Quantum Algorithms
Lecture 19
Physically realizable transformations of density matrices I

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Introduction

In this section we introduce a formalism for the description of irreversible quantum processes. We will not use it in full generality (so some of the results are superfluous=unnecessary), but the basic concepts and examples will be helpful.

Physically realizable superoperators: characterization

General linear map

All transformations of density matrices we will encounter can be represented by linear maps between operator spaces, $L(N) \to L(M)$. A general linear map of this type is called a superoperator. We now describe those superoperators that are admissible from the physical point of view.

Unitary operator

1. A unitary operator takes the density matrix of a pure state $\rho = |\xi\rangle\langle\xi|$ to the matrix $\rho' = U|\xi\rangle\langle\xi|U^{\dagger}$. It is natural to assume (by linearity) that such a formula also yields the action of a unitary operator on an arbitrary density matrix:

$$\rho \xrightarrow{U} U\rho U^{\dagger}$$

Partial trace

2. A second type of transformation is the operation of taking the partial trace. If $\rho \in L(N \otimes F)$, then the operation of discarding the second subsystem is described by the superoperator

$$Tr_F\colon \rho \to Tr_F \rho$$

Isometric embedding

3. We recall that it has been useful to us to borrow qubits in the state $|0\rangle$. Let the state $\rho \in (B^{\otimes n})$. We consider the isometric (preserving the inner product) embedding $V\colon B^{\otimes n} \to B^{\otimes N}$ in a space of larger dimension, given by the formula $|\xi\rangle \xrightarrow{V} |\xi\rangle \otimes |0^{N-n}\rangle$. The density matrix ρ is transformed thereby into $\rho \otimes \left|0^{N-n}\right\rangle\!\left\langle 0^{N-n}\right|$. For any isometric embedding V we similarly obtain a superoperator $V \cdot V^\dagger$ that acts as follows:

$$V \cdot V^\dagger\colon \rho \to V\rho V^\dagger$$

Physically realizable superoperator

We postulate that a physically realizable superoperator is a composition of an arbitrary number of transformations of types 2 and 3 (type 1 is a special case of 3).

1. $\rho \xrightarrow{U} U\rho U^\dagger$
2. $Tr_F\colon \rho \to Tr_F\rho$
3. $V \cdot V^\dagger\colon \rho \to V\rho V^\dagger$

Superoperator

A superoperator T is physically realizable if and only if it has the form

$$T = Tr_F(V \cdot V^{\dagger}) : \rho \to Tr_F(V\rho V^{\dagger})$$

where $V\colon N \to N \otimes F$ is an isometric embedding.

Operator sum decomposition

A superoperator T is physically realizable if and only if it can be represented in the form

$$T = \sum_m A_m \cdot A_m^\dagger \colon \rho \to \sum_m A_m \rho A_m^\dagger$$

where $\sum_m A_m^\dagger A_m = I$.

Forgetting subsystem

The operation of taking the partial trace means forgetting (discarding) one of the subsystems. We show that such an interpretation is reasonable, specifically that the subsequent fate of the discarded system in no way influences the quantities characterizing the remaining system.

Forgetting subsystem

Let us take a system consisting of two subsystems, which is in some state $\rho \in L(N \otimes F)$. If we discard the second subsystem (to the trash), then it will be subjected to uncontrollable influences. Suppose we apply some operator U to the first subsystem. We will then obtain a state $\gamma = (U \otimes Y)\rho(U \otimes Y)^{\dagger}$, where Y is an arbitrary unitary operator (the action of the trash bin on the trash).

