Transfer of 0-order coherence matrix along spin-1/2 chain

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Abstract

In this work, we study transfer of coherence matrices along spin-1/2 chains of various length. Unlike higher order coherence matrices, 0-order coherence matrix can be perfectly transferred if its elements are properly fixed. In certain cases, to provide the perfect transfer, an extended receiver together with optimized its unitary transformation has to be included into the protocol. In this work, the asymptotic perfectly transferable 0-order coherence matrix for an infinitely long chain is considered and deviation of a perfectly transferred state from this asymptotic state is studied as a function of the chain length for various sizes of the extended receiver. The problem of arbitrary parameter transfer via the nondiagonal elements of the 0-order coherence matrix is also considered and optimized using the unitary transformation of the extended receiver.

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I. INTRODUCTION

The methods of quantum state transfer cover an important area of quantum communication and demonstrate advantages of quantum mechanics approach in comparison with classical one. The problem of state transfer between different nodes of a multiparticle quantum system is motivated not only by the needs of long-distance exchange of quantum information but also by the needs of exchanging quantum information among different quantum devices transferring the output state of a particular circuit (sender) to the input register of another circuit (receiver). Similar problems appear in the general field of optimal quantum control [1]. However, in general, quantum evolution leads to spread of the initial quantum state of the sender over the whole system. Therefore, we need a mechanism which would lead to the collapse of the transferred state at the receiver. This motivates development of the models serving for either perfect or high-probability state transfer. The phenomenon of perfect state transfer (PST) was intensively investigated after the state transfer problem was formulated in Ref. [2]. It turned out that PST in spin chains is achievable in very specific cases [3, 4] and can be easily destroyed by small perturbations of the interaction Hamiltonian. In this case, PST becomes high probability state transfer (HPST) [5]. HPST is simpler for realization [6, 7] and it demonstrates stability with respect to small perturbations of the Hamiltonian [8]. Of course, the privileged carriers for long-distance communications are photons [9–11]. However, spin-states can also serve for this purpose in compact quantum devices [12, 13]. This motivates our study in that direction.

One has to emphasize that the main idea of PST is to use such coupling constants in the Hamiltonian that provide proper rational numbers for all ratios of eigenvalues of the Hamiltonian. For instance, those coupling constants D_n between the *n*th and (n + 1)th nodes were found to be $D_n = \lambda \sqrt{n(N-n)}$ (λ is a normalization constant) in [3] for the XX Hamiltonian with the nearest neighbor interaction. Of course, this requirement is very sensitive to the variations in the environment, but nevertheless it serves a reference point in many state-transfer protocols.

The high-probability state transfer uses different principle. While all eigenvalues of the Hamiltonian contribute to the state-transfer probability in the perfect state transfer, highprobability state transfer is based on selecting several eigenvalues of the interaction Hamiltonian (typically two or three) which yields the main contribution to the state-transfer probability. The most popular way to reach this aim is using the weak bonds between the end nodes and the main body of the chain (the weak end-bond model) [6, 8, 14]. However, a specially adjusted local magnetic field can be also used [15]. Application of these two methods can be found in Refs.[16–18]. Many other aspects of state transfer process were considered in [19–27].

Although HPST is more reliable then PST, the state transfer fidelity decreases with the chain length. One of the methods to partially overcome this obstacle is to use the extended receiver (i.e., receiver joined with its few nearest nodes) together with a special unitary transformation, which was also effective in remote state preparation [28].

Recently the concept of transfer of non-interacting multi-quantum coherence matrix was introduced [29]. Then, it was pointed in [30] that the zero-order coherence matrix of special form can be perfectly transferred from the sender to the receiver along the tripartite spin system (which includes sender S, transmission line TL, and receiver R) with the only requirements that the Hamiltonian is conserving the excitation number of the spin system and, in addition, the initial state of $TL \cup R$ must be a 0-order coherence matrix (it is a thermodynamic equilibrium state in [30]). Notice that the unitary transformation of the extended receiver was not used in [30]. Next, in [31], general statements regarding the perfect transfer of a 0-order coherence matrix were formulated for the case of the ground initial state of the subsystem $TL \cup R$. In that case, an additional unitary transformation should be applied to the final receiver's state which exchanges two elements of the receiver density matrix: the elements corresponding to 0- and maximal excitation number. The important feature of that transformation is that it does not conserve the excitation number of the spin system.

Continuing the results of Refs.[29–32], the concept of optimal state transfer was formulated. This optimal state transfer is the structural restoring of the higher order coherence matrices of the initial sender's state and perfect transfer of the 0-order coherence matrix, or, if desired, the structural restoring of the whole nondiagonal part of the receiver's initial state and perfect transfer of its diagonal part. Structural restoring of some blocks of the transferred density matrix means that each element of this block in the receiver's density matrix differs from the appropriate element of the sender's density matrix by a multiplicative factor. Such restoring is achievable due to using the optimizing unitary transformation of the extended receiver which plays a crucial role in the optimal state transfer. We emphasize that the above factors in the restored state as well as the optimizing transformation are universal objects which are defined by the interaction Hamiltonian and time instant for the receiver's state registration and they do not depend on the particular sender's initial state to be transferred.

All this motivates the detailed study of the 0-order coherence matrix which is the subject of our paper. The basic problems to be explored are the following.

1. As a preliminary step, study the general block-structure of density matrices involved into the state-transfer process preserving the excitation number:

> initial sender's density matrix $\rho^{(S)}(0) \rightarrow$ (1) density matrix of the whole evolutionary system $\rho(t) \rightarrow$ receiver's density matrix at certain time instant t_0 , $\rho^{(R)}(t_0)$.

- Determine the structure of the perfectly transferable 0-order coherence matrix (PTZ) in an infinitely long chain (the asymptotic PTZ) and study deviation of the PTZ from the asymptotic one.
- 3. Explore and optimize the protocol for an arbitrary parameter transfer via encoding parameters in the elements of the 0-order coherence matrix. Remark, that the possibility of encoding free parameters in the nondiagonal part of 0-order coherence matrix was shown in [32]. Here we show that arbitrary parameters can be encoded into all elements of one-excitation block of 0-order coherence matrix.

The paper is organized as follows. In Sec. II we discuss the general block structure of a density matrix of spin system and evolution of this structure. In Sec. III, we study the structure of 0-order coherence matrix and the perfect transfer of this matrix from the sender to the receiver. The asymptotic perfectly transferable state for infinitely long chain is proposed, and the difference between the norms of the asymptotic state and the perfectly transferred state is studied as a function of the chain length. A particular case of the perfect transfer of the 0-order coherence matrix including only two blocks corresponding to 0- and 1-excitation is explored in Sec. IV. The arbitrary parameter transfer using the elements of the one-excitation block is also considered in that section. Conclusions are provided in Sec. V. Some important details regarding the structure of the transfer matrix (i.e., of the matrix which transfers the initial sender state to the final receiver state) are collected in Appendix, Sec. VI.

II. GENERAL STRUCTURE OF DENSITY MATRIX

Any density matrix ρ of a spin chain can be represented as the sum of multi-quantum (MQ) coherence matrices:

$$\rho = \sum_{n=-N}^{N} \rho^{(n)}, \quad \text{such that} \quad [I_z, \rho^{(n)}] = n \rho^{(n)},$$
(2)

where $\rho^{(n)}$ is the *n*-order coherence matrix, $I_z = \sum_i I_{zi}$ is the *z*-projection of the total spin of the chain, I_{zi} is the *z*-projection of the *i*th spin. Notice that the matrix $\rho^{(n)}$ in (2) collects the probability amplitudes of state transitions which increase (for n > 0) or decrease (for n < 0) the excitation number of states by *n*. There are 2N + 1 such matrices in the sum.

According to the definition of $\rho^{(n)}$, the N-qubit density matrix ρ , has the following block-structure:

	$\sigma_{0,0}^{(0)}$	$\sigma_{0,1}^{(1)}$	$\sigma_{0,2}^{(2)}$		$\sigma_{0,N-1}^{(N-1)}$	$\sigma_{0,N}^{(N)}$				
	$\sigma_{1,0}^{(-1)}$	$\sigma_{1,1}^{(0)}$	$\sigma_{1,2}^{(1)}$	•••	$\sigma_{1,N-1}^{(N-2)}$	$\sigma_{1,N}^{(N-1)}$				
0 —	$\sigma_{2,0}^{(-2)}$	$\sigma_{2,1}^{(-1)}$	$\sigma_{2,2}^{(0)}$		$\sigma_{2,N-1}^{(N-3)}$	$\sigma_{2,N}^{(N-2)}$			$\sigma_{ij}^{(-k)} = (\sigma_{ji}^{(k)})^{\dagger}.$	(3)
$\rho =$				•••				,	$O_{ij} = (O_{ji})$.	(0)
	$\sigma_{N-1,0}^{(-N+1)}$	$\sigma_{N-1,1}^{(-N+2)}$	$\sigma_{N-1,2}^{(-N+3)}$	•••	$\sigma_{N-1,N-1}^{(0)}$	$\sigma_{N-1,N}^{(1)}$				
	$\sigma_{N,0}^{(-N)}$	$\sigma_{N,1}^{(-N+1)}$	$\sigma_{N,2}^{(-N+2)}$		$\sigma_{N,N-1}^{(-1)}$	$\sigma_{N,N}^{(0)}$)			

Each block $\sigma_{i,j}^{(n)}$ is included into the *n*-order coherence matrix and has dimension $D_i \times D_j$ (n = j - i), where D_i is the dimension of the *i*-excitation subspace which, for the *N*-qubit system, reads:

$$D_k = \begin{pmatrix} N \\ k \end{pmatrix}, \quad k = 0, 1, \dots, N.$$
(4)

In particular, $D_0 = D_N = 1$, $D_1 = D_{N-1} = N$. Therefore, the blocks in (3) are in general not square matrices.

