Collection of useful notions from QM

[To be periodically updated as needed]

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1 Useful exponential formulae

- Baker-Campbell-Hausdorff formula:

$$e^A e^B = \exp\Big(A + B + \frac{1}{2}[A,B] + \frac{1}{12}\left([A,[A,B]] + [B,[B,A]]\right) \tag{1}$$

$$- \frac{1}{24}[B,[A,[A,B]]] - \frac{1}{720}\left([B,[B,[B,[B,A]]]] + [A,[A,[A,[A,B]]]]\right) + \dots\Big) \ . \tag{2}$$

- Defining $\mathrm{ad}_A^k(B) = [A,[A,[\dots,[A,B]]\dots]$ with k nested commutators (and k appearances of A),

$$e^A B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!}\mathrm{ad}_A^n(B) \ , \tag{3}$$

$$= B + [A,B] + \frac{1}{2}[A,[A,B]] + \frac{1}{3!}[A,[A,[A,B]]] + \dots \ . \tag{4}$$

- For an explicitly time-dependent operator $A(t)$,

$$\frac{\partial e^{A(t)}}{\partial t} e^{-A(t)} = \sum_{n=0}^{\infty} \frac{1}{(n+1)!}\mathrm{ad}_{A(t)}^n \frac{\partial A(t)}{\partial t} \tag{5}$$

$$= \frac{\partial A(t)}{\partial t} + \frac{1}{2}\left[A(t), \frac{\partial A(t)}{\partial t}\right] + \frac{1}{6}\left[A(t), \left[A(t), \frac{\partial A(t)}{\partial t}\right]\right] + \dots \ . \tag{6}$$

2 Dimensionless Schrödinger equation

If it often convenient to represent the Schrödinger equation in dimensionless/unitless form, for example because

- the relevant parameter distiguishing different physical regimes of the system is typically the ratio between different characteristic energy (or, e.g., time) scales. For instance, we can think of the ratio between the strength of a perturbation and the energy gaps in the system in perturbation theory. It is thus convenient to cast the problem in a representation where this ratio appears explicitly, instead of the individual physical quantities;
- We might want to simplify the notation by avoiding to carry on constants such as $\hbar$;
- If one plans to use numerical tools to solve the equation on a computer, the (digital, at least) computer works with pure numbers and not physical units.

A dimensionless form of the Schrödinger equation is obtained as follows. Assume that g is a characteristic energy scale of the system, which could be a coupling constant entering the Hamiltonian. Then, we can re-define the Hamiltonian in dimensionless form by re-scaling it with g:

$$H \to H_g = H/g \ . \tag{7}$$

In other words, we use g as our unit of energy. The Schrödinger equation changes according to

$$i\hbar\frac{\partial\,|\psi\rangle}{\partial t} = gH_g\,|\psi\rangle\,. \tag{8}$$

We next define a dimensionless time τ through the rescaling

$$\tau = gt/\hbar. \tag{9}$$

It is indeed dimensionless, since g has the unit of energy, t has the unit of time, and $\hbar$ is a unit of action, that is, energy times time. With this substitution, we obtain the Schrödinger equation in dimensionless form

$$i\frac{\partial\,|\psi\rangle}{\partial \tau} = H_g\,|\psi\rangle\,. \tag{10}$$

With a slight abuse of notation, in Eq. (10), $|\psi\rangle$ and H_g are now understood as functions of τ.

Example. A harmonic oscillator, with Hamiltonian $H_0 = Ea^\dagger a$ (see Sec. 4 if needed) is perturbed by $V = \lambda(a+a^\dagger)$, where λ denotes the strength of the perturbation and $a^\dagger$ and a are creation and annihilation operators. We choose E as the unit of energy and rescale the Hamiltonian accordingly, as $H_0 \to H_0/E$. We then define the dimensionless time $\tau = Et/\hbar$, arriving at the dimensionless Schrödinger equation

$$i\frac{\partial\,|\psi\rangle}{\partial t} = \left[a^\dagger a + \lambda_E(a+a^\dagger)\right]|\psi\rangle\,, \tag{11}$$

where we introduced $\lambda_E = \lambda/E$. As anticipated, this form of the Schrödinger equation highlights the key role of the ratio $\lambda_E = \lambda/E$ between the strength of the perturbation and the internal energy scale of the system.

3 Two-level systems

- The Hilbert space is $\mathbb{H} = \mathbb{C}^2$, where $\mathbb{C}$ is the set of complex numbers.
- The canonical basis of $\mathbb{C}^2$ is given by the vectors

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \qquad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}\,. \tag{12}$$

- a generic normalize state $|\psi\rangle$ of the two-level system can be parametrized as

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}\,|1\rangle\,, \tag{13}$$

  Being determined by the two angles θ and ϕ, it can be represented on the surface of a sphere, dubbed the *Bloch sphere*, where θ and ϕ represent the polar and azimuthal angles, respectively (see the Fig.).

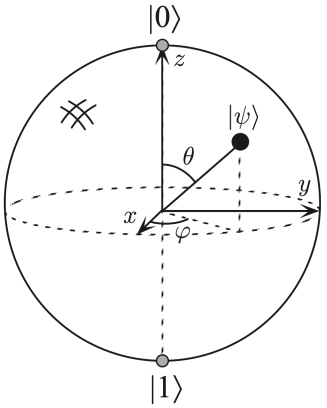

Fig. Bloch sphere representation of the state of a two-level system (image borrowed from the book of Nielsen and Chuang, Quantum Computation and Quantum Information).

- A basis of operators acting on $\mathbb{H}$ is given by the Pauli matrices

$$\sigma_0 = \mathbb{1} = \begin{pmatrix}1&0\\0&1\end{pmatrix}, \quad \sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix} \quad \sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix} \quad \sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{14}$$

  We will also use the notation $\sigma_x = \sigma_1$, $\sigma_y = \sigma_2$, $\sigma_z = \sigma_3$.

  The Pauli matrices are Hermitian, $\sigma_i^\dagger = \sigma_i$, and satisfy

  - the commutation relations $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$, for $i, j = 1, 2, 3$.
  - the anti-commutation relation $\{\sigma_i, \sigma_j\} = 0$, for $i \neq j$ and $i, j = 1, 2, 3$.

– they square to the identity, $\sigma_i^2 = \mathbb{1}$. Hence, they have eigenvalues ± 1.