Forgetting subsystem

If we wish to find the probability for some subspace $M \subseteq N$ pertaining to the first subsystem (the trash doesn't interest us), then the result does not depend on Y and equals

$$P(\gamma, M \otimes F) = P(Tr_F \gamma, M) = P(U(Tr_F \rho)U^\dagger, M)$$

Forgetting subsystem

$$P(\gamma, M \otimes F) = P(Tr_F \gamma, M) = P\left(U(Tr_F \rho)U^\dagger, M\right)$$

Here the first equality is the property 4q of quantum probability, whereas the second equality represents a new property:

$$Tr_F((U \otimes Y)\rho(U \otimes Y)^\dagger) = U(Tr_F \rho)U^\dagger$$

Quantum probability
4^q. In the quantum case, the restriction to one of the subsystems is described by taking a *partial trace* (see below). Thus, even if the initial state was pure, the resulting state of the subsystem may turn out to be mixed: $\mathbf{P}(\rho, \mathcal{M}_1 \otimes \mathcal{N}_2) = \mathbf{P}(\mathrm{Tr}_{\mathcal{N}_2}\, \rho, \mathcal{M}_1)$.

Superoperator

Let us write a superoperator T: $L(N) \to L(M)$ in the coordinate form:

$$T(|j\rangle\langle k|) = \sum_{j',k'} T_{(j'j)(k'k)} |j'\rangle\langle k'|$$

The physical realizability of T is equivalent to the set of three conditions:

a) $\sum_l T_{(lj)(lk)} = \delta_{jk}$ (Kronecker symbol)

b) $T^*_{(j'j)(k'k)} = T_{(k'k)(j'j)}$

c) The matrix $(T_{(j'j)(k'k)})$ is nonnegative (each of the index pairs is regarded as a single index).

Kronecker delta/symbol

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$$

n \ k	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	1	0	−1	0	−1	0	1	0	1	0	−1	0	−1	0	1	0	1	0	−1	0	−1	0	1	0	1	0	−1	0	−1	0
3	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0
4	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0
5	1	−1	−1	1	0	1	−1	−1	1	0	1	−1	−1	1	0	1	−1	−1	1	0	1	−1	−1	1	0	1	−1	−1	1	0
6	1	0	0	0	1	0	1	0	0	0	1	0	−1	0	0	0	−1	0	−1	0	0	0	−1	0	1	0	0	0	1	0
7	1	1	−1	1	−1	−1	0	1	1	−1	1	−1	−1	0	1	1	−1	1	−1	−1	0	1	1	−1	1	−1	−1	0	1	1
8	1	0	−1	0	−1	0	1	0	1	0	−1	0	−1	0	1	0	1	0	−1	0	−1	0	1	0	1	0	−1	0	−1	0
9	1	1	0	1	1	0	1	1	0	1	1	0	1	1	0	1	1	0	1	1	0	1	1	0	1	1	0	1	1	0
10	1	0	1	0	0	0	−1	0	1	0	−1	0	1	0	0	0	−1	0	−1	0	−1	0	−1	0	0	0	1	0	−1	0
11	1	−1	1	1	1	−1	−1	−1	1	−1	0	1	−1	1	1	1	−1	−1	−1	1	−1	0	1	−1	1	1	1	−1	−1	−1
12	1	0	0	0	−1	0	1	0	0	0	−1	0	1	0	0	0	−1	0	1	0	0	0	−1	0	1	0	0	0	−1	0
13	1	−1	1	1	−1	−1	−1	−1	1	1	−1	1	0	1	−1	1	1	−1	−1	−1	−1	1	1	−1	1	0	1	−1	1	1
14	1	0	1	0	1	0	0	0	1	0	−1	0	1	0	1	0	−1	0	1	0	0	0	1	0	1	0	1	0	−1	0
15	1	1	0	1	0	0	−1	1	0	0	−1	0	−1	−1	0	1	1	0	1	0	0	−1	1	0	0	−1	0	−1	−1	0
16	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0
17	1	1	−1	1	−1	−1	−1	1	1	−1	−1	−1	1	−1	1	1	0	1	1	−1	1	−1	−1	−1	1	1	−1	−1	−1	1
18	1	0	0	0	−1	0	1	0	0	0	−1	0	−1	0	0	0	1	0	−1	0	0	0	1	0	1	0	0	0	−1	0
19	1	−1	−1	1	1	1	1	−1	1	−1	1	−1	−1	−1	−1	1	1	−1	0	1	−1	−1	1	1	1	1	−1	1	−1	1
20	1	0	−1	0	0	0	−1	0	1	0	1	0	−1	0	0	0	−1	0	1	0	1	0	−1	0	0	0	−1	0	1	0
21	1	−1	0	1	1	0	0	−1	0	−1	−1	0	−1	0	0	1	1	0	−1	1	0	1	−1	0	1	1	0	0	−1	0
22	1	0	−1	0	−1	0	−1	0	1	0	0	0	1	0	1	0	−1	0	1	0	1	0	1	0	1	0	−1	0	1	0
23	1	1	1	1	−1	1	−1	1	1	−1	−1	1	1	−1	−1	1	−1	1	−1	−1	−1	−1	0	1	1	1	1	−1	1	−1
24	1	0	0	0	1	0	1	0	0	0	1	0	−1	0	0	0	−1	0	−1	0	0	0	−1	0	1	0	0	0	1	0
25	1	1	1	1	0	1	1	1	1	0	1	1	1	1	0	1	1	1	1	0	1	1	1	1	0	1	1	1	1	0
26	1	0	−1	0	1	0	−1	0	1	0	1	0	0	0	−1	0	1	0	1	0	1	0	1	0	1	0	−1	0	−1	0
27	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0	1	−1	0
28	1	0	−1	0	−1	0	0	0	1	0	1	0	−1	0	1	0	−1	0	−1	0	0	0	1	0	1	0	−1	0	1	0
29	1	−1	−1	1	1	1	1	−1	1	−1	−1	−1	1	−1	−1	1	−1	−1	−1	1	−1	1	1	1	1	−1	−1	1	0	1
30	1	0	0	0	0	0	−1	0	0	0	1	0	1	0	0	0	1	0	−1	0	0	0	1	0	0	0	0	0	1	0