A. Evolution conserving excitation number

We consider the evolution of the spin chain governed by the XX-Hamiltonian

$$H = \sum_{j>i} D_{ij} (I_{i;x} I_{j;x} + I_{i;y} I_{j;y}),$$
(5)

where $D_{ij} = \gamma^2 \hbar / r_{ij}^3$ is the coupling constant between the *i*th and *j*th spins (the magnetic field is directed along the chain), γ is the gyromagnetic ratio, and \hbar is the Planck constant. For the homogeneous chain we have $r_{i,i+1} = r$ and therefore the coupling constants between the nearest neighbors are the same. Hereafter we consider the homogeneous spin chain. Hamiltonian (5) satisfies the commutation relation

$$[H, I_z] = 0, (6)$$

and therefore has the following block-diagonal structure:

$$H = \operatorname{diag}(H^{(0)}, H^{(1)}, \dots, H^{(N)}), \tag{7}$$

where the dimension of the block $H^{(n)}$ is $D_n \times D_n$. In this formula, the *n*th block governs the evolution of the subspace of the *n*-excitation states, and there are N + 1 such blocks. The evolution operator $V(t) = e^{-iHt}$ generated by the Hamiltonian (7) also has the blockdiagonal structure

$$V = \operatorname{diag}(V^{(0)}, V^{(1)}, \dots, V^{(N)}), \quad V^{(n)} = e^{-iH^{(n)}t}$$
(8)

and the dimension of the block $V^{(n)}$ is the same as the dimension of $H^{(n)}$. This means that each block $\sigma_{i,j}^{(n)}$ in (3) evolves independently:

$$\rho(t) = V(t)\rho(0)V^{\dagger}(t) \quad \Rightarrow \quad \sigma_{i,j}^{(n)}(t) = V^{(i)}(t)\sigma_{i,j}^{(n)}(0)(V^{(j)}(t))^{+}.$$
(9)

B. State transfer along spin chain

Now we consider the communication line including the sender S, transmission line TLand receiver R and describe the state propagation from the sender to the receiver. Suppose that we have K-excitation initial state of the $N^{(S)}$ -qubit sender, $K \leq N^{(S)}$:

	$\left(s_{0,0}^{(0)} \right)$	$s_{0,1}^{(1)}$	$s_{0,2}^{(2)}$		$s_{0,K-1}^{(K-1)}$	$s_{0,K}^{(K)}$ \)
	$s_{1,0}^{(-1)}$	$s_{1,1}^{(0)}$	$s_{1,2}^{(1)}$	• • •	$s_{1,K-1}^{(K-2)}$	$s_{1,K}^{(K-1)}$	
$o^{(S)} =$	$s_{2,0}^{(-2)}$	$s_{2,1}^{(-1)}$	$s_{2,2}^{(0)}$	• • •	$s_{2,K-1}^{(K-3)}$	$s_{2,K}^{(K-2)}$. (10)
p - p				• • •			. (10)
	$s_{K-1,0}^{(-K+1)}$	$s_{K-1,1}^{(-K+2)}$	$s_{K-1,2}^{(-K+3)}$	•••	$s_{K-1,K-1}^{(0)}$	$s_{K-1,K}^{(1)}$	
	$s_{K,0}^{(-K)}$	$s_{K,1}^{\left(-K+1\right)}$	$s_{K,2}^{(-K+2)}$	•••	$s_{K,K-1}^{(-1)}$	$s_{K,K}^{(0)}$ /)

The dimension of each block $s_{i,j}^{(k)}$ is $D_i^{(S)} \times D_j^{(S)}$,

$$D_k^{(S)} = \begin{pmatrix} N^{(S)} \\ k \end{pmatrix}, \quad k = 0, 1, \dots, K.$$

$$(11)$$

As was shown in [29], to arrange the independent propagation of the MQ-coherence matrices from the sender to the receiver, two following sufficient conditions must be imposed on the initial state.

1. The initial state should have tensor-product form:

$$\rho(0) = \rho^{(S)}(0) \otimes \rho^{(TL,R)}(0), \tag{12}$$

where $\rho^{(S)}(0)$ and $\rho^{(TL,R)}(0)$ are, respectively, the initial states of the sender and transmission line joined with the receiver.

2. The initial state $\rho^{(TL,R)}(0)$ should include only 0-order coherence matrix; it is the ground state in our paper.

Then the evolution of the state of the whole N-qubit system $S \cup TL \cup R$ is described by the density matrix ρ having the block-structure (3). We emphasize that the excitation number remains the same, and the elements of the particular block $s_{i,j}^{(n)}$ appear only in the appropriate block $\sigma_{i,j}^{(n)}$, i.e., we have the following block-map:

$$s_{ij}^{(k)} \to \sigma_{ij}^{(k)}, \ k = 1, \dots, K,$$
 (13)

where dimensions of σ -blocks are larger than dimensions of s-blocks.

Next, the state of the receiver at some time instant t reads

$$\rho^{(R)} = \operatorname{Tr}_{S,TL}\rho(t) = \begin{pmatrix}
\frac{r_{0,0}^{(0)} & r_{0,1}^{(1)} & r_{0,2}^{(2)} & \cdots & r_{0,K-1}^{(K-1)} & r_{0,K}^{(K)} \\
\hline r_{1,0}^{(-1)} & r_{1,1}^{(0)} & r_{1,2}^{(1)} & \cdots & r_{1,K-1}^{(K-2)} & r_{1,K}^{(K-1)} \\
\hline r_{2,0}^{(-2)} & r_{2,1}^{(-1)} & r_{2,2}^{(0)} & \cdots & r_{2,K-1}^{(K-3)} & r_{2,K}^{(K-2)} \\
\hline \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\hline r_{K-1,0}^{(-K+1)} & r_{K-1,1}^{(-K+2)} & r_{K-1,2}^{(-K+3)} & \cdots & r_{K-1,K-1}^{(0)} & r_{K-1,K}^{(1)} \\
\hline r_{K,0}^{(-K)} & r_{K,1}^{(-K+1)} & r_{K,2}^{(-K+2)} & \cdots & r_{K,K-1}^{(-1)} & r_{K,K}^{(0)}
\end{pmatrix},$$
(14)

i.e., we have another map

$$\sigma_{ij}^{(k)} \to r_{ij}^{(k)}.\tag{15}$$

Again, matrix (14) includes up to K-excitation blocks and map (15) decreases the dimension of each block reducing it from $D_i \times D_j$ to $D_i^{(R)} \times D_j^{(R)}$, $D_i^{(R)} < D_i$,

$$D_k^{(R)} = \begin{pmatrix} N^{(R)} \\ k \end{pmatrix}, \quad k = 0, 1, \dots, K.$$
 (16)

In particular, if $N^{(S)} = N^{(R)}$, then $D_i^{(R)} = D_i^{(S)}$. Notice that calculating $\operatorname{Tr}_{TL,S} \rho$ we calculate the trace of each block $\sigma_{i,j}^{(k)}$. Since j = i + k in the notation $\sigma_{i,j}^{(k)}$ and the coherence order of each particular block is conserved by trace operation [29], we can write

$$\operatorname{Tr}_{S,TL}\sigma_{i,i+k}^{(k)} = \sum_{l=0}^{i} \tilde{\sigma}_{l,l+k}^{(k;i)}, \quad i = 0, \dots, K-k,$$
(17)

where each term $\tilde{\sigma}_{l,l+k}^{(k;i)}$ contributes into the block $r_{l,l+k}^{(k)}$. Therefore we have

$$r_{l,l+k}^{(k)} = \sum_{i=0}^{K-k} \tilde{\sigma}_{l,l+k}^{(k,i)}.$$
(18)

Hereafter we concentrate on the evolution of the 0-order coherence matrix. We show that the perfectly transferable 0-order coherence matrix can be constructed for the case $K = N^{(S)}$ without involving extended receiver, while for the case $K < N^{(S)}$ we have to involve special unitary transformation of the extended receiver to reach the goal.

III. TRANSFER OF 0-ORDER COHERENCE MATRIX

Hereafter we study the 0-order coherence matrix and adopt the following notation:

$$s_{k,k}^{(0)} = s^{(k)},$$

$$r_{k,k}^{(0)} = r^{(k)},$$

$$\sigma_{k,k}^{(0)} = \sigma^{(k)}.$$
(19)

Therefore, below the subscripts mean a particular elements of the appropriate block, for instance $s_{ij}^{(k)}$. In the case of the sender initial state including only 0-order coherence matrix formulae (10), (3), (14) read, respectively,

$$\rho^{(S)} = \text{diag}(s^{(0)}, \dots, s^{(K)}), \tag{20}$$

$$\rho = \operatorname{diag}(\sigma^{(0)}, \dots, \sigma^{(K)}), \tag{21}$$

$$\rho^{(R)} = \text{diag}(r^{(0)}, \dots, r^{(K)}).$$
(22)

and formulas (17) reduce to

$$\operatorname{Tr}_{S,TL}\sigma^{(i)} = \sum_{l=0}^{i} \tilde{\sigma}^{(i;l)}, \ i = 0, \dots, K,$$
(23)

where each term $\tilde{\sigma}^{(i;l)}$ contributes to the block $r^{(l)}$, and (18) gets the form

$$r^{(l)} = \sum_{i=l}^{K} \tilde{\sigma}^{(i;l)}.$$
(24)

Thus, for a fixed l, each block $r^{(l)}$ depends not only on the elements of the block $\sigma^{(l)}$, but on the elements of the blocks $\sigma^{(j)}$ with j > l. In particular, the block $r^{(N^{(R)})}$ has no contributions from any σ -block, while the block $r^{(0)}$ includes contributions from all σ -blocks.

