5. