Open quantum systems – lecture 2

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Chapter 1

Open quantum systems

We typically imagine an open quantum system as part of a larger, closed, quantum system. One could in principle tackle such problems by just solving the dynamics of the von-Neumann equation for the complete system, described by the full Hamiltonian

$$\dot{\rho}_{\text{tot}} = -\mathrm{i}\left[H_S + H_I + H_B, \rho_{\text{tot}}\right] . \tag{1.1}$$

If it was possible to obtain the global solution $\rho_{\text{tot}}(t)$, one could obtain any observable of the system via $\langle A\rangle_t = \mathrm{Tr}\left\{A\rho_{\text{tot}}(t)\right\}$. Unfortunately, a typical reservoir reservoir has an enormously large number of degrees of freedom, and the dimension of the Hilbert space scales even worse. Therefore, apart from some particular examples (some of which we will discuss), this path is typically not taken. Instead, since we are typically only interested in the dynamics of a small part (that we call system) of the whole universe, and we are interested in finding a time-dependent solution for the density matrix of that local part $\rho_S(t)$. In general, this cannot be a von-Neumann equation

$$\dot{\rho}_S \neq -\mathrm{i}\left[H_{\text{eff}}(t), \rho_S(t)\right] , \tag{1.2}$$

since the solution to these equations is always unitary, preserving information on the initial state. However, realistic reservoirs exchange information, energy and possibly also matter with a quantum system. Thus, we are looking for a general evolution equation for the local system density matrix.

1.1 Kraus map

One approach to this is based on formal requirements: Any evolution equation should preserve all properties (trace, hermiticity, and positivity) of the density matrix.

The most general evolution preserving all the nice properties of a density matrix is the so-called **Kraus map**. A density matrix ρ (Hermitian, positive definite, and with trace one) can be mapped to another density matrix ρ' via

$$\rho' = \sum_{\alpha\beta} \gamma_{\alpha\beta} A_\alpha \rho A_\beta^\dagger , \qquad \text{with} \qquad \sum_{\alpha\beta} \gamma_{\alpha\beta} A_\beta^\dagger A_\alpha = \mathbf{1} , \tag{1.3}$$

where the prefactors $\gamma_{\alpha\beta}$ form a Hermitian ($\gamma_{\alpha\beta} = \gamma^*_{\beta\alpha}$) and positive definite ($\sum_{\alpha\beta} x^*_\alpha \gamma_{\alpha\beta} x_\beta \geq 0$ or equivalently all eigenvalues of $(\gamma_{\alpha\beta})$ are non-negative) matrix. It is straightforward to see that the above map preserves trace and Hermiticity of the density matrix.

We first rewrite the map in a simpler way. Since the matrix $\gamma_{\alpha\beta}$ is Hermitian, it can be diagonalized by a suitable unitary transformation, and we introduce the new operators $A_\alpha = \sum_{\alpha'} U_{\alpha\alpha'} \bar{K}_{\alpha'}$

$$\begin{aligned}\rho' &= \sum_{\alpha\beta}\sum_{\alpha'\beta'} \gamma_{\alpha\beta} U_{\alpha\alpha'} \bar{K}_{\alpha'} \rho U^*_{\beta\beta'} K^\dagger_{\beta'} = \sum_{\alpha'\beta'} \bar{K}_{\alpha'} \rho \bar{K}^\dagger_{\beta'} \underbrace{\sum_{\alpha\beta} U_{\alpha\alpha'} \gamma_{\alpha\beta} U^*_{\beta\beta'}}_{\gamma_{\alpha'}\delta_{\alpha'\beta'}} \\ &= \sum_\alpha \gamma_\alpha \bar{K}_\alpha \rho \bar{K}^\dagger_\alpha \,, \end{aligned} \tag{1.4}$$

where $\gamma_\alpha \geq 0$ represent the eigenvalues of the matrix $(\gamma_{\alpha\beta})$. Since these are by construction positive, we introduce further new operators $K_\alpha = \sqrt{\gamma_\alpha}\bar{K}_\alpha$ to obtain the simplest representation of a Kraus map.

$$\rho' = \sum_\alpha K^\dagger_\alpha \rho K_\alpha \qquad : \qquad \sum_\alpha K^\dagger_\alpha K_\alpha = \mathbf{1} \,. \tag{1.5}$$