1. Asymptotic receiver's state as $N \to \infty$

The asymptotic receiver's state $\rho_{\infty}^{(R;0)}$ for infinitely long chain is prompt by formula (24) and by the fact that all elements ρ_{ij} vanish with an increase in the chain length for a fixed sender's dimension $N^{(S)}$. In other words, the asymptotic state of the receiver is expected to be the ground state because the 0-excitation block of $\rho^{(R)}$ gathers elements from the higher-excitation blocks due to the partial trace. Thus

$$\rho_{\infty}^{(R;0)} = \text{diag}(1,0,\dots,0).$$
(25)

A. Unitary transformation of the extended receiver

To handle the structure of the nondiagonal elements of the zero-order coherence matrix, we use the unitary transformation U of the so-called extended receiver (the receiver joined with its several neighboring spins). The unitary transformation of the $N^{(ER)}$ -qubit extended receiver has also the diagonal block structure:

$$U(\varphi) = \text{diag}(1, U^{(1)}(\varphi^{(1)}), \dots, U^{(N^{(ER)}}(\varphi^{(N^{(ER)})})),$$
(26)

where $\varphi = (\varphi^{(1)}, \dots, \varphi^{(N^{(ER)})})$, and $\varphi^{(k)}$ are the sets of free parameters in the block $U^{(k)}$: $\varphi^{(k)} = (\varphi_1^{(k)}, \dots, \varphi_{F^{(k)}}^{(k)})$. Here $F^{(k)}$ is the parameter defined below in Eq. (29).

The parametrization of a particular block $U^{(k)}$ can be done as follows. Let us enumerate the nondiagonal elements of the upper triangular submatrix of a $D_k \times D_k$ matrix as follows. The nondiagonal element in the *k*th row and *l*th column, l > k, prescribes the index *n*,

$$n = \sum_{m=1}^{k-1} (D_k - m) + l - k.$$
(27)

Then the block $U^{(k)}$ of the unitary transformation can be parameterized as follows:

$$U^{(k)} = \prod_{n=1}^{F^{(k)}} e^{i\sigma_{xn}^{(k)}\varphi_n^{(k)}} \prod_{n=1}^{F^{(k)}} e^{i\sigma_{yn}^{(k)}\varphi_n^{(k)}}.$$
(28)

Here $\sigma_{xn}^{(k)}$ with *n* defined in (27) is the matrix with two units in the *k*th row and *l*th column and in the *l*th row and *k*th column. Similarly, $\sigma_{yn}^{(k)}$ with *n* defined in (27) is the matrix with -i ($i^2 = -1$) in the *k*th row and *l*th column and *i* in the *l*th row and *k*th column.

As was stated in Ref. [32], only nondiagonal elements of U are effective. Therefore the number of free real non-diagonal parameters in the kth block of U is

$$F^{(k)} = D_k^{(ER)} (D_k^{(ER)} - 1), \quad k = 0, \dots, N^{(ER)}.$$
(29)

Thus, the total number of free parameters is (since $F^{(0)} = F^{(N)} = 0$) is

$$F = \sum_{n=1}^{N-1} F^{(n)}.$$
 (30)

However, only blocks of U with up to K excitations are effective, where K is the excitation number in $\rho^{(S)}(0)$. Therefore, the number of effective parameters is

$$F_{eff} = \sum_{n=1}^{K} F^{(n)}.$$
 (31)

We combine the evolution operator V and transformation U into the single operator W:

$$W(t) = \left(\mathbb{I}_{S,TL'} \otimes U\right) V(t), \tag{32}$$

where TL' is the transmission line without the nodes of the extended receiver. Of course, W has the block-structure similar to (8):

$$W = \text{diag}(W^{(0)}, W^{(1)}, \dots, W^{(N)})$$
(33)

with scalar blocks $W^{(0)}$ and $W^{(N)}$.

Although using the unitary transformation we can not completely restore the diagonal elements of the 0-order coherence matrix, but we can use these parameters to restore the nondiagonal elements of the 0-order coherence matrix. This can be useful, in particular, to keep the required form of the zero-order coherence matrix, as will be used below.

B. Perfect transfer of the 0-order coherence matrix

1. Complete state space of the sender

First we consider $N^{(S)}$ -excitation initial state of the $N^{(S)}$ -qubit sender and transfer this state to the $N^{(R)} = N^{(S)}$ -qubit receiver, i.e., the transferred density matrix consists of all blocks related with the excitation numbers from 0 to $N^{(S)}$ (the complete state space of sender).

In this case, the sender and receiver states are

$$\rho^{(S)} = \operatorname{diag}(s^{(0)}, s^{(1)}, \dots, s^{(N^{(S)})}), \quad \rho^{(R)}(t) = \operatorname{diag}(r^{(0)}(t), r^{(1)}(t), \dots, r^{(N^{(S)})}(t)), \quad (34)$$

where $s^{(0)}$, $s^{(N^{(S)})}$, $r^{(0)}$ and $r^{(N^{(S)})}$ are scalars with $r^{(N)}(t) = |W^{(N)}(t)|^2 s^{(N)}$. We select the time instant for state registration $t^{(N^{(S)})}$ corresponding to the maximum of $|W^{(N)}(t)|^2$ (the probability of the $N^{(S)}$ -excitation state transfer from the sender to the receiver [31]):

$$\max_{t} \left(|W^{(N)}(t)|^2 \right) = |W^{(N)}(t^{(N^{(S)})})|^2.$$
(35)

This time instant is almost a linear function of the chain length N, as is demonstrated in Table I for the XX-Hamiltonian (5) with $N^{(S)} = 2$, see also Fig.2.

Ν	1	0 1	5 2	20 2	25 3	30 3	5 4	0 4	5 5	0 5	5
$t^{(2)}$	12.8	896 18.2	2026 23.4	4171 28.5	5937-33.7	7448 38.8	3736 43.9	9842 49.0	820 54.1	709 59.2	2527
	N	60	65	70	75	80	85	90	95	100	
	$t^{(2)}$	64.3271	69.3941	74.4548	79.5106	84.5620	89.6089	94.6516	99.6898	104.724	

TABLE I: Time instants for state registration for spin chain of different chain length N governed by XX-Hamiltonian (5) with 2-qubit sender including up to two excitations.

For a long homogeneous chain one has $|W^{(N^{(S)})}|^2 < 1$, and therefore the equality $\rho^{(R)}(t) = \rho^{(S)}(0)$ is impossible. But we can find such $s^{(0)}(0)$ that (see [31])

$$r^{(N^{(S)})}(t^{(N^{(S)})}) = s^{(0)}(0).$$
(36)

We also require the elements of $s^{(k)}(0)$ $(k \neq 0, N^{(S)})$ to satisfy the following equations at the time instant $t^{(N^{(S)})}$:

$$r^{(k)}(t^{(N^{(S)})}) = s^{(k)}(0), \ 1 \le k \le N^{(S)} - 1.$$
 (37)

Then $\rho^{(R)}(t^{(N^{(S)})})$ coincides with $\rho^{(S)}(0)$ up to the exchange of two elements of blocks with zero and $N^{(S)}$ excitations. This exchange can be performed by the unitary transformation U^{ex} such that

$$[U^{ex}, I_z] \neq 0. \tag{38}$$

An interesting question is the dependence of the elements of the perfectly transferred zeroorder coherence matrix on the chain length N. The asymptotic receiver's state (25) allows to assume that the sender state found as a solution of the system (36), (37) in view of the unitary transformation U^{ex} tends to

$$\rho_{\infty}^{(R)} = \rho_{\infty}^{(S)} = \text{diag}(0, 0, \dots, 0, 1)$$
(39)

in a long chain. The graph of the deviation

$$\delta = ||\rho_{\infty}^{(S)} - \rho^{(S)}(N)||, \tag{40}$$

where $||A|| = \sqrt{\text{Tr}(AA^{\dagger})}$ is the Frobenius (or the Hilbert–Schmidt) norm, as a function of N for the 2-qubit sender at time instants taken from Table I is shown in Fig. 1. In this case we have three blocks in the sender and receiver density matrices.

