S-matrix approach to the construction of decoherence-free subspaces

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Analyzing the *S* matrices associated with a host of relaxation processes allows one, using extra ''chaperon'' states, to construct a decoherence-free subspace (DFS) that is immune to the effects of relaxation. The method does not require knowledge of the system-bath Hamiltonian, which is rarely known. Thus, a DFS can be constructed directly from experimentally determined relaxation and dephasing rates of the relevant decoherence processes. Although the method requires resetting the coefficients of the chaperon states at various times, this resetting does not require determining the coefficients of the states belonging to the DFS that one uses for control, computations, or information storage.

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Quantum computation [1] and coherent control [2,3] of material and photonic processes require the creation and maintenance of coherent quantum superposition states for relatively long times. Decoherence, i.e., dephasing and relaxation of a *system* due to collisions with atoms or molecules of a *bath*, which is detrimental to all processes that require coherence and rely on quantum interferences, can pose a serious obstacle to realizing quantum computation devices [1] and quantum control. The construction of superposition states that belong to a subspace that is immune (or is relatively insensitive) to decoherence, the so-called decoherence-free subspace (DFS) [4,5], would, if realizable, alleviate much of the decoherence problem.

In this paper, we describe a procedure for constructing a DFS, based on knowledge of the *S* matrices associated with all the processes contributing to decoherence. More explicitly, we show that we can construct a DFS by adding additional states (which we term chaperon states) to a subspace of interest. Although the coefficients of the chaperon states, which by themselves are susceptible to decoherence, must be reset from time to time, no such resetting needs to be done to the smaller subspace of interest, which, due to interferences with the chaperon states, becomes immune to decoherence. The effectiveness of chaperon states is due to a property shown in our previous work on the suppression of reactive tunneling [6], if the number of final states that are energetically accessible to a given scattering process is less than the number of initial states in the space of interest, then one can construct subspaces in which the given scattering process is suppressed.

Focus then on the *system* states $|A\rangle$ in a Hilbert subspace $\{\alpha\}$ that undergo transitions to states $|B\rangle$ in the Hilbert subspace $\{\beta\}$ due to the action of an external perturbation, such as that exerted by a bath. The subspaces $\{\alpha\}$ and $\{\beta\}$ may be equal, or may differ from one another. We show that by utilizing states in another subspace, which undergo transitions to $\{\beta\}$ and possibly other states, we can modify $\{\alpha\}$ to be decoherence-free. This, as shown below, is due to quantum interference effects.

We assume that in the absence of the interaction with the bath, the system dynamics is described by the system Hamiltonian H_s, whose eigenstates are denoted by $|i\rangle$. Here we focus on *energetically degenerate* subspaces of H_s, i.e., states of the same system energy E_s. For example, we might consider a situation in which the system is comprised of a set of $j=1,\ldots,N$ $s_j=\pm 1/2$ spinors, kept sufficiently far apart from one another, such that their spin-spin interaction is negligible. In this case we will write states $|i\rangle$ as either

$$|i\rangle=\Pi_{j=1}^{N}|s_j^{(i)}\rangle \tag{1}$$

or as entangled linear combinations of such states.

Standard scattering theory [7] gives the probability P_{fi} of making a transition to a final state $|f\rangle$ having started in the initial state $|i\rangle$ due to a collision with a bath atom of energy E_b (i.e., at total energy $E=E_s+E_b$), as

$$P_{fi}(E)=|T_{fi}(E)|^2, \tag{2}$$

where $T_{fi}(E)\equiv\langle f|T(E)|i\rangle$. Here $T(E)$ is the transition operator defined as $T(E)\equiv S(E)-I$, where $S(E)$ is the scattering operator and I is the unit operator. The total probability $P_{\beta\leftarrow i}(E)$ of executing a transition into the entire subspace $\{\beta\}$ that is comprised of M_β energetically degenerate final states is given by

$$P_{\beta\leftarrow i}=\sum_{f=1}^{M_\beta}|T_{fi}|^2, \tag{3}$$

where, for brevity, we have suppressed the energy index E.