Here, it is very simple to see that ρ' inherits the positivity from ρ. We simply insert the spectral representation of $\rho = \sum_n \lambda_n |n\rangle \langle n|$

$$\begin{aligned}\langle\Psi|\,\rho'\,|\Psi\rangle &= \sum_\alpha \langle\Psi|\,K_\alpha \rho K^\dagger_\alpha\,|\Psi\rangle = \sum_n \lambda_n \sum_\alpha \langle\Psi|\,K_\alpha\,|n\rangle\,\langle n|\,K^\dagger_\alpha\,|\Psi\rangle \\ &= \sum_n \underbrace{\lambda_n}_{\geq 0} \underbrace{\sum_\alpha \left|\langle n|\,K^\dagger_\alpha\,|\Psi\rangle\right|^2}_{\geq 0} \geq 0 \,. \end{aligned} \tag{1.6}$$

That means, a positive definite matrix ρ (with $\lambda_n \geq 0$) will map to a positive definite matrix ρ'.

In short, the Kraus map

$$\rho(t+\Delta t) = \sum_\alpha K_\alpha(t,\Delta t)\rho(t)K^\dagger_\alpha(t,\Delta t) \tag{1.7}$$

with Kraus operators $K_\alpha(t,\Delta t)$ obeying the relation $\sum_\alpha K^\dagger_\alpha(t,\Delta t)K_\alpha(t,\Delta t) = \mathbf{1}$ preserves Hermiticity, trace, and positivity of the density matrix.

Obviously, both unitary evolution and the average evolution under measurement are just special cases of a Kraus map. Though Kraus maps are heavily used in quantum information, they are not often very easy to interpret. For example, it is not straightforward to identify the unitary and the non-unitary part induced by the Kraus map.

1.2 Lindblad master equation

Any dynamical evolution equation for the density matrix should (at least in some approximate sense) preserve its interpretation as density matrix, i.e., trace, Hermiticity, and positivity must be preserved. By construction, the measurement postulate and unitary evolution preserve these properties. However, more general evolutions are conceivable.

It is convenient to use a differential equation for the density matrix as the desired evolution equation. The most general first order differential equation that is time-local, linear in ρ, and has time-independent coefficients that preserves the density matrix properties is known as **Lindblad form** (sometimes also Lindblad-Gorini-Kossakowski-Sudarshan – LGKS generator).

1.2.1 General properties

Def. 1 (Lindblad form). *In an N-dimensional system Hilbert space, a master equation of LGKS form [1, 2] has the structure*

$$\dot{\rho} = -\mathrm{i}\,[H,\rho] + \sum_{\alpha,\beta=1}^{N^2-1} \gamma_{\alpha\beta}\left(A_\alpha \rho A_\beta^\dagger - \frac{1}{2}\left\{A_\beta^\dagger A_\alpha, \rho\right\}\right) \equiv \mathcal{L}\rho\,, \tag{1.8}$$

where the Hermitian operator $H = H^\dagger$ can be interpreted as an effective Hamiltonian and $\gamma_{\alpha\beta} = \gamma_{\beta\alpha}^*$ is a positive semidefinite matrix, i.e., it fulfills $\sum_{\alpha\beta} x_\alpha^* \gamma_{\alpha\beta} x_\beta \geq 0$ for all vectors x (or, equivalently that all eigenvalues of $(\gamma_{\alpha\beta})$ are non-negative $\gamma_i \geq 0$). After suitable transformations, this can be written as

$$\dot{\rho} = -\mathrm{i}\,[H,\rho] + \sum_{\alpha}^{N^2-1} \left(L_\alpha \rho L_\alpha^\dagger - \frac{1}{2}\left\{L_\alpha^\dagger L_\alpha, \rho\right\}\right) \equiv \mathcal{L}\rho\,. \tag{1.9}$$

To see that the first Lindblad master equation can be written in simpler form, follow the same steps as for the Kraus map: As the dampening matrix γ is Hermitian, it can be diagonalized by a suitable unitary transformation. Its non-negative eigenvalues can therefore be absorbed in the Lindblad operators, which yields the second, simpler form of the Lindblad master equation.