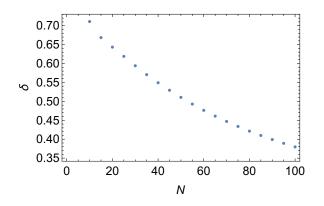


FIG. 1: Deviation δ of the perfectly transferred 2-qubit state $\rho^{(S)}$ $(N^{(S)} = 2)$ from the asymptotic density matrix $\rho_{\infty}^{(S)}$.

a. Effect of PTZ on the structure of the restorable higher-order coherence matrices. We emphasize that the unitary transformation U^{ex} interchanges the first column (respectively, first row) with the last column (respectively, last row) of the matrix $\rho^{(R)}$. Therefore, using the proposed protocol for the perfect transfer of the 0-order coherence matrix in combination with the structural restoring of the higher order coherence matrices imposes a restriction on the structure of the optimally transferable sender's state [31]. Namely, the sender's density matrix (10) now should have the following form (using notation (19) for the diagonal blocks):

$$\rho^{(S)} = \begin{pmatrix}
\frac{s^{(0)} & 0_{0,1}^{(1)} & 0_{0,2}^{(2)} & \cdots & 0_{0,N^{(S)}-1}^{(N^{(S)}-1)} & 0_{0,N^{(S)}}^{(N^{(S)})} \\
\frac{0_{1,0}^{-1} & s^{(1)} & s_{1,2}^{(1)} & \cdots & s_{1,N^{(S)}-1}^{(N^{(S)}-2)} & 0_{1,N^{(S)}}^{(N^{(S)}-1)} \\
\frac{0_{2,0}^{(-2)} & s_{2,1}^{(-1)} & s^{(2)} & \cdots & s_{2,N^{(S)}-1}^{(N^{(S)}-3)} & 0_{2,N^{(S)}}^{(N^{(S)}-2)} \\
\frac{\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\frac{0_{N^{(S)}-1,0}^{(-N^{(S)}+1)} & s_{N^{(S)}-1,1}^{(-N^{(S)}+2)} & s_{N^{(S)}-1,2}^{(-N^{(S)}+3)} & \cdots & s^{(N^{(S)}-1)} & 0_{N^{(S)}-1,N^{(S)}}^{(1)} \\
\frac{0_{N^{(S)},0}^{(-N^{(S)})} & 0_{N^{(S)},1}^{(-N^{(S)}+1)} & 0_{N^{(S)},2}^{(-N^{(S)}+2)} & \cdots & 0_{N^{(S)},N^{(S)}-1}^{(-1)} & s^{(N^{(S)})} \\
\end{pmatrix},$$
(41)

where $0_{i,j}^{(n)}$ is the block $s_{i,j}^{(n)}$ with all zeros. The diagonal blocks in (41) correspond to 0-order coherence matrix; for the blocks of non-zero order coherence matrices we keep the notations introduced in (10). Formula (41) shows that the first column (respectively, row) and the last column (respectively, row) of the whole matrix $\rho^{(S)}(0)$ must be zero except of their diagonal elements. Otherwise, the final unitary transformation U^{ex} will mix some elements of coherence matrices of different orders.

2. Restricted state space of the initial sender's state

Suppose that the state of the $N^{(S)}$ -qubit sender includes $K < N^{(S)}$ excitations. Then, instead of (34) we have

$$\rho^{(S)} = \operatorname{diag}(s^{(0)}, s^{(1)}, \dots, s^{(K)}), \ \rho^{(R)} = \operatorname{diag}(r^{(0)}, r^{(1)}, \dots, r^{(K)}).$$
(42)

The state in the form (42) can not be perfectly transferred using the method in Sec. III B 1. In fact, this method assumes that the final unitary transformation U^{ex} exchanges the positions of $r^{(0)}$ and one more diagonal element, say $r_{11}^{(K)}$. But such transformation does not conserve the excitation number (see Eq. (38)), it unavoidably exchanges rows and columns associated with the two mentioned diagonal elements and thus creates higher-order coherence matrices which are not desirable. To avoid this effect, we have to impose a special restriction on the structure of the blocks $s^{(K)}$ and $r^{(K)}$. Namely, let all the elements in the row and the column of the diagonal element $s_{11}^{(K)}$ (i.e., all the elements of the first column and first row of the Kth block) be zeros except the single diagonal element $s_{1,1}^{(K)}$, i.e.

$$s_{i,1}^{(K)} = s_{1,i}^{(K)} = 0, \ 1 < i \le D_K^{(S)}.$$
 (43)

Then the structure of $s^{(K)}$ reduces to the following one:

$$s^{(K)} = \left(\frac{s_{1,1}^{(K)} \quad 0_{1,D_K^{(S)}-1}}{0_{D_K^{(S)}-1,1} \quad \tilde{s}^{(K)}} \right), \tag{44}$$

and

$$\tilde{s}^{(K)} = \begin{pmatrix} s_{2,2}^{(K)} & \dots & s_{2,D_K^{(S)}}^{(K)} \\ \dots & \dots & \dots \\ (s_{2,D_K^{(S)}}^{(K)})^* & \dots & s_{D_K^{(S)},D_K^{(S)}}^{(K)} \end{pmatrix},$$
(45)

where $0_{i,j}$ is the $i \times j$ zero matrix. Recall that the subscripts in (43)-(45) are indexes of matrix elements.

Now we can replace the system (37) with the following one:

$$r^{(k)} = s^{(k)}, \ 1 \le k \le K - 1,$$
(46)

$$r_{i,j}^{(K)} = s_{i,j}^{(K)}, \ 2 \le i \le D_K^{(S)}, \ 2 \le i \le D_K^{(S)},$$
 (47)

$$s_{1,i}^{(K)} = 0, \ 2 \le i \le D_K^{(S)},$$
(48)

$$r_{1,1}^{(K)} = s^{(0)},\tag{49}$$

$$r_{1,i}^{(K)} = 0, \ 2 \le i \le D_K^{(S)}.$$
 (50)

However, in the receiver density matrix $\rho^{(R)}$, the elements $r_{i,1}^{(K)}$ are non-zero at t > 0because of the mixing of the elements during the evolution. That is why Eq. (50) is valuable. Therefore, we have to involve the unitary transformation of the extended receiver with parameters φ to make these elements zero at certain time instant $t_K^{(N^{(S)})}$ (this time instant will be specified below). To write the system for the set of parameters φ of the unitary transformation, we use the results of [31] and write the relation between $r^{(k)}$ and $s^{(k)}$ as

$$r_{i,j}^{(k)}(t,\varphi) = \sum_{n,m=1}^{D_k^{(S)}} T_{ij;nm}^{(k)}(t,\varphi) s_{nm}^{(k)}(0), \quad T_{ij;nm}^{(k)}(t,\varphi) = (T_{ji;mn}^{(k)}(t,\varphi))^*.$$
(51)

where $T^{(k)}$ is the transfer matrix of the k-excitation block whose explicit form is not important at the moment. Then system (50) takes the form

$$r_{1,i}^{(k)}(t,\varphi) = \sum_{n,m=1}^{D_k^{(S)}} T_{1i;nm}^{(k)}(t,\varphi) s_{nm}^{(k)}(0) = 0.$$
(52)

This system of equations is satisfied if the parameters φ at $t = t_K^{(N^{(S)})}$ satisfy the following system (taking into account (48)):

$$T_{1,n;i,i}^{(K)}(t^{(N_K^{(S)})},\varphi) = 0, \quad 2 \le n \le D_K^{(S)} \quad 1 \le i \le D_K^{(S)}, \tag{53}$$

$$T_{1,n;i,j}^{(K)}(t_K^{(N^{(S)})},\varphi) = 0, \ 2 \le n \le D_K^{(S)}, \ 2 \le i \le D_K^{(S)}, \ 2 \le j \le D_K^{(S)}, \ i \ne j.$$
(54)

Notice, that the asymptotic PTZ has the form (39) as well.

Remark. In principle, the system (46)–(50) can be solved as the whole for the parameters φ and elements of $r^{(k)}$. But we select Eq. (50), replace it by system (53), (54) and solve the later for φ . After that, the system (46)–(49) can be solved for the elements of $r^{(k)}$.

IV. 0-ORDER COHERENCE MATRIX WITH UP TO ONE EXCITATION

A. Perfect transfer of 0-order coherence matrix

We consider the 0-order coherence matrix including 0- and 1-excitation. According to (41) and (44), the initial sender's density matrix has the following structure:

$$\rho^{(S)} = \left(\frac{s^{(0)} \mid 0^{(1)}_{0,1}}{0^{-1}_{1,0} \mid s^{(1)}}\right), \quad s^{(1)} = \left(\frac{s^{(1)}_{1,1} \mid 0_{1,N^{(S)}-1}}{0_{N^{(S)}-1,1} \mid \tilde{s}^{(1)}}\right), \tag{55}$$

where $\tilde{s}^{(1)}$ is a full matrix of the form (45). Since the only higher order coherence matrices in this case are the ±1-order coherence matrices and they are zeros according to (55), this case doesn't allow to transfer any arbitrary parameter through the higher order coherence matrices. Nevertheless, we consider this case in details to reveal some general features of PTZ.

In this case the system (51) can be written in the simple matrix form

$$r^{(1)}(t,\varphi) = \mathcal{W}(t,\varphi)s^{(1)}\mathcal{W}^{\dagger}(t,\varphi),$$
(56)

see Appendix VI for more detail. Then system (53), (54) with K = 1 and $D_1^{(S)} = N^{(S)}$ reads

$$T_{1,n;i,i}^{(1)}(t_1^{(N^{(S)})},\varphi) = \mathcal{W}_{1i}(t_1^{(N^{(S)})},\varphi)\mathcal{W}_{ni}^*(t_1^{(N^{(S)})},\varphi) = 0,$$

$$2 \le n \le N^{(S)}, \quad 1 \le i \le N^{(S)},$$

$$T_{1,n;i,j}^{(1)}(t_1^{(N^{(S)})},\varphi) = \mathcal{W}_{1i}(t_1^{(N^{(S)})},\varphi)\mathcal{W}_{nj}^*(t_1^{(N^{(S)})},\varphi)0,$$

$$2 \le n \le N^{(S)}, \quad 2 \le i \le N^{(S)}, \quad 2 \le j \le N^{(S)}, \quad i \ne j.$$
(57)
$$(57)$$

This system is satisfied if φ solves the smaller system of $N^{(S)}$ equations

$$\mathcal{W}_{1j} = 0, \ \ j = 1, \dots, N^{(S)},$$
(59)

although solution space of system (57), (58) is richer than that of (59). Notice also that solution of (59) leads to

$$r_{11}^{(1)} = 0$$
 for any $s_{11}^{(1)}$. (60)

We fix the time instant for state registration as the time instant $t_1^{(N^{(S)})}$ maximizing the sum of probabilities of the excitation transfer from any node of the sender to any node of the receiver with $\varphi = 0$, i.e. the maximum of the Frobenious norm of \mathcal{W} :

$$\max_{t} ||\mathcal{W}(t,0)|| = ||\mathcal{W}(t^{(N^{(S)})},0)||.$$
(61)

For the 3- and 4-node sender these time instants $t_1^{(3)}$ and $t_1^{(4)}$ are given in Table II for different chain lengths, see also Fig.2.