- We can define raising and lowering operators $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$, which have thus matrix representation

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{15}$$

and they act on the basis states as

$$\sigma_- |0\rangle = |1\rangle\,, \qquad \sigma_+ |1\rangle = |0\rangle\,, \tag{16}$$
$$\sigma_- |1\rangle = 0, \qquad \sigma_+ |0\rangle = 0\ . \tag{17}$$

They further satisfy the commutation relations

$$[\sigma_z, \sigma_\pm] = \pm 2\sigma_\pm, \quad [\sigma_+, \sigma_-] = \sigma_z. \tag{18}$$

- The Hamiltonian can be chosen to be traceless by re-defining the zero of the energy (which amounts to adding a global phase to the states, which has no impact on the physics),

$$H \to H - \frac{1}{2}\mathrm{tr}(H)\mathbb{1}, \tag{19}$$

and can then be represented as

$$H = \begin{pmatrix} H_{00} & H_{10}^* \\ H_{10} & -H_{00} \end{pmatrix}\ , \tag{20}$$

where $H_{ij} = \langle i| H |j\rangle$. Noting that $H^2 = (H_{00}^2 + |H_{10}|^2)\mathbb{1}$, the eigenvalues are immediately found to be

$$E_\pm = \pm\sqrt{H_{00}^2 + |H_{10}|^2}\ . \tag{21}$$

The energy gap between the two levels is thus $2\sqrt{H_{00}^2 + |H_{10}|^2}$.

- The Hamiltonian can be decomposed on the Pauli matrices,

$$H = \frac{1}{2}\sum_{i=1}^{3} h_i \sigma_i, \qquad h_i = \mathrm{tr}(H\sigma_i). \tag{22}$$

Comparing with Eq. (20), the real components h_i are linked to the matrix elements H_{ij} according to

$$h_1 = \mathrm{Re}(H_{10}), \quad h_2 = \mathrm{Im}(H_{10}), \quad h_3 = H_{00}\ . \tag{23}$$

The Hamiltonian can thus be visualized as a vector $\boldsymbol{h}$ in 3D space, which we can parametrize with two angles θ and ϕ as

$$\boldsymbol{h} = [|h|\sin\theta\cos\phi, |h|\sin\theta\sin\phi, |h|\cos\theta]. \tag{24}$$

The length $|h|$ of the vector is determined by the eigenvalues, $|h| = E_+ = \sqrt{h_1^2 + h_2^2 + h_3^2}$, and the angles are linked to the matrix elements as

$$\tan\theta = \frac{|H_{10}|}{H_{00}}, \quad \phi = \mathrm{Arg}(H_{10})\ , \tag{25}$$

for $0 \le \theta \le \pi/2$. With this parametrization, H reads as

$$H = E_+ \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix}. \tag{26}$$

- The eigenvectors can be written as

$$\begin{bmatrix} |\psi_+\rangle \\ |\psi_-\rangle \end{bmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} & e^{i\phi}\sin\frac{\theta}{2} \\ -e^{-i\phi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{bmatrix} |0\rangle \\ |1\rangle \end{bmatrix}. \tag{27}$$

- The unitary matrix U which diagonalizes H,

$$U^{-1}HU = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}, \tag{28}$$

has thus the form

$$U = |\psi_+\rangle\langle 0| + |\psi_-\rangle\langle 1| = \begin{pmatrix} \cos\frac{\theta}{2} & -e^{-i\phi}\sin\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} . \tag{29}$$

Exercise. Given the vector of Pauli matrices $\boldsymbol{\sigma} = \{\sigma_x, \sigma_y\, \sigma_z\}$, prove the relation

$$\exp\left(-\frac{i}{2}\phi\ \boldsymbol{n}\cdot\boldsymbol{\sigma}\right) = \cos(\phi/2)\mathbb{1} - i(\boldsymbol{n}\cdot\boldsymbol{\sigma})\sin(\phi/2) . \tag{30}$$

Exercise. Work out a matrix representation of $\exp(-i\alpha H)$, where α is a real number.

Exercise. We pointed out that H can be depicted geometrically as a vector $\boldsymbol{h}$ [Eq. (24)]. Consider Eq. (28) and note that, since $E_- = -E_+$, the right-hand-side is also equal to $E_+\sigma_z$. In the light of Eq. (28), can you give a geometric interpretation of the diagonalization matrix U?

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4 Harmonic Oscillator

4.1 Ladder operators

- Hamiltonian of a harmonic oscillator with mass $m > 0$ and frequency $\omega > 0$:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 , \tag{31}$$

with q and p are the position and momentum operators, $[q, p] = i\hbar$.

- Creation and annihilation (ladder) operators can be constructed as

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(q + \frac{i}{m\omega}p\right), \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(q - \frac{i}{m\omega}p\right) \tag{32}$$

and they satisfy $[a, a^\dagger] = 1$. Conversely,

$$q = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger), \qquad p = -i\sqrt{\frac{\hbar m\omega}{2}}(a - a^\dagger) . \tag{33}$$

- The Hamiltonian, rewritten in terms of ladder operators, reads $H = \hbar\omega(a^\dagger a + 1/2)$.

- The *number* operator $N = a^\dagger a$ thus counts the number of excitations in an eigenstate, $N|n\rangle = n|n\rangle$. The creation and annihilation operators are eigen-operators of N, namely

$$[N, a^\dagger] = a^\dagger, \qquad [N, a] = -a . \tag{34}$$

- The ground state is the vacuum state $|n = 0\rangle$, which is annihilated by a, $a|0\rangle = 0$. The action of the ladder operators on the eigenstates $|n\rangle$ is

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle , \tag{35}$$

$$a|n\rangle = n|n-1\rangle \ , \quad n > 0 \tag{36}$$

4.2 Coherent states

- *Coherent (or Glauber) states* are right eigenstates of the annihilation operator,

$$a\,|\alpha\rangle = \alpha\,|\alpha\rangle\,, \tag{37}$$

where α is a complex number (not just real, because a is not Hermitian, $a \neq a^\dagger$). The Hermitian conjugate of Eq. (37) gives

$$\langle\alpha|\,a^\dagger = \alpha^*\,\langle\alpha|\,, \tag{38}$$

Hence, $\langle\alpha|$ is a left eigenstate of $a^\dagger$ with eigenvalue α^*.

- A coherent state *is not* an eigenstate of the number operator $N = a^\dagger a$. It features an average number of excitations $\overline{N}_\alpha = \langle\alpha|\,N\,|\alpha\rangle = |\alpha|^2$. The variance of the excitation number is equal to the average value itself, $\mathrm{var}_\alpha(N) = \langle N^2\rangle_\alpha - \langle N\rangle_\alpha^2 = \overline{N}_\alpha$, where $\langle\star\rangle_\alpha = \langle\alpha|\,\star\,|\alpha\rangle$.