Exercise 1 (Lindblad form). *Show that the Lindblad form master equation preserves trace and Hermiticity of the density matrix.*

The representation of a master equation is not unique. Any other unitary operation would lead to a different non-diagonal form of $\gamma_{\alpha\beta}$ which however describes the same master equation. In addition, we note here that the master equation is not only invariant to unitary transformations of the operators A_α, but in the diagonal representation also to inhomogeneous transformations of the form

$$\begin{aligned} L_\alpha &\to L'_\alpha = L_\alpha + a_\alpha \mathbf{1} \\ H &\to H' = H + \frac{1}{2\mathrm{i}} \sum_\alpha \gamma_\alpha \left(a_\alpha^* L_\alpha - a_\alpha L_\alpha^\dagger\right) + b\mathbf{1}\,, \end{aligned} \tag{1.10}$$

with $a_\alpha \in \mathbb{C}$ and a real number $b \in \mathbb{R}$. The numbers a_α can be chosen such that the Lindblad operators are traceless $\mathrm{Tr}\,\{L_\alpha\} = 0$, which is a popular convention. Choosing b simply corresponds to gauging the energy of the system.

Exercise 2 (Shift invariance). *Show the invariance of the diagonal representation of a Lindblad form master equation (1.9) with respect to the transformation (1.10).*

We would like to demonstrate the preservation of positivity here. Since preservation of Hermiticity follows directly from the Lindblad form, we can – since at any time we know that $\rho = \rho^\dagger$ – formally write the density matrix in its spectral representation

$$\rho(t) = \sum_j \lambda_j(t) \left|\Psi_j(t)\right\rangle \left\langle\Psi_j(t)\right| \tag{1.11}$$

with eigenvalues $\lambda_j(t) \in \mathbb{R}$ (we still have to show that these remain positive) and time-dependent orthonormal eigenstates. The eigenvectors themselves are normalized at all times $\langle\Psi_i(t)|\Psi_j(t)\rangle = \delta_{ij}$, and by acting on this expression with a time derivative we see that $\left\langle\dot{\Psi}_i|\Psi_i\right\rangle + \left\langle\Psi_i|\dot{\Psi}_i\right\rangle = 0$.

Therefore, the time-derivative of the density matrix becomes

$$\dot{\rho} = \sum_j \left[\dot{\lambda}_j \left|\Psi_j\right\rangle \left\langle\Psi_j\right| + \lambda_j \left|\dot{\Psi}_j\right\rangle \left\langle\Psi_j\right| + \lambda_j \left|\Psi_j\right\rangle \left\langle\dot{\Psi}_j\right|\right] , \tag{1.12}$$

and sandwiching the time-derivative above with the eigenvector $|\Psi_i\rangle$ leads to the cancellation of two terms, such that $\langle\Psi_i(t)|\,\dot{\rho}\,|\Psi_i(t)\rangle = \dot{\lambda}_i(t)$. On the other hand, we can also sandwich the right-hand side of the Lindblad equation to obtain

$$\begin{aligned}
\dot{\lambda}_i &= -\mathrm{i} \left\langle\Psi_i\right| H \left|\Psi_i\right\rangle \lambda_i + \mathrm{i}\lambda_i \left\langle\Psi_i\right| H \left|\Psi_i\right\rangle \\
&\quad + \sum_\alpha \left[\left\langle\Psi_i\right| L_\alpha \left(\sum_j \lambda_j \left|\Psi_j\right\rangle \left\langle\Psi_j\right|\right) L_\alpha^\dagger \left|\Psi_i\right\rangle - \left\langle\Psi_i\right| L_\alpha^\dagger L_\alpha \left|\Psi_i\right\rangle \lambda_i\right] \\
&= \sum_j \left(\sum_\alpha \left|\left\langle\Psi_i\right| L_\alpha \left|\Psi_j\right\rangle\right|^2\right) \lambda_j - \sum_j \left(\sum_\alpha \left|\left\langle\Psi_j\right| L_\alpha \left|\Psi_i\right\rangle\right|^2\right) \lambda_i \,.
\end{aligned} \tag{1.13}$$

This is nothing but a rate equation

$$\dot{\lambda}_i = \sum_j R_{j\to i}(t)\lambda_j(t) - \sum_j R_{i\to j}\lambda_i(t) = \sum_j R_{ij}(t)\lambda_j(t) \tag{1.14}$$

with positive but time-dependent transition rates

$$R_{j\to i}(t) = \sum_\alpha \left|\left\langle\Psi_i(t)\right| L_\alpha \left|\Psi_j(t)\right\rangle\right|^2 \geq 0 \,. \tag{1.15}$$