In most situations, the decoherence process cannot be described by a single transition operator. Rather, one finds L distinct processes that operate in a completely independent way from one another. For example, we may have collisions at various bath energies E_b, or contributions from many orbital angular momenta. (We do not consider as being distinct processes that operate simultaneously or in a concerted way. Such processes can be lumped under a single T.) Scattering

theory [7] tells us that for a set of distinct processes, the integral (i.e., angle-averaged) cross section is given as a simple sum of the cross sections associated with each independent process. We can therefore generalize Eq. (3) in a straightforward way to read

$$P_{\beta\leftarrow i}=\sum_{\ell=1}^{L}\sum_{f=1}^{M_\beta}|T_{fi}^{(\ell)}|^2, \tag{4}$$

where $T^{(\ell)}$ is the T operator associated with process ℓ.

Consider now a further generalization in which the initial state is not a single eigenstate, but $|\mathbf{c}\rangle$, an entangled superposition of many eigenstates of the same energy E_s,

$$|\mathbf{c}\rangle=\sum_{i=1}^{K}c_i|i\rangle=\sum_{i=1}^{K}c_i\Pi_{j=1}^{N}|s_j^{(i)}\rangle. \tag{5}$$

Because all these states have the same energy, the probability of forming $|f\rangle$ from this initial state is

$$P_{f\leftarrow\mathbf{c}}=\sum_{\ell=1}^{L}\left|\sum_{i=1}^{K}c_iT_{fi}^{(\ell)}\right|^2, \tag{6}$$

and the total transition probability into subspace $\{\beta\}$, $P_{\beta\leftarrow\mathbf{c}}$, is

$$P_{\beta\leftarrow\mathbf{c}}=\sum_{\ell=1}^{L}\sum_{f=1}^{M_\beta}\left|\sum_{i=1}^{K}c_iT_{fi}^{(\ell)}\right|^2. \tag{7}$$

Note, in Eq. (7), the distinctly different character of the two sums: i.e., the incoherent sum over probabilities to final states and over different processes, and the coherent sum over amplitudes from initial states. The latter sum will, as shown below, allow control over the relaxation process.

Introducing the matrix $\boldsymbol{\sigma}=\Sigma_\ell\mathbf{T}_\beta^{\dagger(\ell)}\cdot\mathbf{T}_\beta^{(\ell)}$ with elements $\sigma_{ij}=\Sigma_{\ell=1}{}^{L}\Sigma_{f=1}^{M_\beta}T_{fj}^{*(\ell)}T_{fi}^{(\ell)}$ allows us to rewrite Eq. (7) as

$$P_{\beta\leftarrow\mathbf{c}}=\mathbf{c}^\dagger\cdot\boldsymbol{\sigma}\cdot\mathbf{c}, \tag{8}$$

where the dagger denotes the Hermitian conjugate. The β subscript on the $\mathbf{T}^{(\ell)}$ symbol indicates that we are dealing with the submatrix of the $\mathbf{T}^{(\ell)}$ containing the transition amplitudes into the $\{\beta\}$ final subspace only.

We now wish to choose optimal sets of $\mathbf{c}$ vectors that minimize the transitions into subspace $\{\beta\}$, consistent with the normalization constraint $\Sigma_{i=1}^{K}|c_i|^2=1$. We obtain the optimal solutions by requiring

$$\frac{\partial}{\partial c_k^*}\left[P_{\beta\leftarrow\mathbf{c}}-\lambda\sum_{i=1}^{K}|c_i|^2\right]=\frac{\partial}{\partial c_k^*}[\mathbf{c}^\dagger\cdot\boldsymbol{\sigma}\cdot\mathbf{c}-\lambda\,\mathbf{c}^\dagger\mathbf{c}]=0, \tag{9}$$

where λ is a Lagrange multiplier. Explicitly taking the derivative gives the result that the optimized coefficients satisfy the eigenvalue equation

$$\boldsymbol{\sigma}\cdot\mathbf{c}^{(\lambda)}=\lambda\mathbf{c}^{(\lambda)}. \tag{10}$$

Note that Eq. (10) also results from taking derivatives in Eq. (9) with respect to c_k, since $\boldsymbol{\sigma}$ is Hermitian.

If there is a zero eigenvalue, i.e., if $\lambda=0$ is an eigenvalue of Eq. (10), with an eigenvector $\mathbf{c}^{(0)}$ satisfying

$$\boldsymbol{\sigma}\cdot\mathbf{c}^{(0)}=0, \tag{11}$$

then [by inserting Eq. (11) into Eq. (8)] we have that $P_{\beta\leftarrow\mathbf{c}^{(0)}}=0$. Therefore, the superposition state with the $\mathbf{c}^{(0)}$ coefficients is completely immune to all scattering processes into subspace $\{\beta\}$, i.e., $|\mathbf{c}^{(0)}\rangle$ is a "decoherence free" state with respect to subspace $\{\beta\}$.