- A coherent state, represented on the number (Fock) basis $|n\rangle$, has the form

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^{+\infty}\frac{\alpha^n}{\sqrt{n!}}\,|n\rangle\ . \tag{39}$$

The occupation probability of the n-th Fock state is thus

$$|\langle n|\alpha\rangle|^2 = \frac{\overline{N}_\alpha^n\ e^{-\overline{N}_\alpha}}{n!}. \tag{40}$$

Hence, the coherent state corresponds to a Poissonian distribution over the Fock states with average $\overline{N}_\alpha$.

- Coherent states are an overcomplete basis. Two coherent states $|\alpha\rangle$ and $|\beta\rangle$ are not orthogonal, but have an overlap

$$\langle\alpha|\beta\rangle = e^{-(\alpha-\beta)^2}\ . \tag{41}$$

- A coherent state is a minimum uncertainty state: it saturates the Heisenberg uncertainty relation,

$$\mathrm{var}_\alpha(q)\mathrm{var}_\alpha(p) = \hbar^2/4\ . \tag{42}$$

In this sense, it is as close as possible to a classical (zero-uncertainty) state.

- The *displacement operator* is defined as

$$D(\alpha) = e^{\alpha a^\dagger - \alpha^* a}. \tag{43}$$

It is unitary and it transforms the ladder operators according to

$$D^\dagger(\alpha)\,a\,D(\alpha) = a + \alpha. \tag{44}$$

Moreover, it displaces the vacuum to the coherent state $|\alpha\rangle$,

$$D(\alpha)\,|0\rangle = |\alpha\rangle\,. \tag{45}$$

Exercise. Using the exponential formulae from Sec. 1 or Taylor expansions, prove the following relations,

$$e^{i\theta a^\dagger a}\,a\,e^{-i\theta a^\dagger a} = e^{-i\theta}a, \tag{46}$$

$$e^{i\theta a^\dagger a}\,a^\dagger\,e^{-i\theta a^\dagger a} = e^{i\theta}a^\dagger, \tag{47}$$

$$D(\alpha) = e^{-|\alpha|^2/2}e^{\alpha a^\dagger}e^{-\alpha^* a}. \tag{48}$$

Exercise. Derive Eq. (39), by imposing Eq. (37) on an ansatz for $|\alpha\rangle$ as a generic decomposition on Fock states, $|\alpha\rangle = \sum_n c_n\,|n\rangle$.

Exercise. Prove Eqs. (44) and (45).

Exercise. A light source is in a coherent state $|\alpha\rangle$. Consider the occupation probability of a Fock state $|n\rangle$. Show that, if n is within one standard deviation $\Delta\overline{N}_\alpha = \sqrt{\mathrm{var}_\alpha(N)}$ from the average photon number $\overline{N}_\alpha$ and $\overline{N}_\alpha \gg 1$, then the occupation probability of $|n\rangle$ and of its neighboring Fock states $|n \pm 1\rangle$ is approximately the same.

Exercise. Study the dynamics of an oscillator initiated in its vacuum state $|0\rangle$ and driven by the Hamiltonian (in units of $\hbar$)

$$H = \omega a^\dagger a + \mathcal{E}(a + a^\dagger) \tag{49}$$

How does the state at time t look like? *Hint:* One approach is to initially displace the oscillator using the displacement operator $D(\alpha)$. Choose α such that, in the displaced Hamiltonian, all terms which are linear in ladder operators cancel out. Solving what remains should then be easier. (see also Sec. 5.1 if needed)

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5 Time evolution

5.1 Autonomous systems

- A system governed by the Hamiltonian H evolves according to the Schrödinger Eq.

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H |\psi(t)\rangle , \tag{50}$$

  given an initial condition $|\psi(t_0)\rangle$, at the initial time $t = t_0$.

- The solution of the Schrödinger Eq. has the form

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle , \tag{51}$$

  where $U(t, t_0)$ is the evolution operator or propagator.

- The evolution operator $U(t, t_0)$ satisfies as well the Schrödinger Eq.

$$i\hbar \frac{\partial U(t, t_0)}{\partial t} = HU(t, t_0), \qquad U(t_0, t_0) = \mathbb{1}. \tag{52}$$

  For a time-independent Hamiltonian, Eq. (52) has the solution

$$U(t, t_0) = \exp\left(-\frac{i}{\hbar}(t - t_0)H\right). \tag{53}$$

  Once the system energies E_n and eigenvectors $|E_n\rangle$ are found by solving the eigenvalue equation

$$H |E_n\rangle = E_n |E_n\rangle , \tag{54}$$

  the evolution operator can be represented in the energy eigenbasis as

$$U(t, t_0) = \sum_n e^{-\frac{i}{\hbar}E_n(t-t_0)} |E_n\rangle\langle E_n| \ . \tag{55}$$

  As a consequence, by decomposing the initial state in the energy eigenbasis as

$$|\psi(t_0)\rangle = \sum_n c_n |E_n\rangle , \tag{56}$$

  with $c_n = \langle E_n|\psi(t_0)\rangle$, the time-evolved state has the form

$$|\psi(t)\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t} |E_n\rangle \ . \tag{57}$$

  The occupation probability $|\langle E_n|\psi(t)\rangle|^2$ of the eigenstates is conserved over time,

$$\partial_t |\langle E_n|\psi(t)\rangle|^2 = \partial_t |c_n|^2 = 0, \tag{58}$$

  which reflects the conservation of the energy in the system, $\partial_t \langle\psi(t)| H |\psi(t)\rangle = 0$. In order to modify the eigenstate occupations, we need to perturb the system.

Exercise. A two-level system is at time $t_0 = 0$ in the state $|\psi(t_0)\rangle = |0\rangle$. It then evolves with the Hamiltonian $H = (\omega/2)\sigma_x$. How does the probability of being in $|\psi(t_0)\rangle$ change over time?