The rate matrix in the rate equation $\dot{\boldsymbol{\lambda}} = R(t)\boldsymbol{\lambda}(t)$ contains the rates as

$$\left(R(t)\right)_{ij} = \begin{cases} R_{j\to i}(t) & : \; j \neq i \\ -\sum_{j\neq i} R_{i\to j} & : \; j = i \end{cases} . \tag{1.16}$$

Therefore, only the diagonal entries of the rate matrix are negative. From this, it follows first that the sum of all eigenvalues (i.e., the trace of ρ) is conserved and second, that all eigenvalues remain positive. To see this, assume that one eigenvalue approaches zero $\lambda_{\bar{n}} \to 0$ while all others are still positive. Then, the time derivative if $\lambda_{\bar{n}}$ is always positive, i.e., it can never become negative. From this, it follows that the positivity of the eigenvalues $\lambda_j(t)$ (and thereby that of the density matrix) is granted for all times, a valid initialization provided. This can be seen by considering the time derivative of an eigenvalue $\bar{n}$ that vanishes at a certain time $\lambda_{\bar{n}}(t^*) = 0$ while all other

eigenvalues are non-negative $\lambda_{n\neq\bar{n}}(t*) \geq 0$. From this, it follows that the time derivative of the monitored critical eigenvalue is

$$\dot{\lambda}_{\bar{n}}|_{t=t^*} = \sum_n R_{\bar{n}n}(t^*)\lambda_n(t^*) = \sum_{n\neq\bar{n}} R_{n\to\bar{n}}(t^*)\lambda_n(t^*) \geq 0\,, \tag{1.17}$$

i.e., the eigenvalue will increase again, if it ever reaches zero. Thereby, it can never become negative (and we can repeat the argument for the other eigenvalues), such that the density matrix remains positive at all times. The argument fails, of course, if some eigenvalues are already negative (i.e., for an invalid initial condition), such that the Lindblad evolution can only preserve the density matrix properties, but not cure them.

Unfortunately, the basis within which this simple rate equation holds is time-dependent and also only known after solving the master equation and diagonalizing the solution. The rate equation representation is therefore not very practical, unless the eigenbasis is constant in time.

1.2.2 Example: Master Equation for a cavity in a thermal bath

Consider the Lindblad form master equation

$$\begin{aligned}\dot{\rho} = &-\mathrm{i}\left[\Omega a^\dagger a, \rho\right] + \Gamma(1+n_B)\left[a\rho a^\dagger - \frac{1}{2}a^\dagger a\rho - \frac{1}{2}\rho a^\dagger a\right] \\ &+ \Gamma n_B\left[a^\dagger\rho a - \frac{1}{2}aa^\dagger\rho - \frac{1}{2}\rho aa^\dagger\right]\,,\end{aligned} \tag{1.18}$$

with bosonic operators $\left[a, a^\dagger\right] = \mathbf{1}$ and Bose-Einstein bath occupation $n_B = \left[e^{\beta\Omega} - 1\right]^{-1}$ (we consider $\mu = 0$) and cavity frequency $\Omega > 0$. Finally, $\Gamma > 0$ is a constant (spontaneous emission rate).

Steady state solution

In Fock-space representation, these operators act as $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$ (where $0 \leq n < \infty$), such that the above master equation couples only the diagonals of the density matrix $\rho_n = \langle n|\,\rho\,|n\rangle$ to each other. This is directly visible by sandwiching the master equation with $\langle n|\ldots|n\rangle$

$$\begin{aligned}\dot{\rho_n} &= \Gamma(1+n_B)\left[(n+1)\rho_{n+1} - n\rho_n\right] + \Gamma n_B\left[n\rho_{n-1} - (n+1)\rho_n\right] \\ &= \Gamma n_B n\rho_{n-1} - \Gamma\left[n + (2n+1)n_B\right]\rho_n + \Gamma(1+n_B)(n+1)\rho_{n+1}\,,\end{aligned} \tag{1.19}$$

which shows that the rate equation arising for the diagonals even has a simple tri-diagonal form. That makes it particularly easy to calculate its stationary state recursively, since the boundary solution $n_B\bar{\rho}_0 = (1+n_B)\bar{\rho}_1$ implies for all n the relation

$$\frac{\bar{\rho}_{n+1}}{\bar{\rho}_n} = \frac{n_B}{1+n_B} = e^{-\beta\Omega}\,, \tag{1.20}$$

i.e., if the off-diagonal matrix elements (coherences) vanish, the stationary state is a thermalized Gibbs state with the same temperature as the reservoir.