Superoperator

A superoperator $T: L(N) \to L(M)$ is physically realizable if and only if it satisfies the following three conditions:

a) $Tr(TX) = TrX$ for any $X \in L(N)$;
b) $(TX)^{\dagger} = TX^{\dagger}$ for any $X \in L(N)$;
c) T is completely positive. Namely, for any additional space G the superoperator $T \otimes I_{L(G)}: L(N \otimes G) \to L(M \otimes G)$ maps nonnegative operators to nonnegative operators.

Calculation of the probability for quantum computation

Calculating the probability

Now, since we have the general definitions of quantum probability and of a physically realizable transformation of density matrices, there are two ways to calculate the probability that enters the definition of quantum computation.

Calculating the probability

Suppose we use a supplementary subsystem. After we no longer need it, we can discard it to the trash and, in counting the probability, take the partial trace over the state space of the supplementary subsystem.

Calculating the probability

Or else we may hold all the trash until the very end and consider the probability of an event of the form $M_1 \otimes N_2$ (once we have stopped using the second subsystem, no details of its existence are of any importance to us and we are not interested in what precisely happens to it in the trash bin). As already stated, these probabilities are equal:

$$P(\rho, M_1 \otimes N_2) = P(Tr_{N_2}\rho, M_1)$$

Remark

It is not difficult to define a more general model of quantum computation in which suitable physically realizable superoperators (not necessarily corresponding to unitary operators) serve as the elementary gates. Such a model of computation with mixed states is more adequate in the physical situation where the quantum computer interacts with the surrounding environment.

Remark

In particular, one can consider things like combination of classical and quantum computation. From the complexity point of view, the new model is polynomially equivalent to the standard one, if a complete basis is used in both cases.

Remark

Completeness in the new model is most comprehensively defined as the possibility to effect arbitrary unitary operators on “encoded qubits” (Remark 8.3 on page 74).

We also note that in the model of computation with mixed states a more natural definition of a probabilistic subroutine is possible. We will not give this definition here, but refer interested readers to [D. Aharonov, A. Kitaev, and N. Nisan, Quantum circuits with mixed states, STOC’29, 1997; e-print quant-ph/9806029].