Exercise. Consider a two-level system evolving for a time $t \in [0, T]$. The system is subjected to a Hamiltonian which changes abruptly at an intermediate time

$$H(t) = \begin{cases} \frac{\Omega_z}{2}\sigma_z & \text{for } 0 \leq t < T/2, \\ \frac{\Omega_x}{2}\sigma_x & \text{for } T/2 \leq t \leq T. \end{cases} \tag{59}$$

(i) Determine the evolution operators corresponding to the two Hamiltonians pertaining to the case in which
   - the evolution starts at time $t_0 = 0$, and we consider an evolution interval $0 \leq t < T$;
   - the evolution starts at time $t_0 = T/2$, and we consider an evolution interval $T/2 \leq t \leq T$;

(ii) Determine the matrix representation of the operators computed in (i).

(iii) Building on the result of (i) and (ii), determine the evolution operator of the system at a time $t > T/2$, given the initial time $t_0 = 0$ (in matrix representation).

(iv) Can this evolution operator be expressed as

$$U(t, t_0) = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')\right) ? \tag{60}$$

5.2 Pictures

Consider the Schrödinger equation

$$i\hbar\frac{\partial U(t, t_0)}{\partial t} = HU(t, t_0), \tag{61}$$

for the evolution operator $U(t, t_0)$.

- In *Schrödinger picture*, states evolve as $|\psi(t)\rangle = U(t, t_0)\,|\psi(t_0)\rangle$, while operators do not. The time-evolved state is found by solving the Schrödinger equation

$$i\hbar\frac{\partial\,|\psi(t)\rangle}{\partial t} = H\,|\psi(t)\rangle\,. \tag{62}$$

  Expectation values at time t of an observable O are determined by sandwiching the time independent O with the time-evolved state $|\psi(t)\rangle$,

$$\langle O\rangle(t) = \langle\psi(t)|\,O\,|\psi(t)\rangle\,. \tag{63}$$

- In *Heisenberg picture*, states do not evolve and the time-dependence is moved to operators instead. Given an observable O, its time-propagated form is

$$O(t, t_0) = U^\dagger(t, t_0)OU(t, t_0)\ . \tag{64}$$

  Accordingly, the time-evolved operator $O(t, t_0)$ is found by solving the Heisenberg equation of motion

$$\frac{\partial O(t, t_0)}{\partial t} = \frac{i}{\hbar}[H, O(t, t_0)]\ . \tag{65}$$

  Expectation values of O at time t are thus found by sandwitching the propagated operator $O(t)$ with the initial state $|\psi(t_0)\rangle$,

$$\langle O\rangle(t) = \langle\psi(t_0)|\,O(t)\,|\psi(t_0)\rangle\ \ . \tag{66}$$

- *Generic gauge transformation.* We can represent the evolving states in a different time-dependent reference frame, defined by a unitary transformation $V(t)$, as

$$|\psi_V(t)\rangle = V(t)\,|\psi(t)\rangle = U_V(t,t_0)\,|\psi(t_0)\rangle\,, \tag{67}$$

where I defined $U_V(t,t_0) = V(t)U(t,t_0)$. Correspondingly, by expressing $U(t,t_0)$ as $U(t,t_0) = V^\dagger(t)U_V(t,t_0)$, we can write the Schrödinger equation in the new frame, which reads as

$$i\hbar\frac{\partial U_V(t,t_0)}{\partial t} = \left[V(t)HV^\dagger(t) - i\hbar V(t)\frac{\partial V^\dagger(t)}{\partial t}\right]U_V(t,t_0). \tag{68}$$

It involves the transformed Hamiltonian

$$H_V(t) = V(t)HV^\dagger(t) - i\hbar V(t)\frac{\partial V^\dagger(t)}{\partial t}\ , \tag{69}$$

which includes an instantaneous change of basis $V(t)HV^\dagger(t)$ and the inertial or centrifugal term $i\hbar V(t)\frac{\partial V^\dagger(t)}{\partial t}$. To preserve the expectation value $\langle O\rangle(t) = \langle\psi(t_0)|\,U^\dagger(t,t_0)OU(t,T_0)\,|\psi(t_0)\rangle$ of the observables under the change of frame, both states and operators must evolve:

$$\langle O\rangle(t) = \langle\psi_V(t)|\,O_V(t)\,|\psi_V(t)\rangle\ \ , \tag{70}$$

with

$$O_V(t) = V(t)OV^\dagger(t)\ . \tag{71}$$

- *Interaction (or Dirac) picture.* Assume that the Hamiltonian decomposes as $H = H_0 + H_I$ into a free (or unperturbed) part H_0 and an interaction (or perturbation) part H_I. In the interaction picture, we represent the dynamics in a frame where the free part H_0 has been integrated out. Namely, we choose

$$V(t) = e^{\frac{i}{\hbar}H_0 t} \tag{72}$$

in Eqs. (67) and (68), such that the centrifugal contribution $i\hbar V(t)\partial_t V^\dagger(t)$ precisely cancels H_0 in the transformed Hamiltonian (69). From Eq. (69), the interaction-picture Hamiltonian is then

$$H_I(t) = e^{\frac{i}{\hbar}H_0 t}H_I e^{-\frac{i}{\hbar}H_0 t}\ . \tag{73}$$

To preserve the expectation value of the observables under the change of picture, both states and operators must evolve, as in Eqs. (67) and (71).

Exercise. Derive the Heisenberg equation of motion from the Schrödinger equation.

Exercise. Let the Hamiltonian of a two-level system be given by $H = H_0 + H_1$ with

$$H_0 = \frac{\omega}{2}\sigma_z, \qquad H_1 = \frac{\Omega}{2}\sigma_x\ . \tag{74}$$

Compute the representation of the Hamiltonian in the interaction picture.

5.3 Time-dependent Hamiltonians: the Dyson series

In this section, we derive formal expressions for the time-evolution operator generated by a Hamiltonian which features an explicit time-dependence.