Exercise 3 (Moments)**.** *Calculate the expectation value of the number operator $\hat{n} = a^\dagger a$ and its square $\hat{n}^2 = a^\dagger a a^\dagger a$ in the stationary state of the master equation (1.18).*

In general, the matrix elements of the density matrix $\rho_{nm} = \langle n| \rho |m\rangle$ will obey

$$\begin{aligned}
\dot{\rho}_{nm} &= -\mathrm{i}\Omega(n-m)\rho_{nm} + \Gamma(1+n_B)\left[\sqrt{(n+1)(m+1)}\rho_{n+1,m+1} - \frac{n+m}{2}\rho_{nm}\right] \\
&\quad + \Gamma n_B\left[\sqrt{nm}\rho_{n-1,m-1} - \frac{n+1+m+1}{2}\rho_{nm}\right] \\
&= \left[-\mathrm{i}\Omega(n-m) - \Gamma\frac{(1+n_B)(n+m) + n_B(n+1+m+1)}{2}\right]\rho_{nm} \\
&\quad + \Gamma(1+n_B)\sqrt{(n+1)(m+1)}\rho_{n+1,m+1} + \Gamma n_B\sqrt{nm}\rho_{n-1,m-1}\,,
\end{aligned} \tag{1.21}$$

and it is straightforward to see that vanishing coherences (off-diagonal matrix elements) $\bar{\rho}_{n\neq m} = 0$ are a valid steady-state solution. Not being aware of the Lindblad form we may nevertheless ask whether there are other solutions. The above equation shows that among the coherences, only few couple, and by arranging them in a favorable form we can write these equations in matrix form with infinite-dimensional tri-diagonal matrices (for brevity we use $\gamma = \Gamma n_B$ and $\bar{\gamma} = \Gamma(1+n_B)$)

$$W = \begin{pmatrix}
 & \vdots & & \\
\ddots & +\bar{\gamma}\sqrt{nm} & 0 & \\
\ldots\ +\gamma\sqrt{nm} & \left[-\mathrm{i}\Omega(n-m) - \bar{\gamma}\frac{n+m}{2} - \gamma\frac{n+1+m+1}{2}\right] & +\bar{\gamma}\sqrt{(n+1)(m+1)} & \ldots \\
0 & +\gamma\sqrt{(n+1)(m+1)} & \ddots & \\
 & \vdots & &
\end{pmatrix}. \tag{1.22}$$

By examining every column in detail, we see that the real part of the diagonal entries has always larger magnitude than the sum of the off-diagonal entries, since

$$\bar{\gamma}\frac{n+m}{2} + \gamma\frac{n+1+m+1}{2} \geq +\bar{\gamma}\sqrt{nm} + \gamma\sqrt{(n+1)(m+1)}\,. \tag{1.23}$$

The above equation naturally follows from $(x-y)^2 = x^2 + y^2 - 2xy \geq 0$, with $x^2 \to \bar{\gamma}n$ and $y^2 \to \bar{\gamma}m$ or $x^2 \to \gamma(n+1)$ and $y^2 \to \gamma(m+1)$, respectively. Furthermore, we see that equality actually only holds for the diagonal elements ($n = m$). From Gershgorins circle theorem, we can therefore conclude that all the eigenvalues of the matrix W have for $n \neq m$ a negative real part. Consequently, the coherences must decay and the stationary state only contains populations in the Fock space representation.