Decoherence

Irreversible degradation

The term “decoherence” is generally used to denote irreversible degradation of a quantum state caused by its interaction with the environment. This could be an arbitrary physically realizable superoperator that takes pure states to mixed states. For the purpose of our discussion, decoherence means the specific superoperator D that “forgets” off-diagonal matrix elements:

$$\rho = \sum_{j,k} \rho_{jk} \, |j\rangle\langle k| \xrightarrow{D} \sum_{k} \rho_{kk} \, |k\rangle\langle k|$$

Irreversible degradation

$$\rho = \sum_{j,k} \rho_{jk} \, |j\rangle\langle k| \xrightarrow{D} \sum_{k} \rho_{kk} \, |k\rangle\langle k|$$

This superoperator is also known as an extreme case of a “phase damping channel”. We will show that it is physically realizable. For simplicity, let us assume that D acts on a single qubit.

Action of D

The action of D on a density matrix ρ can be performed in three steps. First, we append a null qubit:

$$\rho \to \rho \otimes |0\rangle\langle 0|$$

Then we "copy" the original qubit into the ancilla. This can be achieved by applying the operator

$$\Lambda(\sigma^x): |a, b\rangle \to |a, a \oplus b\rangle$$

Action of D

We get

$$\rho \otimes |0\rangle\langle 0| \xrightarrow{\Lambda(\sigma^x)} \sum_k \rho_{jk} \, |j,j\rangle\langle k,k|$$

Finally, we take the partial trace over the ancilla, which yields the diagonal matrix

$$\sum_k \rho_{kk} \, |k\rangle\langle k|$$

Copying operation

The “copying operation” we considered:

$$|j\rangle \rightarrow |j, j\rangle$$

$$\sum_{j,k} \rho_{jk} \, |j\rangle\langle k| \rightarrow \sum_{k} \rho_{jk} \, |j, j\rangle\langle k, k|$$

(the composition of the first two transformations) in fact copies only the basis states. We note that the copying of an arbitrary quantum state is a nonlinear operator and so cannot be physically realized. (This statement is called a “no-cloning theorem”.)

No-cloning theorem

In physics, the no-cloning theorem states that it is impossible to create an independent and identical copy of an arbitrary unknown quantum state.

The no-cloning theorem prevents us from using classical error correction techniques on quantum states. For example, we cannot create backup copies of a state in the middle of a quantum computation, and use them to correct subsequent errors.

Copying operation

We will take the liberty of calling the operator of the form

$$\sum_j c_j |\eta_j\rangle \to \sum_j c_j |\eta_j\rangle \otimes |\eta_j\rangle$$

copying relative to the orthonormal basis $\{|\eta_j\rangle\}$.

Link between classical and quantum

So, the decoherence superoperator D translates any state into a classical one (with diagonal density matrix) by copying qubits. This can be interpreted as follows: if we constantly observe a quantum system (make copies), then the system will behave like a classical one. Thus the copying operation, together with “forgetting” about the copy (i.e., the partial trace), provides a conceptual link between quantum mechanics and the classical picture of the world.

Random dephasing

In the case of a single qubit, the decoherence superoperator (the off-diagonal matrix elements set to zero) can be also obtained if we apply the operator σ^z with probability $1/2$:

$$\rho \to \frac{1}{2}\rho + \frac{1}{2}\sigma^z \rho \sigma^z$$

Such a process is called random dephasing: the state $|1\rangle$ is multiplied by the phase factor -1 with probability $1/2$. Thus, the dephasing leads likewise to the situation that the system behaves classically.

Superoperator + subspace

Suppose we have a physically realizable superoperator $T: L(N) \to L(N \otimes F)$ with the following property:

$$Tr_F\,(T\rho) = \rho$$

for any pure state ρ. Then $TX = X \otimes \gamma$ (for any operator X), where γ is a fixed density matrix on the space F.

