization condition and the unimportant global phase).

The generalized HR is defined as

$$\mathbf{M}(v;\varphi) = \mathbf{I} + \left(e^{i\varphi} - 1\right)|v\rangle\langle v|,\tag{11}$$

where  $\varphi$  is an arbitrary phase. The standard HR (10) is a special case of the generalized HR (11) 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  $\mathbf{M} = e^{i\varphi}$ .

It was shown earlier [5, 8] that the standard and generalized HR can be realized in an *N*-pod quantum system, wherein *N* degenerate states are coupled to an ancillary state, as shown in figure 1, or by using a similar coupling scheme and a STIRAP process [25]. We will now briefly review the implementation of HR, and then show how it can be improved by CPs. Let us assume that the couplings  $\Omega_j$  in figure 1 have the same time dependence f(t), but different



**Figure 1.** Level scheme for the *N*-pod, which realizes the Householder transformation. (bottom) The level scheme after the Morris– Shore transformation.

amplitudes  $\chi_i$  and phases  $\beta_i$ ,

$$\Omega_j(t) = \chi_j f(t) \mathrm{e}^{\mathrm{i}\beta_j}.$$
 (12)

Such a system is described by the Hamiltonian

$$\mathbf{H} = \frac{\hbar}{2} \begin{bmatrix} 0 & 0 & \cdots & 0 & \Omega_{1}(t) \\ 0 & 0 & \cdots & 0 & \Omega_{2}(t) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \Omega_{N}(t) \\ \Omega_{1}^{*}(t) & \Omega_{2}^{*}(t) & \cdots & \Omega_{N}^{*}(t) & 2\Delta(t) \end{bmatrix}.$$
(13)

By using the Morris–Shore transformation [26] one can reduce this (N + 1)-state problem to a set of N - 1 uncoupled states and a two-state system (figure 1, bottom) with a Hamiltonian, which involves the same detuning  $\Delta$  as in equation (13) and the coupling is the root-mean-square (rms) Rabi frequency<sup>1</sup>  $\Omega(t) = \sqrt{\sum_{j=1}^{N} |\Omega_j(t)|^2}$ ,

$$\mathbf{H}_{\rm MS} = \frac{\hbar}{2} \begin{bmatrix} 0 & \Omega(t) \\ \Omega(t) & 2\Delta(t) \end{bmatrix}.$$
(14)

Explicitly, the new basis states after the MS transformation read (written in the basis  $|1\rangle$ ,  $|2\rangle$ , ...,  $|N\rangle$ ,  $|e\rangle$ )

$$|d_1\rangle = \frac{1}{X_2} \Big[\chi_2, -\chi_1, 0, 0, ..., 0\Big]^T$$
 (15a)

$$|d_2\rangle = \frac{1}{X_2 X_3} \Big[ \chi_1 \chi_3, \chi_2 \chi_3, -X_2^2, 0, ..., 0 \Big]^T$$
(15b)

$$|d_3\rangle = \frac{1}{X_3 X_4} \Big[ \chi_1 \chi_4, \chi_2 \chi_4, \chi_3 \chi_4, -X_3^2, 0, \dots, 0 \Big]^T \quad (15c)$$

$$|d_{N-1}\rangle = \frac{1}{X_{N-1}X_N} \Big[ \chi_1 \chi_N, \chi_2 \chi_N, \dots, -X_{N-1}^2, 0 \Big]^T \quad (15d)$$

<sup>1</sup> We have chosen the MS basis such that the rms Rabi frequency is real. However, a common phase shift in the couplings  $\Omega_k$  would still translate as a phase shift in the rms Rabi frequency  $\Omega$ .

$$|b\rangle = \frac{1}{X_N} [\chi_1, \chi_2, ..., \chi_N, 0]^T$$
 (15e)

$$e\rangle = [0, ..., 0, 1]^T,$$
 (15f)

where

$$X_n = \sqrt{\sum_{k=1}^n \chi_k^2} \quad (n = 2, 3, ..., N).$$
(16)