Transient dynamics

A simpler way to solve the particular master equation at hand is by using it to calculate the expectation value $\langle n\rangle = \mathrm{Tr}\left\{a^\dagger a\rho\right\}$ of the particle number operator

$$\begin{aligned}\frac{d}{dt}\langle n\rangle &= \langle a^\dagger a\dot\rho\rangle \\ &= +\Gamma(1+n_B)\mathrm{Tr}\left\{\left[a^\dagger a^\dagger aa - \left(a^\dagger a\right)^2\right]\rho\right\} \\ &\quad + \Gamma n_B \mathrm{Tr}\left\{\left[aa^\dagger aa^\dagger - \frac{1}{2}a^\dagger aaa^\dagger - \frac{1}{2}aa^\dagger a^\dagger a\right]\rho\right\}\,, \end{aligned} \tag{1.24}$$

where we have used the invariance of the trace under cyclic permutations to move the density matrix to the right. Further using the bosonic commutation relations we get the very simple equation

$$\frac{d}{dt}\langle n\rangle = -\Gamma\left(1+n_B\right)\langle n\rangle + \Gamma n_B\left(1+\langle n\rangle\right)\,, \tag{1.25}$$

which yields the same steady state solution

$$\frac{\bar n}{1+\bar n} = \frac{n_B}{1+n_B} = e^{-\beta\Omega}\,, \tag{1.26}$$

which we had before in Eq. (1.20). Likewise, the dynamics of the creation and annihilation operators becomes

$$\begin{aligned}\frac{d}{dt}\langle a\rangle &= \left[-\mathrm{i}\Omega - \frac{\Gamma}{2}\right]\langle a\rangle\,, \\ \frac{d}{dt}\langle a^\dagger\rangle &= \left[+\mathrm{i}\Omega - \frac{\Gamma}{2}\right]\langle a^\dagger\rangle\,, \end{aligned} \tag{1.27}$$

such that these expectation values will in the long run approach the origin. Considering observables like

$$\langle x\rangle = \frac{1}{\sqrt{2m\Omega}}\langle a^\dagger + a\rangle\,, \qquad \langle p\rangle = \mathrm{i}\sqrt{\frac{m\Omega}{2}}\langle a^\dagger - a\rangle\,, \tag{1.28}$$

we see that position and momentum are damped to the origin, since they obey the coupled equations

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle - \frac{\Gamma}{2}\langle x\rangle\,, \qquad \frac{d}{dt}\langle p\rangle = -m\Omega^2\langle x\rangle - \frac{\Gamma}{2}\langle p\rangle\,. \tag{1.29}$$

Mostly, one is not as fortunate as in this case, where the resulting evolution equations close with just a few variables, but deriving and solving equations of motion for observables from master equations is a popular tool for solving them.

1.3 Microscopic Lindblad Derivation

1.3.1 Mathematical Prerequisites

Master equations are often used to describe the dynamics of systems interacting with one or many large reservoirs (baths). To derive them from microscopic models – including the Hamiltonian of the full system – requires to review some basic mathematical concepts.

Tensor Product

The greatest advantage of the density matrix formalism is visible when quantum systems composed of several subsystems are considered. Roughly speaking, the tensor product represents a way to construct a larger vector space from two (or more) smaller vector spaces.

Def. 2 (Tensor Product). *Let V and W be Hilbert spaces (vector spaces with scalar product) of dimension m and n with basis vectors $\{|v\rangle\}$ and $\{|w\rangle\}$, respectively. Then $V \otimes W$ is a Hilbert space of dimension $m \cdot n$, and a basis is spanned by $\{|v\rangle \otimes |w\rangle\}$, which is a set combining every basis vector of V with every basis vector of W.*

Mathematical properties

- *Bilinearity* $(z_1 |v_1\rangle + z_2 |v_2\rangle) \otimes |w\rangle = z_1 |v_1\rangle \otimes |w\rangle + z_2 |v_2\rangle \otimes |w\rangle$ *as well as* $|v\rangle \otimes (z_1 |w_1\rangle + z_2 |w_2\rangle) = z_1 |v\rangle \otimes |w_1\rangle + z_2 |v\rangle \otimes |w_2\rangle$
- *operators acting on the combined Hilbert space $A \otimes B$ act on the basis states as* $(A \otimes B)(|v\rangle \otimes |w\rangle) = (A |v\rangle) \otimes (B |w\rangle)$
- *any linear operator on $V \otimes W$ can be decomposed as* $C = \sum_i c_i A_i \otimes B_i$
- *the scalar product is inherited in the natural way, i.e., one has for* $|a\rangle = \sum_{ij} a_{ij} |v_i\rangle \otimes |w_j\rangle$ *and* $|b\rangle = \sum_{k\ell} b_{k\ell} |v_k\rangle \otimes |w_\ell\rangle$ *the scalar product* $\langle a|b\rangle = \sum_{ijk\ell} a^*_{ij} b_{k\ell} \langle v_i|v_k\rangle \langle w_j|w_\ell\rangle = \sum_{ij} a^*_{ij} b_{ij}$