Superoperator + subspace

Think of N as a system one wants to observe, and F as an "observation record". Then the condition $Tr_F\,(T\rho) = \rho$ indicates that the superoperator T does not perturb the system, whereas $TX = X \otimes \gamma$ means that the obtained record γ does not carry any information about ρ. Thus, it is impossible to get any information about an unknown quantum state without perturbing the state.

Decoherence in physics

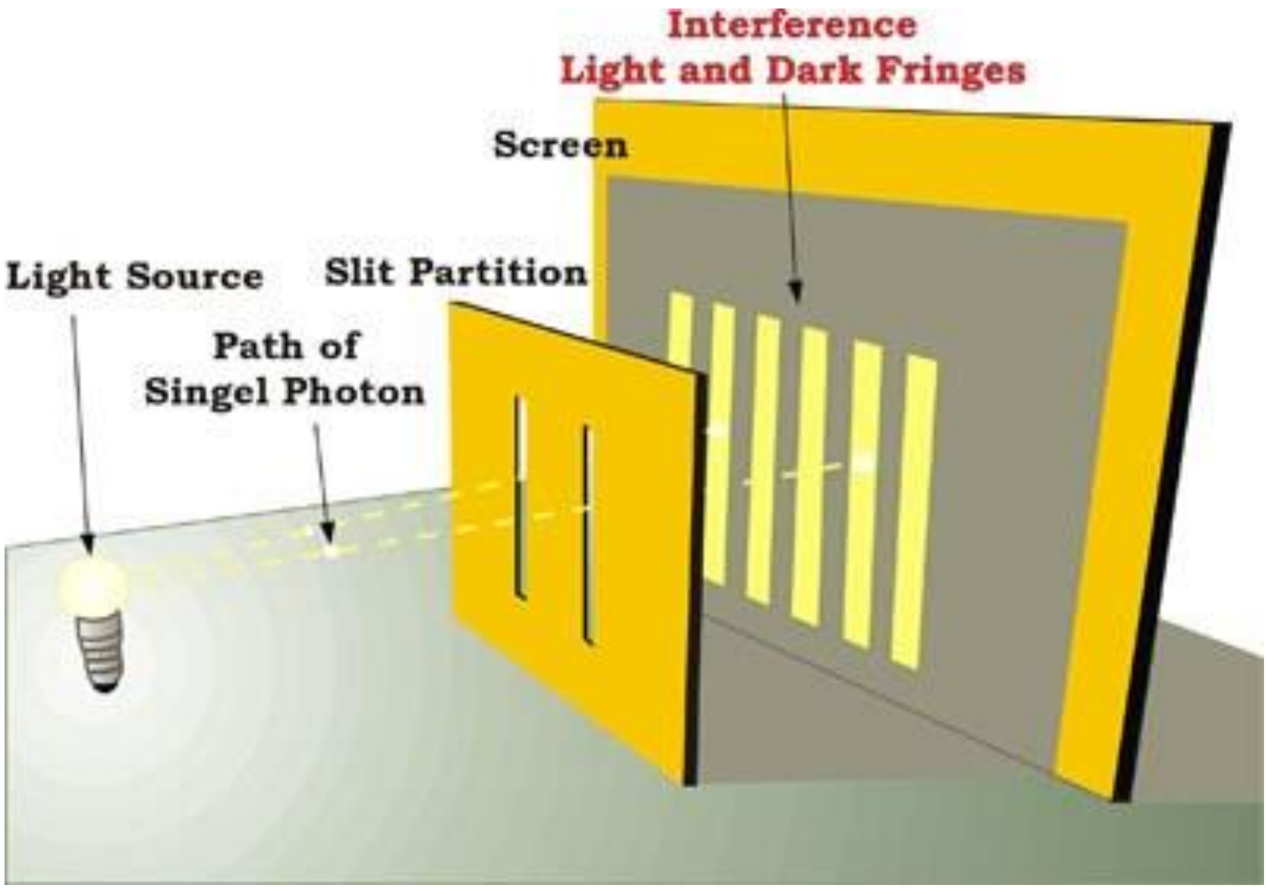
Copying to the environment

In Nature, decoherence by “copying to the environment” is very common and, of course, does not require a human observer. Let us consider one famous example of quantum phenomenon — an interference pattern formed by a single photon.