Clearly, $\lambda=0$ is obtained if

$$\det(\boldsymbol{\sigma})=\det\sum_\ell(\mathbf{T}_\beta^{(\ell)\dagger}\cdot\mathbf{T}_\beta^{(\ell)})=\det(\mathcal{T}_\beta^\dagger\cdot\mathcal{T}_\beta)=0, \tag{12}$$

where $\mathcal{T}$ is a super T matrix, including the ℓ different processes as a subscript,

$$\mathcal{T}_{\ell,f;i}\equiv\mathbf{T}_{f,i}^{(\ell)}. \tag{13}$$

Equation (12) holds if the number of initial states K comprising the initial superposition [Eq. (5)] is greater than LM_β. To see this result, note that, under these circumstances, $\boldsymbol{\sigma}$ is a matrix of order $K\times K$ and the $\mathcal{T}_\beta$ matrix is of order $K\times LM_\beta$. If $K>LM_\beta$, then we can construct a $K\times K$ order matrix $\mathcal{A}_\beta$ by adding a submatrix of $(K-LM_\beta)$ rows of zeros to the lower part of each $\mathcal{T}_\beta$. Then

$$\begin{aligned}\det(\boldsymbol{\sigma})&=\det(\mathcal{T}_\beta^\dagger\cdot\mathcal{T}_\beta)=\det(\mathcal{A}_\beta^\dagger\cdot\mathcal{A}_\beta)\\&=\det(\mathcal{A}_\beta^\dagger)\det(\mathcal{A}_\beta)=0.\end{aligned} \tag{14}$$

The last equality holds because the determinants of $\mathcal{A}_\beta$ and $\mathcal{A}_\beta^\dagger$ are zero.

The number of decoherence-free states with respect to subspace $\{\beta\}$, i.e., the degeneracy of the $\lambda=0$ eigenvalue of Eq. (11), is $K-\mathrm{rank}(\boldsymbol{\sigma})=K-\mathrm{rank}(\mathcal{T}_\beta)$. Given the dimensionality of $\mathcal{T}_\beta$, and that $K>LM_\beta$, the degeneracy is at least, and typically, $K-LM_\beta$. This result leads immediately to the development of a strategy of constructing a DFS of dimension M_α. That is, we first identify the subspace $\{\beta\}$ of dimension M_β that is coupled to the subspace $\{\alpha\}$ by the L scattering processes considered above. We now use a larger space, of dimension $K=LM_\beta+M_\alpha$, to construct the superposition states $|\mathbf{c}^{(0)}\rangle$ all having, according to Eq. (10), zero eigenvalues and hence zero transition probabilities to subspace $\{\beta\}$. We call the extra LM_β states "chaperon" states.

In order to create the desired DFS, we choose the M_α degenerate $\mathbf{c}^{(0)}$ eigenvectors satisfying Eq. (11) to be of the form

$$\begin{aligned}\mathbf{c}^{(0,1)\mathsf{T}}&=(1,0,\ldots,0,c_{M_\alpha+1}^{(0,1)},c_{M_\alpha+2}^{(0,1)},\ldots,c_K^{(0,1)}),\\\mathbf{c}^{(0,2)\mathsf{T}}&=(0,1,\ldots,0,c_{M_\alpha+1}^{(0,2)},c_{M_\alpha+2}^{(0,2)},\ldots,c_K^{(0,2)}),\\&\vdots\\\mathbf{c}^{(0,M_\alpha)\mathsf{T}}&=(0,\ldots,0,1,c_{M_\alpha+1}^{(0,M_\alpha)},c_{M_\alpha+2}^{(0,M_\alpha)},\ldots,c_K^{(0,M_\alpha)}),\end{aligned} \tag{15}$$

written for typographical convenience in terms of the matrix transpose T.

The $c^{(0,i)}_{M_\alpha+1},\ldots,c^{(0,i)}_{K}$, $i=1,\ldots,M_\alpha$ coefficient matrix is determined by substituting Eq. (15) into Eq. (11) and solving it. The resulting set of vectors $\mathbf{c}^{(0,i)}$, $i=1,\ldots,M_\alpha$ spans a DFS of dimension M_α that is immune to the L bath-induced $\{\alpha\}\rightarrow\{\beta\}$ transitions. Note that the structure of Eq. (15) arises from the fact that each vector has LM_β free coefficients plus the number one in one of the entries. This is exactly the number of coefficients (normalization is of no consequence) needed to satisfy Eq. (11). Each of the M_α null eigenvectors thus generated is different from the other, because the one is placed in a different position.