If more than just two vector spaces are combined to form a larger vector space, the dimension of the joint vector space grows rapidly, as e.g. exemplified by the case of a qubit: Its Hilbert space is just spanned by two vectors $|0\rangle$ and $|1\rangle$. The joint Hilbert space of two qubits is four-dimensional, of three qubits 8-dimensional, and of n qubits 2^n-dimensional. Eventually, this exponential growth of the Hilbert space dimension for composite quantum systems is at the heart of quantum computing.

Exercise 4 (Tensor Products of Operators). *Let $\boldsymbol{\sigma}$ denote the Pauli matrices, i.e.,*

$$\sigma^1 = \begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix} \qquad \sigma^2 = \begin{pmatrix} 0 & -\mathrm{i} \\ +\mathrm{i} & 0 \end{pmatrix} \qquad \sigma^3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}$$

Compute the trace of the operator

$$\begin{aligned} \Sigma &= a\mathbf{1} \otimes \mathbf{1} + \sum_{i=1}^{3} \alpha_i \sigma^i \otimes \mathbf{1} + \sum_{j=1}^{3} \beta_j \mathbf{1} \otimes \sigma^j + \sum_{i,j=1}^{3} a_{ij} \sigma^i \otimes \sigma^j \\ &\equiv a + \sum_{i=1}^{3} \alpha_i \sigma_1^i + \sum_{j=1}^{3} \beta_j \sigma_2^j + \sum_{i,j=1}^{3} a_{ij} \sigma_1^i \sigma_2^j \,. \end{aligned}$$

Since the scalar product is inherited, this typically enables a convenient calculation of the trace

in case of a few operator decomposition, e.g., for just two operators

$$\begin{aligned}\mathrm{Tr}\left\{A\otimes B\right\} &= \sum_{n_A,n_B}\left\langle n_A,n_B\right| A\otimes B\left|n_A,n_B\right\rangle \\ &= \left[\sum_{n_A}\left\langle n_A\right| A\left|n_A\right\rangle\right]\left[\sum_{n_B}\left\langle n_B\right| B\left|n_B\right\rangle\right] \\ &= \mathrm{Tr}_A\{A\}\mathrm{Tr}_B\{B\}\,, \end{aligned} \tag{1.29}$$

where $\mathrm{Tr}_{A/B}$ denote the trace in the Hilbert space of A and B, respectively.

The partial trace

Whereas the full trace maps a matrix to a number, one could also imagine a **partial trace** to reduce a full density matrix (or statistical operator) to a matrix acting only on a subspace. This is done with the partial trace.

Def. 3 (Partial Trace)**.** *Let $|a_1\rangle$ and $|a_2\rangle$ be vectors of state space A and $|b_1\rangle$ and $|b_2\rangle$ vectors of state space B. Then, the partial trace over state space B is defined via*

$$\mathrm{Tr_B}\left\{\left|a_1\right\rangle\left\langle a_2\right|\otimes\left|b_1\right\rangle\left\langle b_2\right|\right\} = \left|a_1\right\rangle\left\langle a_2\right|\mathrm{Tr}\left\{\left|b_1\right\rangle\left\langle b_2\right|\right\}\,. \tag{1.30}$$

Notation-wise, we note that an index can be suppressed when the normal trace is considered, such that the dimension is clear from the operator.

The partial trace is linear, such that the partial trace of arbitrary operators is calculated similarly. One may therefore calculate the most general partial trace via

$$\mathrm{Tr_B}\left\{C\right\} = \sum_\alpha c_\alpha \mathrm{Tr_B}\left\{A_\alpha\otimes B_\alpha\right\} = \sum_\alpha c_\alpha A_\alpha \mathrm{Tr}\left\{B_\alpha\right\}\,. \tag{1.31}$$

Exercise 5 (Partial Trace)**.** *Compute the partial trace of a pure density matrix $\rho = |\Psi\rangle\langle\Psi|$ in the bipartite state*

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right) \equiv \frac{1}{\sqrt{2}}\left(|0\rangle\otimes|1\rangle + |1\rangle\otimes|0\rangle\right)$$

The reduced density matrix

For composite systems, it is usually not necessary to keep all information of the complete system in the density matrix. Rather, one would like to have a density matrix that encodes all the information on a particular subsystem only. Obviously, the map $\rho \to \mathrm{Tr_B}\left\{\rho\right\}$ to such a reduced density matrix should leave all expectation values of observables A acting only on the considered subsystem invariant.