Consider the Schrödinger Eq. with an explicitly time-dependent Hamiltonian $H(t)$ for the evolution operator $\mathcal{U}(t,t_0)$,

$$i\hbar\frac{\partial\mathcal{U}(t,t_0)}{\partial t} = H(t)\mathcal{U}(t,t_0). \tag{75}$$

We want to construct the formal solution for $\mathcal{U}(t,t_0)$. To this end, we start by integrating Eq. (75) in time with the initial condition $\mathcal{U}(t_0,t_0) = \mathbb{1}$, obtaining

$$\mathcal{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 H(t_1)\mathcal{U}(t_1,t_0)\ . \tag{76}$$

This is a so-called Volterra-type equation, namely an integral equation where the variable enters as an integral extremum. We can solve it through a recursion: We use the right-hand-side of this expression to represent the evolution operator appearing under integration on the right-hand side,

$$\mathcal{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 H(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 H(t_1)H(t_2)\mathcal{U}(t_2,t_0) \ . \tag{77}$$

Iterating this procedure by substituting every evolution operator appearing under integration with Eq. (76), we obtain an infinite series involving nested integrals of products of the Hamiltonian $H(t)$ evaluated at different time points,

$$\mathcal{U}(t,t_0) = \mathbb{1} + \sum_{n=1}^{+\infty} \left(-\frac{i}{\hbar}\right)^n \mathcal{I}_n(t,t_0) \ , \tag{78}$$

with

$$\mathcal{I}_n(t,t_0) = \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n \ H(t_1)\dots H(t_n) \ . \tag{79}$$

Since each nested integral runs over an interval of times which are smaller than the value of time set by an outer integral (i.e., t_n is always smaller than t_{n-1}, which is always smaller than t_{n-2} and so on), the product of Hamiltonians in the argument of Eq. (78) has a time ordering: if $m < n$, then $H(t_n)$ appears to the left of $H(t_m)$. This property can be used to simplify the integration extrema and obtain a more compact representation. We introduce the *time-ordering operator* $\mathcal{T}$, which orders products of operators by decreasing time argument. For two operators, it reads

$$\mathcal{T}\big\{H(t_i)H(t_j)\big\} = \begin{cases} H(t_i)H(t_j) & \text{if } t_i > t_j, \\ H(t_j)H(t_i) & \text{if } t_i < t_j. \end{cases} \tag{80}$$

We next note that

$$\mathcal{T}\left(\int_{t_0}^{t} dt' H(t')\right)^2 = \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \mathcal{T}\big\{H(t_1)H(t_2)\big\}, \tag{81}$$

$$= \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ H(t_1)H(t_2) + \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 \ H(t_2)H(t_1), \tag{82}$$

$$= \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ H(t_1)H(t_2) + \int_{t_0}^{t} dt_2 \int_{t_2}^{t} dt_1 \ H(t_1)H(t_2), \tag{83}$$

$$= 2\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ H(t_1)H(t_2) \ . \tag{84}$$

The step leading to Eq. (83) can be understood by considering the integration region in a (t_1, t_2) plane, shown in Fig. 1. By choosing suitable integration boundaries, one is free to choose which variable between t_1 and t_2 to integrate first. Generalizing this reasoning, one finds that

$$\int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1)\dots H(t_n) = \frac{1}{n!}\mathcal{T}\left(\int_{t_0}^{t} dt' \ H(t')\right)^n , \tag{85}$$

which can be proved by induction. The factor of $n!$ arises from all the possible permutation of the integration variables. Inserting Eq. (85) into Eq. (78) and recognizing the emerging Taylor series for the exponential, we obtain a compact representation of the evolution operator as a time-ordered exponential,

$$\mathcal{U}(t,t_0) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt' \ H(t')\right). \tag{86}$$

The series representation of this expression is usually called the *Dyson series*.

For a sufficiently short time, the series can be used as a perturbative expansion, which can be truncated to a desired order, yielding an approximation to the time-evolution operator (as used in time-dependent perturbation theory),

$$\mathcal{U}_m(t,t_0) = \mathbb{1} + \sum_{n=1}^{m} \left(-\frac{i}{\hbar}\right)^n \mathcal{I}_n(t,t_0) \ . \tag{87}$$

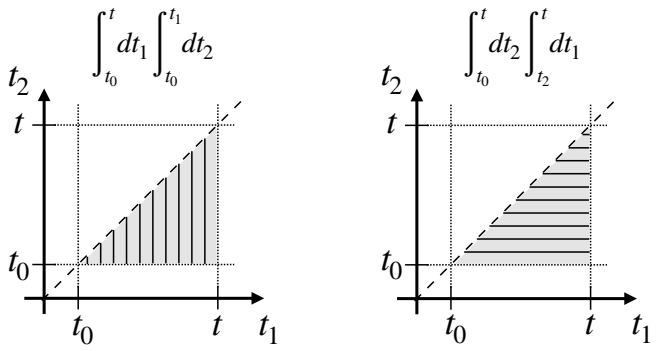

Figure 1: Different integration order for nested integrals.

The error entailed in the truncation can estimated as

$$\|\mathcal{U}(t,t_0) - \mathcal{U}_m(t,t_0)\| \leq \frac{t^{m+1}}{(m+1)!}(\max_{t'\in[t_0,t]}\|H(t')\|)^{m+1} \ . \tag{88}$$

An important property of the Dyson expansion is that, being an expansion of the unitary operator, it *does not preserve unitarity*. In other words, when applied to states, it does not preserve their norm (i.e., the total probability). We will see next a different expansion, which rather expands the generator of the unitary, thus preserving unitarity.

Exercise (Response of a harmonic oscillator). Consider a harmonic oscillator with free Hamiltonian $H_0 = \hbar\omega_0(a^\dagger a + 1/2)$, with $\omega_0 > 0$, which is perturbed by

$$V(t) = \hbar\omega_0\gamma(t)(a + a^\dagger) \ . \tag{89}$$

(i) Determine the interaction-picture representation $V_I(t)$ of $V(t)$. Compute the commutator $[V_I(t), V_I(t')]$.

(ii) Compute the evolution operator in the interaction picture using first-order time-dependent perturbation theory (Dyson expansion) for the particular case

$$\gamma(t) = \gamma_0\Theta(t)\exp(-t\tau), \tag{90}$$

with $\tau > 0$ and where $\Theta(t)$ is the Heaviside Theta function.

(iii) Assuming that the oscillator is its ground state $|0\rangle$ at the initial time, use this evolution operator to compute the probability that the oscillator is in the excited state $|n\rangle$ at long times, $t \gg \tau$.