The nature of the elements in the $\mathbf{c}^{(0,i)}$ is of interest. Note that the first M_α coefficients in each of these vectors (which span the original $\{\alpha\}$ subspace) cannot change under relaxation processes. This is because they correspond to states which could only go to the subspace $\{\beta\}$ under the decoherence processes, and transitions to $\{\beta\}$ have been eliminated by the above construction. By contrast, the chaperon states can make transitions to states other than those in $\{\beta\}$ and can therefore change under decoherence. If we fail to maintain the original values of the chaperon coefficients, the initial $\{\alpha\}$ subspace will no longer be ''protected'' and will cease to be immune to relaxation. However, because these coefficients are known to us, we can reset the values of the chaperon coefficients from time to time, as needed, thereby guaranteeing that the DFS constructed remains a DFS for as long as we wish.

In a similar way we can reset the values of the chaperon coefficients for any superposition state in $\{\alpha\}$. Storing classically the $\mathbf{d}$ matrix of chaperon coefficients, $d_{i,j}\equiv c^{(0,i)}_{M_\alpha+j}$, $i=1,\ldots,M_\alpha$, $j=1,\ldots,LM_\beta$, we can write a general vector in $\{\alpha\}$, of the form $\mathbf{a}=\Sigma_{i=1}^{M_\alpha}a_i\mathbf{c}^{(0,i)}$, as

$$\mathbf{a}^{\mathsf{T}}=\Big(a_1,a_2,\ldots,a_{M_\alpha},\sum_i a_i d_{i,1},\times\sum_i a_i d_{i,2},\ldots,\sum_i a_i d_{i,LM_\beta}\Big). \tag{16}$$

In order to maintain the protective effect of the chaperon states, thereby guaranteeing that we retain a true DFS, all we need is to reset from time to time the values of the chaperon coefficients to be the vector product of the first M_α qbits, whose values need not be determined, times the (classically stored) $\mathbf{d}$ matrix. Because the first M_α coefficients are expected to be very stable, as they can begin to change only after the chaperon coefficients change, this resetting can be done at a rate which is expected to be much smaller than the relaxation rates themselves. Thus, for example, to do quantum computing in the DFS we would perform operations on vectors in the entire space, but use for computing only the first M_α elements of the vectors. Like other error corrections methods, one need never measure anything about the first M_α coefficients with which computations or information storage are done. Rather, whatever operation was performed on the M_α-dimensional DFS subspace can be performed on a vector prepared with the prestored chaperon coefficients of the $d_{i,j}$ matrix to reset the coefficients, without measuring the a_i values.

In order for the procedure to work in practice, we need to know the $\boldsymbol{\sigma}$ relaxation matrix, or more specifically, the $T^{*(\ell)}_{fj}T^{(\ell)}_{fi}$ products. Traditional scattering experiments yield directly only the absolute values $|T^{(\ell)}_{fi}|$. As a consequence, the phases of $T^{*(\ell)}_{fj}T^{(\ell)}_{fi}$ must be extracted using one of a number of methods. For example, one can obtain the complex transition amplitudes from differential cross sections using ''inverse-scattering'' methods and generalized unitarity relations [8,9], or by using coherently controlled scattering [10], which is sensitive to the phases of T matrix elements. Alternatively, one may perform a ''forward'' fitting procedure, in which one optimizes a set of parameter-dependent phases to fit all the experimentally available differential cross-sections data. Although this is not a trivial task, it is one that is doable.

Finally, error producing effects that may well effect the efficacy of this approach (e.g., errors in resetting subspace coefficients, etc.) need be studied in detail within the framework of *particular scenarios*. This work is currently ongoing.

In conclusion, we have presented a method of constructing decoherence-free subspaces via quantum interference that is immune to the action of L different scattering processes with a bath. The method has the great advantage that the system-bath Hamiltonian, which is very difficult to extract and is therefore rarely known, is not needed. Neither is the method dependent on any special form of the system-bath Hamiltonian. Applications of this method to various systems are currently under study.

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