Def. 4 (Reduced density matrix)**.** *Let ρ_{AB} be a density matrix in the composite Hilbert space $A \otimes B$ with dimension $N_A \cdot N_B$*

$$\rho_{AB} = \sum_{n_A,m_A=1}^{N_A} \sum_{n_B,m_B=1}^{N_B} \rho_{(n_A,n_B),(m_A,m_B)} \left|n_A\right\rangle \left\langle m_A\right| \otimes \left|n_B\right\rangle \left\langle m_B\right| . \tag{1.32}$$

Then, the reduced density matrix

$$\rho_A = \sum_{n_A,m_A=1}^{N_A} \left[\sum_{n_B}^{N_B} \rho_{(n_A,n_B),(m_A,n_B)}\right] \left|n_A\right\rangle \left\langle m_A\right| = \sum_{n_A,m_A=1}^{N_A} \rho^{(A)}_{n_A,m_A} \left|n_A\right\rangle \left\langle m_A\right| \tag{1.33}$$

is a valid density matrix in A, and for all local observables we have $\mathrm{Tr}\left\{A\rho_A\right\} = \mathrm{Tr}\left\{A \otimes \mathbf{1}\rho_{AB}\right\}$.

This definition is the only linear map that respects the invariance of expectation values while mapping a large density matrix ρ_{AB} to a reduced one ρ_A. Its analog in the classical context is the computation of a marginal probability distribution via $P_i = \sum_j P_{ij}$.

We check these statements explicitly by using the density matrix properties of ρ_{AB}

- The trace of the reduced density matrix is one

$$\mathrm{Tr}\left\{\rho_A\right\} = \sum_{n_A} \rho^{(A)}_{n_A,n_A} = \sum_{n_A} \sum_{n_B} \rho_{(n_A n_B),(n_A n_B)} = \mathrm{Tr}\left\{\rho_{AB}\right\} = 1 . \tag{1.34}$$

- The reduced density matrix is hermitian

$$\rho_A^\dagger = \sum_{n_A,m_A} \sum_{n_B} \rho^*_{(n_A n_B),(m_A n_B)} \left|m_A\right\rangle \left\langle n_A\right| = \sum_{n_A,m_A} \sum_{n_B} \rho_{(m_A n_B),(n_A n_B)} \left|m_A\right\rangle \left\langle n_A\right| = \rho_A , \tag{1.35}$$

  which we can see by exchanging $n_A \leftrightarrow m_A$ in the last line.

- The reduced density matrix is positive

$$\left\langle \Psi_A\right| \rho_A \left|\Psi_A\right\rangle = \sum_{n_A,m_A} \sum_{n_B} \rho_{(n_A n_B),(m_A n_B)} \left\langle \Psi_A|n_A\right\rangle \left\langle m_A|\Psi_A\right\rangle = \sum_{n_B} \left\langle \Psi_A, n_B\right| \rho_{AB} \left|\Psi_A, n_B\right\rangle \geq 0 . \tag{1.36}$$

- Finally, expectation values of local observables, i.e., those that act trivially on Hilbert space B, only depend on the reduced density matrix

$$\begin{aligned} \mathrm{Tr}\left\{(A \otimes \mathbf{1})\rho_{AB}\right\} &= \sum_{n_A,n_B} \left\langle n_A, n_B\right| A \otimes \mathbf{1}\rho_{AB} \left|n_A, n_B\right\rangle = \sum_{n_A,\bar{n}_A} \left\langle n_A\right| A \left|\bar{n}_A\right\rangle \left[\sum_{n_B} \rho_{(\bar{n}_A n_B),(n_A n_B)}\right] \\ &= \mathrm{Tr}\left\{A\rho_A\right\} , \end{aligned} \tag{1.37}$$

  i.e., the object defined in this way makes sense.

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