The system (46)-(49) must be replaced with the following one:

$$\begin{aligned} r_{i,j}^{(1)} &= s_{i,j}^{(1)}, \ 2 \leq i, j \leq N^{(S)}, \\ s_{i,1}^{(1)} &= 0, \ 2 \leq i \leq N^{(S)}, \\ r_{1,1}^{(1)} &= s^{(0)}. \end{aligned}$$
(62)

Ν]	10	1	15	6 4	20	4	25		30	÷	35	2	40	4	45	Ę	50	5	5
$t_1^{(3)}$	12.	1286	17.5	2800	22.	6386	27.	9575	33.	2243	38.	4457	43.	6308	48.	7867	53.	9178	59.0	261
$t_1^{(4)}$	12.	0631	17.	6689	23.	2101	28.	5882	33.	8054	38.	8500	43.	7263	48.	5206	53.	3406	58.2	072
	N	60)	65	5	7	0	75	5	80)	85	5	90)	95	5	1()0	
	$t_1^{(3)}$	64.1	135	69.1	819	74.2	338	79.2	704	84.2	923	89.29	997	94.2	938	99.2	753	104.	.245	
	$t_1^{(4)}$	63.10	042	68.0	181	72.9	414	77.80	690	82.7	979	87.72	267	92.6	558	97.5	861	102.	5179	

TABLE II: Time instants for state registration for spin chain of different chain length N governed by XX-Hamiltonian (5) with 3- and 4-qubit sender including up to one excitation.

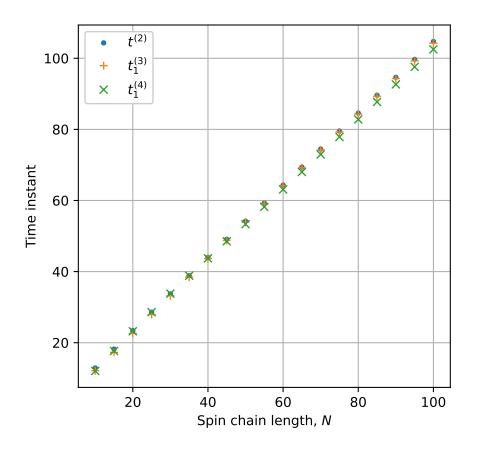


FIG. 2: Time instants for registration of a state transferred along the spin chain governed by XX-Hamiltonian (5) in dependence on chain length N. The data correspond to Tables I and II. Circle, crosses, pluses correspond to, respectively, 2-qubit sender including up to two excitations, 3- and 4-qubit sender including up to one excitation. Note, that transmission time slightly depend on the dimension of the sender.

In this case the general form of the block $s^{(1)}$ of the initial density matrix of the $N^{(S)}$ qubit sender is (44) and (45) with K = 1. Unitary transformation U (26) includes the only nontrivial block $U^{(1)}$ with parameters $\varphi = \varphi^{(1)}$,

$$U(\varphi) = \operatorname{diag}(1, U^{(1)}(\varphi)).$$
(63)

1. Numerical optimization

Since the solution space of the system (57), (58) is larger than the solution space of the reduces system (59), we use the former in the numerical optimization protocol.

The construction of the matrix that can be perfectly transferred consists of the three steps.

- Step 1: Solve system (57), (58) (64) to fix the parameters φ of the unitary transformation (63)
- Step 2: Solve system (62)

for the elements of the initial density matrix of the sender

Step 3: Perform the unitary transformation U^{ex} exchanging positions of $r^{(0)}$ and $r^{(1)}_{1,1}$

The solution $\varphi = \varphi_0$ of the system (57), (58) obtained at the first step provides the required structure of $r^{(1)}(t_0, \varphi_0)$, but this solution is not unique because the number of φ -parameters is, generally, lager then the number of equations in the system (57), 58). Therefore we can select a desired one. Namely, we are interested in such optimal $\varphi = \varphi^{\text{opt}}$ parameters of the unitary transformation (63) that provide the PTZ state obtained as a solution of (62) with the maximal deviation $\delta^{\max} = \delta|_{\varphi=\varphi^{\text{opt}}}$, where

$$\delta(\varphi) = ||\rho_{\infty}^{(S)} - \rho^{(R)}(\varphi)||, \qquad (65)$$

compare with Eq. (40). In Fig.3, δ^{\max} is given as a function of the chain length N for $N^{(S)} = 3$, 4 and different lengths of the extended receiver $N^{(ER)}$. This figure demonstrates that δ^{\max} increases with an increase in the dimension of the extended receiver and slowly decreases with length of the chain, see inset in the right-low corner of Fig.3a. Fig.3a demonstrates that the proposed optimization protocol works in the whole range of the considered chain

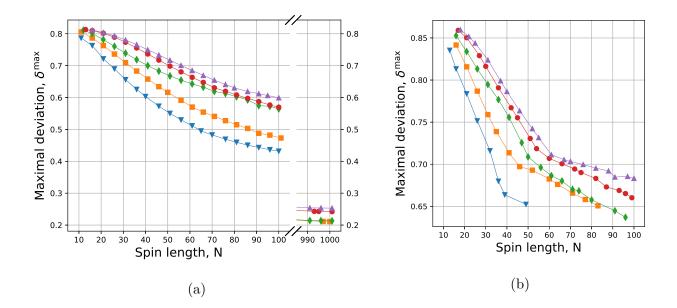


FIG. 3: Deviation δ^{\max} of PTZ $\rho^{(S)}$ from the asymptotic PTZ $\rho_{\infty}^{(S)}$ as a function of N. Optimization is performed for each spin length N and fixed number of ancillary spins $N^{(A)}$ in the extended receiver with size $N^{(ER)} = N^{(S)} + N^{(A)}$. Triangles, rhombus, circles, squares, inverted triangles correspond to, respectively, $N^{(A)} = 5$, $N^{(A)} = 4$, $N^{(A)} = 3$, $N^{(A)} = 2$, $N^{(A)} = 1$. (a) $N^{(S)} = 3$, the long-chain values of δ^{max} are shown at $N \sim 1000$ in the right-low corner of the plot; (b) $N^{(S)} = 4$.

length (up to 100) for the 3-qubit receiver (sender). Regarding the case of 4-qubit receiver (sender), the optimization protocol works in the whole range of N only for large enough extended receiver, while the protocol with the minimal applicable dimension of the extended receiver $(N^{(A)} = 1, 2)$ yields the satisfactory results only for $N \leq 50$ ($N^{(A)} = 1$) or $N \leq 80$ ($N^{(A)} = 2$), as shown in Fig.3b. This fact just indicates that including more optimization parameters simplifies the search for the local minima. We emphasize that in all cases the optimization leads to $r_{1,1}^{(1)} = 0$ pointing that the system (59) yields the optimal parameters φ .

We notice that determining the optimal φ^{opt} -parameters is not a trivial problem. The matter is that when constructing the target function we have to take into account the two-fold purpose of the optimization protocol. First, we have to satisfy the system (57), (58). Second, we have to maximize the deviation δ . Therefore, the natural target function is

$$F_T(\varphi) = w_1 S_T(\varphi) - w_2 \delta(\varphi) \tag{66}$$

where

$$S_T(\varphi) = \sum_{l,n,m} \left| T_{l,1;n,m}^{(1)}(t_1^{(N^{(S)})}, \varphi) \right|$$
(67)

(sum of all equations (57) and (58)), w_i , i = 1, 2 are some weights which are fixed below, and sum is over all allowed values of the indexes l, n and m, as in Eqs.(57), (58). Here φ is rather long set of parameters which varies from 12 (4-qubit extended receiver) to 55 (8-qubit extended receiver) parameters. Thus, we combine Step 1 and Step 2 in the 3-step protocol (64).

Let us describe the optimization protocol in more details. First, we replace S_T given by (67) with the following one

$$S_T(\varphi) = \max_{l,n,m} \left| T_{l,1;n,m}^{(1)}(t_1^{(N^{(S)})}, \varphi) \right|,$$
(68)

i.e. we define the residual S_T as the maximal absolute value of the left sides of eqs. (57), (58). This residual removes confrontation among different terms in sum (67) extracting the most important one.

What follows is based on two remarks.

Remark 1. We study optimization task (66), (68) with a differential evolution (DE) algorithm [33–35] which is a kind of a genetic algorithm with crossover and mutation operations. DE is a popular algorithm for a multiparameter optimization problems, including in quantum control [36–38]. We perform calculation with the SciPy package [39] of version 1.4.1. The number of individuals in each population is $15N^{(S)}$. The probability of crossover is CR = 0.7 and probability of mutation randomly varies in the range $F \in [0.5, 1]$. Some experiments were performed with higher population size $1000N^{(S)}$, higher mutation F = 1.9, and lower recombination CR = 0.3 values to ensure finding the global minimum.