Light beam

It is known from classical optics that a light beam passing through two parallel slits forms a pattern of bright and dark stripes on a screen placed behind the slits. This pattern can be recorded if one uses a photographic film as the screen. When the light is dim, the photographic image consists of random dots produced by individual photons (i.e., quanta of light). The probability for a dot to appear at a given position x is the probability that a photon hits the film at the point x.

Light beam


Interference
Light and Dark Fringes
Screen
Light Source
Slit Partition
Path of
Singel Photon

Light photon

What will happen if the light is so dim that only one photon reaches the film? Quantum mechanics predicts that the photon arrives in a certain superposition $|\psi\rangle = \sum_x c_x |x>$, so the above probability equals $|c_x|^2$.

Light photon

Thus, the quantum state of the photon is transformed into a classical object — a dot, located at a particular place (although the appearance of the dot at a given position x occurs with the probability related to the corresponding amplitude c_x). When and how does this transition happen?

Remark

We think of the position on the film as a discrete variable; specifically, it refers to a grain of light-sensitive substance. The whole grain either turns dark (if it caught a photon) or stays white when the film is developed. Speaking about photons, we have oversimplified the situation for illustrative purposes. In modern films, a single photon does not yet produce a sufficient change to be developed, but several (3 or more) photons per grain do. For single photon detection, physicists use other kinds of devices, e.g., ones based on semiconductors.

Defect

When the photon hits the film, it breaks a chemical bond and generates a defect in a light-sensitive grain (usually, a small crystal of silver compound). The photon is delocalized in space, so a superposition of states with the defect located at different places is initially created. Basically, this is the same state $|\psi\rangle = \sum_x c_x |x>$, but x now indicates the position of the defect.

Defect

The transition from the quantum state $|\psi\rangle$ to the classical state $\sum_x |c_x|^2 |x\rangle\langle x|$ is decoherence. It occurs long before anyone sees the image, even before the film is developed. About every 10^{-12} seconds since the defect was created, it scatters a phonon (a quantum of sonic vibrations). This has the effect of "copying" the state of the defect to phonon degrees of freedom relative to the position basis.

Discard of the copy

The above explanation is based on the assumption that the phonon scattering (or whatever causes the decoherence) is irreversible. But what does this assumption mean if the scattering is just a unitary process which occurs in the film? In the preceding mathematical discussion, the irreversible step was the partial trace; it was justified by the fact that the copy was “discarded”, i.e., never used again.

Discard of the copy

On the contrary, the scattered phonon stays around and can, in principle, scatter back to “undo the copying”. In reality, however, the scattering does not reverse by itself. One reason is that the phonons interact with other phonons, causing the “copies” to multiply. The quantum state quickly becomes so entangled that it cannot be disentangled.

Discard of the copy

Well, this argument is more empirical than logical; it basically says that things can be lost and never found — a true fact with no “proof” whatsoever. For some particular classes of Hamiltonians, some assertions about irreversibility, like “information escapes to infinity”, can be formulated mathematically. Proving this kind of statements is a difficult and generally unsolved problem.

Physics interpretation

Some irreversibility postulate or assumption is necessary to give an interpretation of quantum mechanics, i.e., to introduce a classical observer. It seems that the exact nature of irreversibility is the real question behind many philosophical debates surrounding quantum mechanics. Another thing that is not fully understood, is the meaning of probability in the physical world. Both problems exist in classical physics as well; quantum mechanics just makes them more evident.

Physics interpretation

Fortunately (especially to mathematicians), the theory of quantum computation deals with an ideal world where nothing gets lost. If we observe something, we can also “un-observe”, unless we explicitly choose to discard the result or to keep it as the computation output. As far as probabilities are concerned, we deal with them formally rather than trying to explain them by something else.

Thank you for your attention!