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6 Mixed states

- Uncertainty about the exact pure state of the system is described by a density operator (or statistical operator, or mixed state) ρ.
- A density operator ρ is a positive-semidefinite Hermitian operator with unit trace,
  - (i) $\rho = \rho^\dagger$, [$\Rightarrow$ can be diagonalized and has real eigenvalues]
  - (ii) $\rho \geq 0$, [$\Rightarrow$ the eigenvalues are non-negative]
  - (iii) $\mathrm{tr}[\rho] = 1$, [$\Rightarrow$ the sum of the eigenvalues normalizes to 1]
- The density operator describes a *statistical mixture* (or *ensemble*) $\{p_i, |\psi_i\rangle\}$ of *pure* states $|\psi_i\rangle$ associated with probabilities $p_i \geq 0$, $\sum_i p_i = 1$. It is defined as

$$\rho = \sum_i p_i \, |\psi_i\rangle \langle\psi_i| \ . \tag{91}$$

- The *purity* $\mathrm{tr}(\rho^2)$ can tell us whether the state is pure or mixed: $\mathrm{tr}(\rho^2) = 1$ only for pure states, otherwise $\mathrm{tr}(\rho^2) < 1$.
- In a given basis $\{|i\rangle\}$, the off-diagonal elements $\rho_{ij} = \langle i|\,\rho\,|j\rangle$ are called *coherences* (in that basis), while the diagonal terms are called *populations*.
- Example (thermal state) Consider a system in equilibrium with a thermal bath at inverse temperature $\beta = 1/k_B T$ in the canonical ensemble. Thermal fluctuations create uncertainty about the microscopic pure state of the system. The equilibrium state is thus constructed by attributing probabilities p_i to the system eigenstates $|E_i\rangle$ which are given by (normalized) Boltzmann factors,

$$\rho_\beta = \sum_i p_i\,|E_i\rangle\langle E_i|\,, \qquad p_i = \frac{e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}\ . \tag{92}$$

  This state has thus the form

$$\rho_\beta = \frac{1}{Z_\beta} e^{-\beta H}\ , \tag{93}$$

  where $Z_\beta = \mathrm{tr}[\exp(-\beta H)]$ is the partition function.
- Example: The system is initially in a pure state $|\psi\rangle$. We measure an observable $M = \sum_i m_i\,|M_i\rangle\langle M_i|$, but we do not record the outcome. From measurement theory, the measurement projects the system in state $|M_i\rangle$ with probability $p_i = |\langle\psi|M_i\rangle|^2$. Even if we know that the state has collapsed, we do not know in which state $|M_i\rangle$ the system has been projected, since we did not keep the information about the outcome. We express this statistical uncertainty by associating p_i to the ith possible outcome, thus constructing the post-measurement state ρ_{PM} given by

$$\rho_{PM} = \sum_i p_i\,|M_i\rangle\langle M_i|\ . \tag{94}$$

- Note that different ensembles can give rise to the same density operator. As an example, this is the case for the following ensembles for a two-level system,

$$\text{Ensemble 1}: \qquad \left\{\left(p_0 = \frac{3}{4}, |\psi_0\rangle = |0\rangle\right), \left(p_1 = \frac{1}{4}, |\psi_1\rangle = |1\rangle\right)\right\}, \tag{95}$$

$$\text{Ensemble 2}: \qquad \left\{\left(p_0 = \frac{1}{2}, |\psi_0\rangle = \sqrt{\frac{3}{4}}\,|0\rangle + \sqrt{\frac{1}{4}}\,|1\rangle\right), \left(p_1 = \frac{1}{2}, |\psi_1\rangle = \sqrt{\frac{3}{4}}\,|0\rangle - \sqrt{\frac{1}{4}}\,|1\rangle\right)\right\}\ . \tag{96}$$

- The state describing maximal uncertainty is the fully mixed (or totally unpolarized, or infinite-temperature) state $\rho = \mathbb{1}/d$, where d is the dimension of the Hilbert space.
- From the Schrödinger Eq. follows that ρ evolves according to the Liouville-von Neumann Eq.,

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}[H, \rho(t)]\ . \tag{97}$$

- The (von Neumann) entropy of a density operator ρ is defined as

$$S(\rho) = -\mathrm{tr}[\rho \ln \rho]\ . \tag{98}$$

  Given a spectral decomposition of ρ as $\sum_i \rho_i\,|\rho_i\rangle\langle\rho_i|$, the entropy is

$$S(\rho) = -\sum_i \rho_i \ln \rho_i\ . \tag{99}$$

  Hence, the von Neumann entropy equals the Shannon entropy (with natural log) of the classical probability distribution associated with the eigenstates of ρ, that is, the eigenvalues of ρ.

Exercise. For a two-level system, is $\rho = p_0\,|0\rangle\,\langle 0| + p_1\,|0\rangle\,\langle 1|$ a valid density matrix?

Exercise. Prove that $\mathrm{tr}(\rho^2) \leq 1$ for a mixed state.

Exercise. For a two-state system:

(i) Compute the density matrix corresponding to a generic pure state $|\psi\rangle = \cos(\theta/2)\,|0\rangle + e^{i\phi}\sin(\theta/2)\,|1\rangle$.

(ii) Write down the matrix representation of the mixture $\rho_w = w_0\,|\psi\rangle\langle\psi| + w_1\,|0\rangle\langle 0|$.

(iii) What conditions need w_0 and w_1 fulfill, for ρ_w to be a valid density matrix?

Exercise. Consider the operator

$$\rho = \frac{1}{3}\begin{pmatrix} 1 & 0 & \beta \\ 0 & 1 & 0 \\ \beta & 0 & 1 \end{pmatrix}, \tag{100}$$

depending on a parameter β. Can ρ describe a valid density operator? In which case would it describe a pure state?

Exercise. Let A be an Hermitian operator, with spectral decomposition $A\,|n\rangle = a_n\,|n\rangle$. Consider the operator $\rho = c\exp(A)$, where c is a normalization constant. To be able to express ρ in the form $\rho = \sum_n w_n\,|n\rangle\,\langle n|$, how should the coefficients w_n be chosen? Determine the constant c.

Exercise. For a two-level system, consider the pure state $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ and the mixed state $\rho = \mathbb{1}/2$. What are the probabilities of the system being in state $|0\rangle$ and $|1\rangle$ for $|\psi\rangle$ and ρ? We now want to determine whether $|\psi\rangle$ or ρ is the correct description of the system. Can you think of a gedanken experiment to determine it?

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7 Composite systems

- Given two system $\mathcal{S}_1$ and $\mathcal{S}_2$, with associated Hilbert spaces $\mathbb{H}_1$ and $\mathbb{H}_2$, the Hilbert space $\mathbb{H}_{12}$ of the composite system jointly describing $\mathcal{S}_1$ and $\mathcal{S}_2$ has the tensor product structure $\mathbb{H}_{12} = \mathbb{H}_1 \otimes \mathbb{H}_2$.