In such a way the Hilbert space is decomposed into two subspaces: an (N - 1)-dimensional dark subspace comprising the states  $|d_1\rangle$ , ...,  $|d_{N-1}\rangle$  and a two-dimensional subspace  $(|b\rangle, |e\rangle)$  orthogonal to the dark subspace. The propagator of the MS two-state system can be written as

$$\mathbf{U}_{\mathrm{MS}} = \begin{bmatrix} c & d \\ -d^* & c^* \end{bmatrix}.$$
 (17)

It is straightforward to verify that if  $c = e^{i\varphi}$  (and hence, d = 0) the propagator of the original *N*-state degenerate manifold is equal to the generalized HR (11),

$$\mathbf{U} = \mathbf{M}(v, \varphi), \tag{18}$$

with

$$v = \frac{1}{\chi} \Big[ \chi_1 e^{i\beta_1}, \chi_2 e^{i\beta_2}, \dots, \chi_N e^{i\beta_N} \Big]^{\mathrm{T}},$$
(19)

where  $\chi = X_N = \sqrt{\sum_{j=1}^N \chi_j^2}$  is the rms peak Rabi frequency and  $\beta_{jm} = \beta_j - \beta_m$ .

The condition  $c = e^{i\varphi}$ , as seen from equations (17) and (6), corresponds exactly to a phase gate in the MS two-state system (14), with  $\alpha = 2\varphi$ . Traditionally, there are several ways to produce such phase shifts. One way is to use a dynamic phase gate [27], which only requires a single far-off-resonant pulsed field. Another basic approach is the geometric phase gate [28], which has certain advantages in terms of robustness against parameter fluctuations that come at the cost of more demanding implementations. An alternative phase gate uses adiabatic passage and relative laser phases [29]. In the present work, we use the approach based on composite pulses, which has been described in [24], and we apply the same approach to construct robust and high-fidelity HRs.

#### 3. Composite Householder reflection

As seen in the previous section, in order to create a generalized HR, we need to set the value of the Cayley–Klein parameter to  $c = e^{i\varphi}$ . This corresponds to the creation of a phase gate, which, as recently demonstrated [24], can be constructed using CPs.

#### 3.1. Composite HR resilient to pulse area errors

As the simplest example, we will first examine the broadband composite HR, which is robust against variations in the pulse area. Such a HR can be produced by a sequence of two broadband CPs. These pulses have been extensively studied and demonstrated in the literature [11]. Here, we use the symmetric resonant pulses, derived in [13], with phases given

by the formula

$$\phi_k = k(k-1)\frac{\pi}{n}$$
 (k = 1, 2, ..., n), (20)

and the phases of the second CP are given by equation (9) for  $\alpha = 2\varphi$ . The phases  $\phi_k$  are the relative phases of the couplings for each pulse, which means that if for the first pulse they are equal to  $\beta_j$  (see equation (12)), then the phases for the *k*th pulse are  $\beta_j + \phi_k$ . Explicitly, the phases of the first few CP pulses are (modulo  $2\pi$ )

$$\left(0,\frac{2}{3},0\right)\pi,\tag{21a}$$

$$\left(0, \frac{2}{5}, \frac{6}{5}, \frac{2}{5}, 0\right)\pi,$$
 (21*b*)

$$\left(0, \frac{2}{7}, \frac{6}{7}, \frac{12}{7}, \frac{6}{7}, \frac{2}{7}, 0\right)\pi,$$
 (21c)

$$\left(0, \frac{2}{9}, \frac{2}{3}, \frac{4}{3}, \frac{2}{9}, \frac{4}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{9}, 0\right)\pi.$$
 (21*d*)

As an example, the propagator of the actual operation for n = 3 is

$$\mathbf{M}'(v, \varphi) = \mathbf{U}(\pi + \varphi)\mathbf{U}(2\pi/3 + \pi + \varphi)$$
$$\times \mathbf{U}(\pi + \varphi)\mathbf{U}(0)\mathbf{U}(2\pi/3)\mathbf{U}(0), \qquad (22)$$

where each of the propagators  $U(\phi_k)$  corresponds to resonant excitation with a rms pulse area equal to  $\pi$ , a Rabi frequency distribution corresponding to the vector v (see equation (19)) and relative phases  $\beta_i + \phi_k$ .