Remark 2. We set in the functional (66) weights as $w_1 = w_2 = 1$, because the natural ratio between S_T and δ appearing during optimization is suitable. For instance, for some $\varphi = \varphi_0^{(approx)}$ we find that the residual is $S_T(\varphi_0^{(approx)}) \approx 10^{-3}$, while the deviation is $\delta(\varphi_0^{(approx)}) \approx$ 1. Both these values are quite reasonable and convergence rates for both of them are admittable. On the contrary, using larger ratio $(w_1S_t)/(w_2\delta)$ obtained for some other weights in the formula (66) leads to a low convergence rate for S_T while using smaller ratio decreases the convergence rate for δ . Thus, when minimizing $F_T(\varphi)$ with S_T from (68) we find an approximation $\varphi = \varphi_0^{\text{approx}}$. Now we polish the result with a local optimization method using $\varphi_0^{(approx)}$ for seed values of the parameters φ and using the same target function F_T given by (66). The set of resulting parameters of unitary transformation we denote as φ^{approx} .

Now we obtain the exact solution φ^{opt} of system (57), (58) in the vicinity of φ^{approx} . This is the last step of the optimization protocol.

Step 3 of protocol (64) can be done directly using the unitary transformation U^{ex} exchanging the positions of $r^{(0)}$ and $r^{(1)}_{1,1}$ in the receiver state.

Notice that increasing the dimension of the extended receiver leads to increasing the dimension of the optimization parameter space. As shown in [40, 41], in this case the number of traps, i.e. local but not global minima of the objective, generally decreases. Thus the control landscape of the considered optimization problem for an *n*-spin extended received is expected to have less traps compared to the control landscape for *m*-spin extended receiver if n > m.

To check the reliability of the global minimization we perform the optimization algorithm using two other global optimization methods: the "brute force" method and Dual Annealing method [42] from SciPy package [39] of the version 1.4.1. In all three cases, the results are the same up to the absolute error of 10^{-3} .

B. Arbitrary parameter transfer via 0-order coherence matrix

Let the unitary transformation of the extended receiver be such that the operator \mathcal{W} is diagonal, i.e.

$$\mathcal{W}_{ij} = 0, \ i \neq j, \ i, j = 1, \dots, N^{(S)}.$$
 (69)

System (69) includes $\frac{1}{2}N^{(S)}(N^{(S)}-1)$ complex equations. In this case

$$T_{ij;nm}^{(1)} = \lambda_{ij}\delta_{in}\delta_{jm}, \quad \lambda_{ij} = (\lambda_{ji})^* \quad , \quad i, j, n, m = 1, \dots, N^{(S)}$$

$$\tag{70}$$

$$\lambda_{ij} = \mathcal{W}_{ii}\mathcal{W}_{jj}^*.\tag{71}$$

Therefore any element in the receiver's one-excitation block is proportional to the appropriate element of the sender's one-excitation block, i.e.

$$r_{i,j}^{(1)} = \lambda_{ij} s_{i,j}^{(1)}, \quad i, j = 1, \dots, N^{(S)},$$
(72)

where λ_{ij} are scale factors, $|\lambda_{ij}| \leq 1$. Formula (72) means the structural restoring of the whole one-excitation block of the 0-order coherence matrix [31, 32]. In this case $r^{(0)}$ (the only element of the zero-excitation block) provides the normalization and therefore can not be proportional to $s^{(0)}$. Unlike in Sec. IV A, we do not exchange positions of any diagonal elements and consequently all elements of the one-excitation block can be non-zero.

Below we consider the cases of 2- and 3-qubit senders and appropriate extended receivers with unitary transformations whose parameters not only solve system (69), but also maximize the scale factors λ_{ij} in (72). Therefore, we consider the minimal of $|\lambda_{ij}|$,

$$\lambda_{opt} = \min_{i,j} |\lambda_{ij}|,\tag{73}$$

as a maximization object and use the global minimization algorithm with the following target function:

$$F_T = \sqrt{\sum_{i \neq j} |\mathcal{W}_{ij}|^2} - \min_{i,j} |\lambda_{ij}|.$$
(74)

At that, the optimization parameters are the parameters of the unitary transformation of the extended receiver φ and time t.

However, to simplify calculation, we perform global optimization over the parameters φ at fixed time instants and find the values of $|\lambda_{opt}|$ inside of the time interval around $t \sim N$ as shown in Fig. 4 for 2-qubit receiver and 3-qubit extended receiver. We see in this figure that there are two local maxima near the optimal time instant. For N < 50 the first local maximum is higher, while the second becomes higher for $N \geq 50$. This leads to a jump in the function $t_{opt}(N)$ and to a small local minimum in the function $|\lambda_{opt}(N)|$ as shown in Fig. 5 for the case $N^{(S)} = 2$ and $N^{(ER)} = 3$. This jump leads to the local minimum on the graph of $|\lambda_{opt}|$ in Fig. 5b. Similar jump appears for the case $N^{(ER)} = 4$, although the graph of $|\lambda_{opt}|$ is monotonic. In the case $N^{(S)} = 3$, $N^{(ER)} = 5$, $|\lambda_{opt}|$ has three local maxima near the optimal time instant, therefore two jumps appear on the graph in Fig. 5. However, unlike the case $N^{(S)} = 2$, the graph of $|\lambda_{opt}|$ remains monotonic. The choice of dimensions of extended receivers is explored in Appendix.

V. CONCLUSIONS

Unlike the elements of the higher-order coherence matrices, not all diagonal elements of the 0-order coherence matrix in general can be structurally restored [31]. This happens due

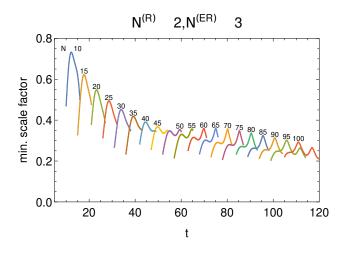


FIG. 4: $N^{(S)} = 2$, $N^{(ER)} = 3$. Dependence of $|\lambda_{opt}|$ (minimal scale factor) on time for different chain lengths from N = 10 to N = 100. Only time intervals around the assumed maxima are considered for each N.

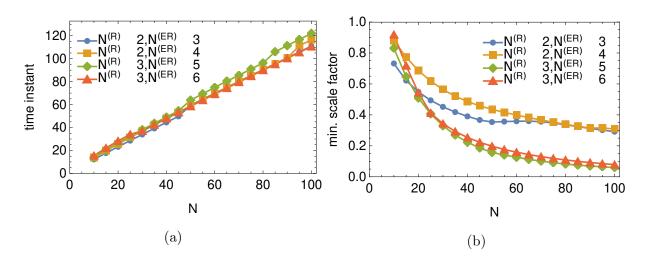


FIG. 5: Time instant t_{opt} (a) and absolute value of the minimal scale factor $|\lambda_{opt}|$ (b) as functions of N for $N^{(S)} = 2$, $N^{(ER)} = 3$, $N^{(S)} = 2$, $N^{(ER)} = 4$ and $N^{(S)} = 3$, $N^{(ER)} = 5$.

to the trace-normalization condition which 0-order coherence matrix must satisfy. However, the normalization condition creates a possibility for the perfect transfer of 0-order coherence matrix with elements fixed in a certain way. We show that the perfect transfer can be produced using one additional unitary transformation applied to the receiver at the time instant of state registration to exchange positions of two diagonal elements. One of these elements is necessarily the only element of the 0-excitation block and another one is, in the simplest case, another one-element block of the receiver density matrix, associated with $N^{(S)}$ -excitation subspaces of the $N^{(S)}$ -qubit receiver. If this element does not exist (this happens if the number of excitations appeared in the receiver state is less then $N^{(S)}$) then any other diagonal element can be taken. This is the case when we need to use the unitary transformation of the extended receiver to provide consistency of the protocol.

We show that, with an increase in the chain length, the perfectly transferable sender density matrix tends to the diagonal matrix $\rho_{\infty}^{(S)}$ with only one non-zero element.

We study the deviation δ of the 0-order coherence matrix perfectly transferred through the N-qubit chain from the limiting matrix $\rho_{\infty}^{(S)}$ for a particular case of transferred states with 0- and 1-excitation blocks of 3- and 4-qubit receiver (and sender) using the $(N^{(S)} + i)$ qubit extended receiver with i = 1, 2, 3, 4, thus verifying that increasing the dimension of the extended receiver we can increase the deviation δ .

For the practical purpose the presence of deviation from the trivial asymptotic is important, because positivity of the density matrix requires vanishing of all elements from the row and column where the zero diagonal element appears. Therefore, the asymptotic 0-order coherence matrix $\rho_{\infty}^{(S)}$ can not transfer any other element.

We also remark, that the simplest case of perfectly transferred 1-excitation 0-order coherence matrix can not be used to transfer the higher order coherence matrices (1-order in this case) because these elements belong to the first row and first column of the receiver's density matrix which are zeros according to Eq.(55).

The 0-order coherence matrix of the receiver state includes one more feature. The elements of the 1-excitation block of this matrix can be restored similarly to the elements of the higher-order coherence matrices. At that, however, the 0-excitation element provides the trace-normalization. This fact allows to use the elements of this block to transfer arbitrary parameters from the sender to the receiver. Of course, there is no perfect transfer of 0-order coherence matrix in this case. We study the absolute value of the minimal of the scale factors ahead of the transferred arbitrary parameters as a function of the chain length for the case of 2- and 3-qubit receiver with the appropriate minimal dimension of the extended receivers.