- Basic properties of the tensor product:

  (i) Given a scalar c and vectors $|\psi_1\rangle \in \mathbb{H}_1$ and $|\psi_2\rangle \in \mathbb{H}_2$,

  $$c(|\psi_1\rangle \otimes |\psi_2\rangle) = (c\,|\psi_1\rangle) \otimes |\psi_2\rangle = |\psi_1\rangle \otimes (c\,|\psi_2\rangle). \tag{101}$$

  (ii) It is linear and distributive with respect to the sum,

  $$\big(\alpha\,|\psi_1\rangle + \beta\,|\phi_1\rangle\big) \otimes |\psi_2\rangle = \alpha\,|\psi_1\rangle \otimes |\psi_2\rangle + \beta\,|\phi_1\rangle \otimes |\psi_2\rangle\,, \tag{102}$$

  $$|\psi_1\rangle \otimes \big(\alpha\,|\psi_2\rangle + \beta\,|\phi_2\rangle\big) = \alpha\,|\psi_1\rangle \otimes |\psi_2\rangle + \beta\,|\psi_1\rangle \otimes |\phi_2\rangle\ . \tag{103}$$

  for scalar α and β, and where $\{|\psi_1\rangle, |\phi_1\rangle\} \in \mathbb{H}_1$, $\{|\psi_2\rangle, |\phi_2\rangle\} \in \mathbb{H}_2$.

- A basis of $\mathbb{H}_{12}$ can be constructed as the tensor product $\{|ij\rangle_{12} \equiv |i\rangle_1 \otimes |j\rangle_2\}$ of a basis $|i\rangle_1$ of $\mathbb{H}_1$ and a basis $|j\rangle_2$ of $\mathbb{H}_2$. If $\mathbb{H}_1$ has dimension d_1 and $\mathbb{H}_2$ has dimension d_2, then $\mathbb{H}_{12}$ has dimension $d_{12} = d_1 \times d_2$. A state $|\psi\rangle_{12} \in \mathbb{H}_{12}$ in the composite Hilbert space can thus be decomposed as

  $$|\psi\rangle_{12} = \sum_{i=1}^{d_1}\sum_{j=1}^{d_2} c_{ij}\,|ij\rangle_{12}\ . \tag{104}$$

  The notation for the states is usually simplified with $|ij\rangle$, dropping the subscripts.

- Operators O_j pertaining to sub-system $\mathcal{S}_i$ are promoted to operators on the tensor-product space by taking their tensor product with identities on the other sub-systems. For example, for a bipartite system, an operator of subsystem $\mathcal{S}_1$ is promoted to $O_1 \otimes \mathbb{1}_2$. Generally, linear operators of the form $O_1 \otimes O_2$ are defined through their action on a state $|v_1\rangle \otimes |v_2\rangle \in \mathbb{H}_{12}$,

  $$(O_1 \times O_2)(|v_1\rangle \otimes |v_2\rangle) = O_1\,|v_1\rangle \otimes O_2\,|v_2\rangle\ . \tag{105}$$

- The matrix representation of the product $A \otimes B$, given the representations a_{ij} and b_{ij} of the $N \times N$ matrices A and B, is obtained via the Kronecker product

$$A \otimes B = \begin{bmatrix} a_{11}B & \dots & a_{1N}B \\ \vdots & \ddots & \vdots \\ a_{N1}B & \dots & a_{NN}B \end{bmatrix} = \begin{bmatrix} a_{11}\begin{pmatrix} b_{11} & \dots & b_{1N} \\ \vdots & \ddots & \vdots \\ b_{N1} & \dots & b_{NN} \end{pmatrix} & \dots & a_{1N}\begin{pmatrix} b_{11} & \dots & b_{1N} \\ \vdots & \ddots & \vdots \\ b_{N1} & \dots & b_{NN} \end{pmatrix} \\ \vdots & \ddots & \vdots \\ a_{N1}\begin{pmatrix} b_{11} & \dots & b_{1N} \\ \vdots & \ddots & \vdots \\ b_{N1} & \dots & b_{NN} \end{pmatrix} & \dots & a_{NN}\begin{pmatrix} b_{11} & \dots & b_{1N} \\ \vdots & \ddots & \vdots \\ b_{N1} & \dots & b_{NN} \end{pmatrix} \end{bmatrix}, \tag{106}$$

$$= \begin{bmatrix} a_{11}b_{11} & \dots & a_{11}b_{1N} & \dots & a_{1N}b_{11} & \dots & a_{1N}b_{1N} \\ \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ a_{11}b_{N1} & \dots & a_{11}b_{NN} & & a_{1N}b_{N1} & \dots & a_{1N}b_{NN} \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ a_{N1}b_{11} & \dots & a_{N1}b_{1N} & & a_{NN}b_{11} & \dots & a_{NN}b_{1N} \\ \vdots & \ddots & \vdots & \dots & \vdots & \ddots & \vdots \\ a_{N1}b_{N1} & \dots & a_{N1}b_{NN} & & a_{NN}b_{N1} & \dots & a_{NN}b_{NN} \end{bmatrix}. \tag{107}$$

- Example: For two spin-1/2 particles, a basis of the composite Hilbert space is obtained from the bases of $\mathbb{C}^2$ as

$$|00\rangle = [1,0,0,0]^T, \quad |01\rangle = [0,1,0,0]^T, \tag{108}$$

$$|10\rangle = [0,0,1,0]^T, \quad |11\rangle = [0,0,0,1]^T\ , \tag{109}$$

  which gives the canonical basis of $\mathbb{H}_{12} = \mathbb{C}^4$.

- The inner product on $\mathbb{H}_{12}$ can be defined through the inner product on $\mathbb{H}_1$ and $\mathbb{H}_2$,

$$\left(\sum_i a_i^* \langle i|_1 \otimes \langle i|_2\right)\left(\sum_j b_j |j\rangle_1 \otimes |j\rangle_2\right) = \sum_{i,j}(a_i^* b_j)\langle i|j\rangle_1 \langle i|j\rangle_2. \tag{110}$$

- Other properties

  (i) $\mathrm{tr}(A \otimes B) = \mathrm{tr}(A)\mathrm{tr}(B)$

  (ii) if A acts on $\mathbb{H}_1$ and B acts on $\mathbb{H}_2$, with $\dim(\mathbb{H}_1) = d_1$ and $\dim(\mathbb{H}_2) = d_2$, then

$$\mathrm{tr}\big(A \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes B\big) = d_2\mathrm{tr}(A) + d_1\mathrm{tr}(B)\ . \tag{111}$$