As already noted, we assume that all the fields, which couple the *N* ground states to the excited one, are produced by a single source. This means that a systematic error in this source will translate into the same systematic error of all the couplings, which allows the treatment of our system to be the same as in the case of the two-state phase gate. Explicitly, we can write the deviations  $\epsilon$  in the Rabi frequencies as

$$\Omega_j(t) = \chi_j f(t) e^{i\beta_j} \to \chi_j(1+\epsilon) f(t) e^{i\beta_j}$$
(23)

and hence the rms Rabi frequency deviates with the same factor  $(1 + \epsilon)$ . The same reasoning is valid for the pulse areas. To test the performance of the composite HRs, we define the infidelity of the actual operation **M**', compared to the desired HR **M**(v,  $\varphi$ ) as

$$D = 1 - \frac{1}{N} \operatorname{abs} \left[ \operatorname{Tr} \left( \mathbf{M}^{\dagger} \mathbf{M}' \right) \right].$$
 (24)

It can be shown that the infidelity does not depend on the target vector  $|v\rangle$ . In figure 2 we plot the infidelity of the BB composite standard and generalized HR, for a phase of  $\varphi = \pi/2$ . One can see that by increasing the number of pulses, the robustness of the operation also increases.

Continuing the analogy between composite phase gates and composite HRs, one can also build an adiabatic composite HR [14], detuning-compensated HRs [13], etc.



**Figure 2.** Infidelity of the broadband HR as a function of the rms pulse area, for N = 3 and n = 1, 3, 5, 9 (from inside to outside). The left frames refer to the standard HR ( $\varphi = \pi$ ) and the right frames to the generalized HR with  $\varphi = \pi/2$ . Lower frames show the same infidelity as upper frames, but in a logarithmic scale.



**Figure 3.** Infidelity of the universal standard HR as a function of the pulse duration and the detuning for N = 3. The pulse shape is rectangular and the composite phases in the bottom frame are  $\phi_k = (0, 11, 2, 11, 0)\pi/6$ .

# 3.2. Composite HR resilient to arbitrary errors

Particularly interesting are the *universal* composite HRs, which allow compensation of systematic errors in *any* parameter of the field. This is achieved by using the recently

developed universal composite pulses [15]. The phases of the universal CPs, for n = 3, 5, 7, are

$$\left(0,\frac{1}{2},0\right)\pi,\tag{25a}$$

$$\left(0, \frac{5}{6}, \frac{1}{3}, \frac{5}{6}, 0\right)\pi,\tag{25b}$$

$$\left(0, \frac{11}{6}, \frac{1}{3}, \frac{11}{6}, 0\right)\pi,$$
 (25c)

$$\left(0, \frac{11}{12}, \frac{5}{6}, \frac{17}{12}, \frac{5}{6}, \frac{11}{12}, 0\right)\pi,$$
(25*d*)

$$\left(0, \frac{23}{12}, \frac{5}{6}, \frac{5}{12}, \frac{5}{6}, \frac{23}{12}, 0\right)\pi, \tag{25e}$$

where for n = 5 and n = 7 we have two different universal CP solutions. A contour plot of the infidelity for the universal composite HR is shown in figure 3. As one can see from the plot, a simple sequence of two single resonant pulses (top frame) cannot achieve high robustness, while using a sequence of n = 5 universal CPs (bottom frame), we can achieve high fidelity for a large range of parameter values.

# 4. Conclusion

We have proposed a fault-tolerant implementation of the Householder reflection operator. The implementation uses the concept of composite (modular) pulses, which is a well developed technology in current experiments, and hence the proposed method is amenable to a relatively simple physical realization. The proposed implementation requires good control of the relative phases of the pulses in the composite sequence and the ratios of the couplings in the *N*-pod system. In return, it is highly accurate and highly insensitive to errors in the other experimental parameters, which makes it suitable for high-fidelity quantum control and quantum information processing. Furthermore, our proposal demonstrates the advantages of using modular design, which is a very popular design approach in engineering, to realize robust quantum operations.

# Acknowledgments

BTT and NVV acknowledge financial support by the EC Seventh Framework Programme under Grant Agreement No. 270843 (iQIT), Bulgarian NSF grants DRila-01/4 and DMU-03/103. EK and BTT acknowledge financial support by an SUTD Start-Up Research Grant, Project No. SRG EPD 2012 029 and an SUTD-MIT International Design Centre (IDC) Grant, Project No. IDG 31300102.

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