We have to emphasize that the perfect transfer of the 0-order coherence matrix implies certain constraints on the structure of the restorable higher-order coherence matrices. Namely, the rows and columns of the transferred matrix corresponding to the diagonal elements which are exchanged by the final unitary transformation of the receiver must be zero, see Eq.(41).

We also shall emphasize that the unitary transformation constructed in Sec. IV A provides the PTZ for a particular 0-order coherence matrix, while the unitary transformation constructed in Sec. IV B for transferring the arbitrary parameters is universal in the sense that the same transformation can be used to transfer parameters of any initial sender's state. The scale factors appearing ahead of the arbitrary parameters in the receiver's state are permanent characteristics of the protocol similar to [31].

To resume, we have studied the structure of the 0-order coherence matrix which can be perfectly transferred along the spin chain. At that the elements of the 1-excitation block of the 0-order coherence matrix can be also used to transfer arbitrary parameters if the unitary transformation of the extended receiver is properly adjusted. Of course, all the transferable arbitrary parameters must keep the positivity of the associated density matrices.

We also emphasize that the proposed protocol of the perfect transfer of the 0-order coherence matrix is not related to just the XX Hamiltonian (5). It can use any Hamiltonian satisfying commutation condition (6), for instance, XXZ Hamiltonian. Although we consider the nearest neighbor interaction, it is not a necessary requirement to the Hamiltonian and we can include the remote node interactions (e.g. dipole-dipole interactions) as far as this step doesn't destroys the above commutation condition. Also the homogeneous chain can be replaced with any non-homogeneous chain since the Hamiltonian for a non-homogeneous chain also satisfies the commutation condition (6). Of course, all the above modifications of the spin system (changing the Hamiltonian, including the remote node interaction and passing to the non-homogeneous chain) change the required unitary transformation U (26) and the form of the perfectly transfered 0-order coherence matrix $\rho^{(S)}$ derived in Sec.IV, but the described protocol of PTZ is stable to all those modifications.

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VI. APPENDIX: REPRESENTATION OF TRANSFER OPERATOR *T* IN TERMS OF EVOLUTION OPERATOR AND UNITARY TRANSFORMATION OF EX-TENDED RECEIVER

According to Ref. [31], the receiver density matrix is defined by two unitary operators. The first one, denoted by V, describes the evolution under certain Hamiltonian H: $V(t) = e^{-iHt}$. This operator acts on the whole system. The second operator U acts only on the extended receiver, it depends on the set of free parameters which are used to satisfy the requirements of the target state creation. These two operators can be combined into the single operator W (32). Therefore, the receiver's density matrix (14) reads

$$\rho^{(R)} = \operatorname{Tr}_{S,TL} \left(W(t,\phi) \left(\rho^{(S)}(0) \otimes \rho^{(TL,R)}(0) \right) W^{\dagger}(t,\varphi) \right).$$
(75)

Now we introduce multiindexes associated with the sender (S), transmission line (TL) and receiver (R) [31]. These indexes are represented by the capital latin letters with appropriate subscript S, TL ar R. Then we write receiver density matrix (75) as

$$r_{N_R,M_R}^{(k)} = \sum_{N_S,N_{TL}} W_{N_S,N_{TL},N_R;I_S,0_{TL},0_R}^{(k)} \rho_{I_S,J_S}^{(S)} (W^{(k)})_{J_S,0_{TL},0_R;N_S,N_{TL},M_R}^{\dagger},$$
(76)
$$k = 0, \dots, N^{(S)}.$$

In the 0- and 1-excitation case, for the elements of the 0-order coherence matrix we have

$$\rho_{0_R,0_R}^{(R)} \equiv r^{(0)} = 1 - \sum_{i=1}^{(N^{(S)})} r_{ii}^{(1)}, \tag{77}$$

$$r_{N_R,M_R}^1 = W_{0_S,0_{TL},N_R;I_S,0_{TL},0_R}^{(1)} s_{I_S,J_S}^{(1)} (W^{(1)})_{J_S,0_{TL},0_R;0_S,0_{TL},M_R}^{\dagger}.$$
(78)

We can introduce $N^{(S)} \times N^{(S)}$ matrix \mathcal{W} passing from the multiindex basis to the computational basis following the rule

$$(\underbrace{0\dots0}_{i-1}1\underbrace{0\dots0}_{N^{(S)}-i}) \to i, \tag{79}$$

so that

$$\mathcal{W}_{ij} = W^{(1)}_{0_S, 0_{TL}, \underbrace{0}_{i-1}, \underbrace{0}_{i-1} \underbrace{1}_{0, \dots, 0; \underbrace{0}_{j-1}, 0}_{N^{(S)}_{i-1}, 0} \underbrace{1}_{0, \dots, 0; 0_{TL}, 0_R} \underbrace{0}_{N^{(S)}_{i-j}}.$$
(80)

and (78) gets the matrix form (56).

Let us estimate the minimal dimension of the extended receiver required to satisfy conditions (59). The number of parameters in the unitary transformation is defined by Eq. (29): $N^{(ER)}(N^{(ER)}-1)$. However, according to Eq.(78) and definition of W (32), only $N^{(S)}$ rows of the unitary transformation U are included into \mathcal{W} . Taking into account the normalization of rows of U and disregarding the common phase in each row, the number of effective free real parameters is

$$\sum_{j=1}^{N^{(S)}} (2N^{(ER)} - 2j) = N^{(S)} (2N^{(ER)} - N^{(S)} - 1).$$
(81)

This number is not less than the number of scalar real equations in (59) (which is $2N^{(S)}$) for $N^{(ER)} \geq \frac{3+N^{(S)}}{2}$. However, $N^{(ER)} \leq N^{(S)}$ means that the extended receiver is not bigger than the receiver, i.e., the unitary transformation U is applied to the receiver state. Then we can write

$$\operatorname{rank}\left(\rho^{(S)}(0)\right) = \operatorname{rank}\left(\operatorname{Tr}_{TL,S}V(t)\rho^{(S)}(0)V^{\dagger}(t)\right)$$
$$> \operatorname{rank}\left(U\operatorname{Tr}_{TL,S}V(t)\rho^{(S)}(0)V^{\dagger}(t)U^{\dagger}\right) = \operatorname{rank}\left(\rho^{(R)}(t)\right).$$
(82)

But the unitary transformation U can not reduce the rank of the matrix. Therefore, $N^{(ER)} \ge N^{(S)}+1$. This inequality is confirmed by the numerical calculations for 3- and 4-qubit receiver in Sec. IV A, Fig. 3.

Now we estimate the minimal dimension of the extended receiver needed to optimize the solution of system (69). By construction, the $N^{(S)} \times N^{(S)}$ matrix \mathcal{W} is a product of two matrices

$$\mathcal{W} = \tilde{U}\tilde{V},\tag{83}$$

where \tilde{U} is a $N^{(S)} \times N^{(ER)}$ matrix of last $N^{(S)}$ rows of the unitary transformation of the extended receiver and \tilde{V} is the $N^{(ER)} \times N^{(S)}$ matrix which is left-down corner block of the evolution matrix V. Let U be composed of the rows a_i , $i = 1, \ldots, N^{(ER)}$, \tilde{U} be composed of the rows a_i , $i = 1, \ldots, N^{(S)}$. Then the diagonal form of \mathcal{W} requires

$$a_i b_j^{\dagger} = 0, \ i \neq j, \ i, j = 1, \dots, N^{(S)}.$$
 (84)

Then we can expand b_i in the basis of a_i as follows

$$b_i = \alpha_{ii}a_i + \sum_{j=N^{(S)}+1}^{N^{(ER)}} \alpha_{ij}a_j, \quad i = 1, \dots, N^{(S)}$$
(85)

where α_{ij} are some constant coefficients.

Now we show that \mathcal{W} can be diagonalized only if $N^{(ER)} \geq 2N^{(S)} - 1$. In fact, suppose that the diagonalization can be done for the case $N^{(ER)} < 2N^{(S)} - 1$ and the system (85) is obtained. We solve first $N^{(ER)} - N^{(S)}$ equations of system (85) for a_j , $j > N^{(S)}$:

$$a_{j} = \sum_{i=1}^{N^{(ER)} - N^{(S)}} \gamma_{ji}(b_{i} - \alpha_{ii}a_{i}).$$
(86)

where the coefficients γ 's depend on α 's. Then the rest $N^{(S)} - (N^{(ER)} - N^{(S)}) = 2N^{(S)} - N^{(ER)}$ vectors b_i we have

$$b_{k} = \alpha_{kk}a_{k} + \sum_{j=N^{(S)}+1}^{N^{(ER)}} \alpha_{kj} \sum_{n=1}^{N^{(ER)}-N^{(S)}} \gamma_{jn}(b_{n} - \alpha_{nn}a_{n}), \qquad (87)$$
$$k = N^{(ER)} - N^{(S)} + 1, \dots, N^{(S)}.$$

or

$$b_{k} - \sum_{j=N^{(S)}+1}^{N^{(ER)}} \sum_{n=1}^{N^{(ER)}-N^{(S)}} \alpha_{kj} \gamma_{jn} b_{n} = \alpha_{kk} a_{k} + \sum_{j=N^{(S)}+1}^{N^{(ER)}} \sum_{n=1}^{N^{(ER)}-N^{(S)}} \alpha_{kj} \gamma_{jn} \alpha_{nn} a_{n}, \quad (88)$$
$$k = N^{(ER)} - N^{(S)} + 1, \dots, N^{(S)}.$$

By virtue of (84), we can write

$$b_k b_j^+ = 0, \ j, k = N^{(ER)} - N^{(S)} + 1, \dots, N^{(S)}, \ j \neq k.$$
 (89)

Notice that system (89) represent the additional relations between b_i . However, the vectors b_i are fixed by the Hamiltonian and they can not satisfy these additional relations in general. Therefore, we have to impose the requirement $N^{(ER)} \ge 2N^{(S)} - 1$. According to this requirement, $N^{(ER)} \ge 3$ for $N^{(S)} = 2$ and $N^{(ER)} \ge 5$ for $N^{(S)} = 3$, which is used in Sec. IV B, see Figs. 4 and 5.