  (iii) $e^{A\otimes\mathbb{1}} = e^A \otimes \mathbb{1}$

  (iv) $e^{A\otimes\mathbb{1}+\mathbb{1}\otimes B} = e^A \otimes e^B$

- The *partial trace* $\mathrm{tr}_n(\star)$ over (the degrees of freedom of) the nth sub-system, say sub-system $\mathcal{S}_2$, is defined by

$$\mathrm{tr}_2[A \otimes B] = \mathrm{tr}(B)A, \tag{112}$$

  where the trace on the right-hand-side is the trace over the second sub-system only. Given the bases $\{|i\rangle_1\}$ of $\mathbb{H}_1$ and $\{|i\rangle_2\}$ of $\mathbb{H}_2$, the partial trace of a generic operator C_{12} acting on $\mathbb{H}_{12}$ can be computed as

$$\mathrm{tr}_2[C_{12}] = \sum_{i,j}\left({}_1\langle i|\,{}_2\langle j|\,C_{12}\,|i\rangle_1 |j\rangle_2\right)|i\rangle_1\langle i| \tag{113}$$

$$= \sum_j {}_2\langle j|\,C_{12}\,|j\rangle_2\,. \tag{114}$$

- If we are given the state ρ_{12} of the combined system and we measure an observable of a sub-system $O_1 \otimes \mathbb{1}_2$, the expectation value is given by

$$\begin{aligned}\langle O_1 \otimes \mathbb{1}_2 \rangle_{12} =& \mathrm{tr}[\rho_{12} O_1 \otimes \mathbb{1}_2] && (115)\\ =& \sum_{i,j} {}_1\langle i|\, {}_2\langle j|\, \rho_{12} O_1 \otimes \mathbb{1}_2\, |i\rangle_1 |j\rangle_2 && (116)\\ =& \sum_i {}_1\langle i| \left(\sum_j {}_2\langle j|\, \rho_{12}\, |j\rangle_2 \, O_1 \right) |i\rangle_1 && (117)\\ =& \mathrm{tr}_1 \left[\mathrm{tr}_2(\rho_{12}) O_1 \right]. && (118)\end{aligned}$$

  Hence, local properties of sub-system $\mathcal{S}_1$ can then be described on the local Hilbert space by using the *reduced density operator*,

$$\rho_1 = \mathrm{tr}_2(\rho_{12}), \tag{119}$$

  according to

$$\langle O_1 \otimes \mathbb{1}_2 \rangle_{12} = \langle O_1 \rangle_1 \equiv \mathrm{tr}(\rho_1 O_1). \tag{120}$$

Exercise. Prove the "Other properties" above.

Exercise. Consider two spin 1/2 systems. A basis of the composite Hilbert space is obtained as $\{|0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle\}$. Compute the matrix representation of $\sigma_1^x \sigma_2^y = \sigma_x \otimes \sigma_y$ from the matrix representations of σ^x and σ^y in the single-spin basis $\{|0\rangle, |1\rangle\}$.

Exercise. Prove that the reduced density operators is actually a valid density operator.

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8 Bi-particle entanglement

- A pure bi-particle state $|\psi\rangle_{AB} \in \mathbb{H}_{AB}$, describing the composite system comprising systems A and B, is *entangled* if it cannot be expressed as a product state,

$$|\psi\rangle_{AB} \neq |\psi_1\rangle_A \otimes |\psi_2\rangle_B, \tag{121}$$

  for any $|\psi_1\rangle_A \in \mathbb{H}_A$ and $|\psi_2\rangle_B \in \mathbb{H}_B$. Otherwise, the state is said to be *separable*.

- Example: For two spin-1/2 particles, having total spin s_{12} and spin projection along the z direction s_{12}^z, the following triplet and singlet states are entangled

$$\left|s_{12}=1, s_{12}^z=0\right\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \qquad \left|s_{12}=0, s_{12}^z=0\right\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}\ . \tag{122}$$

- *Schmidt decomposition.* There exists a basis $\{|\phi_i\rangle_A\}$ of $\mathbb{H}_A$ and a basis $\{|\chi_i\rangle_B\}$ of $\mathbb{H}_B$ such that a given biparticle state $|\psi\rangle_{AB}$ can be expressed as

$$|\psi\rangle_{AB} = \sum_{i=1}^{s} \sqrt{\lambda_i}\, |\phi_i\rangle_A \otimes |\chi_i\rangle_B, \tag{123}$$

  where $s \leq \min(d_1, d_2)$, $\lambda_i > 0$, $\sum_i \lambda_i = 1$. The number s is called the *Schmidt number* and the coefficients $\sqrt{\lambda_i}$ are called *Schmidt coefficients*. Note that the representation is diagonal: the two local bases in the tensor product in Eq. (123) have the same index.

- Observations:

  (i) Some simple criteria for pure-state, bipartite entanglement: a pure state $|\psi\rangle_{AB}$ is entangled iff

  * the Schmidt number is larger than 1;

∗ the reduced density matrices are mixed. In turn, this is the case iff, for $X = A, B$, it holds that $\mathrm{tr}(\rho_X^2) < 1$ or $S(\rho_X) \neq 0$.

(ii) The reduced density matrices have the same eigenvalues, which are the coefficients λ_i,

$$\rho_A = \sum_i \lambda_i \, |\phi_i\rangle_A \langle\phi_i| \,, \qquad \rho_B = \sum_i \lambda_i \, |\chi_i\rangle_B \langle\chi_i| \ . \tag{124}$$

Hence, the Schmidt coefficients characterize common properties of the sub-systems.

- Assume, for simplicity, $d_1 = d_2 \equiv d$. A state is said to be maximally entangled if $s = d$ and $\lambda_i = 1/d$. For such a state, the reduced density operators are fully mixed, $\rho_A = \rho_B = \mathbb{1}/d$. That is, no information on the composite system can be obtained by probing a single sub-system.

- Example: For two spin-1/2 particles, the maximally entangled states are the so-called *Bell's states* or *EPR pairs*

$$|\Phi_\pm\rangle = \frac{|00\rangle \pm |11\rangle}{\sqrt{2}}, \qquad |\Psi_\pm\rangle = \frac{|01\rangle \pm |10\rangle}{\sqrt{2}}. \tag{125}$$

Exercise. Is the two-spin state $(|00\rangle + |01\rangle)/\sqrt{2}$ separable or entangled?

Exercise. Is the two-spin state $(|00\rangle + |01\rangle + |10\rangle + |11\rangle)/2$ separable or entangled?

Exercise. Prove that, if two d-dimensional systems A and B are fully entangled, then the reduced density operators ρ_A and ρ_B are fully mixed.