Data availability statement. The authors confirm that the data supporting the findings of this study are available within the article.

References

 C.P.Koch, U.Boscain, T.Calarco, G.Dirr, S.Filipp, S.J.Glaser, R.Kosloff, S.Montangero, T.Schulte-Herbrüggen, D.Sugny, F.K.Wilhelm, Quantum optimal control in quantum technologies. Strategic report on current status, visions and goals for research in Europe. arXiv:2205.12110 [quant-ph] (2022)

- [2] S.Bose Quantum communication through an unmodulated spin chain, Phys. Rev. Lett. 91 (2003) 207901
- [3] M.Christandl, N.Datta, A.Ekert, and A.J.Landahl, Perfect state transfer in quantum spin networks, Phys.Rev.Lett. 92 (2004) 187902
- [4] P.Karbach, and J.Stolze, Spin chains as perfect quantum state mirrors, Phys.Rev.A. 72 (2005)
 030301(R)
- [5] A.Zwick, G.A.Álvarez, J.Stolze, O.Osenda, Robustness of spin-coupling distributions for perfect quantum state transfer, Phys. Rev. A. 84 (2011) 022311
- [6] G.Gualdi, V.Kostak, I.Marzoli, and P.Tombesi, Perfect state transfer in long-range interacting spin chains, Phys.Rev. A. 78 (2008) 022325
- [7] G.Gualdi, I.Marzoli, P.Tombesi, Entanglement generation and perfect state transfer in ferromagnetic qubit chains, New J. Phys. 11 (2009) 063038
- [8] A.Zwick, G.A.Alvarez, J.Stolze, and O.Osenda, Spin chains for robust state transfer: Modified boundary couplings versus completely engineered chains, Phys. Rev. A. 85 (2012) 012318
- [9] N.A.Peters, J.T.Barreiro, M.E.Goggin, T.-C.Wei, P.G.Kwiat, Remote state preparation: arbitrary remote control of photon polarization, Phys.Rev.Lett. 94, (2005) 150502
- [10] N.A.Peters, J.T.Barreiro, M.E.Goggin, T.-C.Wei, P.G.Kwiat, Remote state preparation: arbitrary remote control of photon polarizations for quantum communication, in: R.E. Meyers, Ya. Shih (Eds.), Quantum Communications and Quantum Imaging III, in: Proc. of SPIE, vol. 5893, SPIE, Bellingham, WA, 2005.
- [11] B. Dakic, Ya.O. Lipp, X. Ma, M. Ringbauer, S. Kropatschek, S. Barz, T. Paterek, V. Vedral, A. Zeilinger, C. Brukner, P. Walther, Quantum discord as resource for remote state preparation, Nat.Phys. 8, (2012) 666
- [12] S. Pouyandeh, F. Shahbazi, A. Bayat, Measurement-induced dynamics for spin-chain quantum communication and its application for optical lattices, Phys.Rev.A 90, (2014) 012337
- [13] L.L.Liu, T. Hwang, Controlled remote state preparation protocols via AKLT states, Quantum Inf. Process. 13, (2014) 1639
- [14] A.Wójcik, T. Luczak, P.Kurzyński, A.Grudka, T.Gdala, and M.Bednarska, Unmodulated spin chains as universal quantum wires, Phys. Rev. A 72, 034303 (2005).

- [15] S.I.Doronin, A.I.Zenchuk, High-probability state transfers and entanglements between different nodes of the homogeneous spin-1/2 chain in an inhomogeneous external magnetic field, Phys. Rev. A 81, (2010) 022321
- [16] S.Paganelli, S.Lorenzo, T.J.G.Apollaro, F.Plastina, and G.L.Giorgi, Routing quantum information in spin chains, Phys. Rev. A 87, 062309 (2013)
- [17] E.B.Fel'dman, A.I.Zenchuk, High-probability quantum state transfer among nodes of an open XXZ spin chain, Phys.Lett.A, V. 373 (2009) 1719
- [18] R.Yousefjani, and A.Bayat, Simultaneous multiple-user quantum communication across a spinchain channel, Phys. Rev. A 102, 012418 (2020)
- [19] T.J.G.Apollaro, L.Banchi, A.Cuccoli, R.Vaia, and P.Verrucchi, 99%-fidelity ballistic quantumstate transfer through long uniform channels, Phys.Rev.A 85, 052319 (2012)
- [20] E.B.Fel'dman, M.G.Rudavets, Exact results on spin dynamics and multiple quantum NMR dynamics in alternating spin-1/2 chains with XY-Hamiltonian at high temperatures, JETP Letters 81 (2005) 47
- [21] E.I.Kuznetsova and E.B. Fel'dman, Exact Solutions in the Dynamics of Alternating Open Chains of Spins s = 1/2 with the XY Hamiltonian and Their Application to Problems of Multiple-Quantum Dynamics and Quantum Information Theory, JETP **102**(6) (2006) 882
- [22] L.C.Venuti, S.M.Giampaolo, F.Illuminati, and P. Zanardi, Long-distance entanglement and quantum teleportation in XX spin chains, Phys. Rev. A 76, (2007) 052328
- [23] A. Bayat and V. Karimipour, Transfer of d-level quantum states through spin chains by random swapping, Phys.Rev.A 75, (2007) 022321
- [24] M.A.Jafarizadeh, R.Sufiani, S.F.Taghavi, and E. Barati, Optimal transfer of a d-level quantum state over pseudo-distance-regular networks, Journal of Physics A: Mathematical and Theoretical, 41, No.47 (2008) 475302
- [25] M.-A. Lemonde, V.Peano, P.Rabl, and D.G. Angelakis, Quantum state transfer via acoustic edge states in a 2D optomechanical array, New J. Phys. 21, 113030 (2019)
- [26] Y.Hong, A.Lucas, Fast high-fidelity multi-qubit state transfer with long-range interactions, Phys. Rev. A 103, 042425 (2021)
- [27] R.Yousefjani, A.Bayat, Parallel entangling gate operations and two-way quantum communication in spin chains, Quantum 5, 460 (2021)
- [28] G.A.Bochkin and A.I.Zenchuk, Optimization of remote one- and two-qubit state creation via

unitary transformations of sender and extended receiver, Theor.Math.Phys. **194**(2), (2018) 295

- [29] E.B.Fel'dman and A.I.Zenchuk, Coherence Evolution and Transfer Supplemented by Sender's Initial-State Restoring, JETP 125(6), (2017) 1042
- [30] G.A.Bochkin, E.B.Fel'dman, and A.I.Zenchuk, Transfer of scaled multiple-quantum coherence matrices, Quant.Inf.Proc. 17, (2018) 218
- [31] E.B. Fel'dman, A.N. Pechen, and A.I.Zenchuk, Complete structural restoring of transferred multi-qubit quantum state, Phys.Let.A 413, (2021) 127605
- [32] A.I.Zenchuk, Partial structural restoring of two-qubit transferred state, Phys.Lett. A. 382 (2018) 324
- [33] R.Storn, and K.Price, Differential Evolution a Simple and Efficient Heuristic for Global Optimization over Continuous Spaces, Journal of Global Optimization, 11, 341 - 359, 1997
- [34] M.Wormington, C.Panaccione, K.M.Matney, D.K.Bowen, Characterization of structures from X-ray scattering data using genetic algorithms, Phil. Trans. R. Soc. Lond. A, 357, 2827-2848, 1999
- [35] J.Lampinen, A constraint handling approach for the differential evolution algorithm. Proceedings of the 2002 Congress on Evolutionary Computation. (Cat. No. 02TH8600). Vol. 2. IEEE, 2002.
- [36] A.Pechen, H.Rabitz, Teaching the environment to control quantum systems, Phys. Rev. A 73 (2006) 0621023
- [37] Bilal, M. Pant, H. Zaheer, L. Garcia-Hernandez, A. Abraham, Differential Evolution: A review of more than two decades of research, Eng. Appl. Artif. Intell. **90** (2020) 103479.
- [38] B.O.Volkov, O.V.Morzhin, A.N.Pechen, Quantum control landscape for ultrafast generation of single-qubit phase shift quantum gates, J. Phys. A: Math. Theor., 54:21 (2021), 215303
- [39] P.Virtanen, R.Gommers, T.E.Oliphant, et al. SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python, Nature Methods, 17(3), 261-272, 2020
- [40] A.N.Pechen, D.J.Tannor, Quantum control landscape for a Lambda-atom in the vicinity of second-order traps, Israel Journal of Chemistry, 52 No.5 (2012), 467-472
- [41] A.Pechen, N.Il'in, Trap-free manipulation in the Landau-Zener system, Phys. Rev. A, 86 (2012), 052117
- [42] Y.Xiang, D.Y.Sun, W.Fan, X.G.Gong, Generalized Simulated Annealing Algorithm and Its

Application to the Thomson Model. Physics Letters A, 233, 216 (1997).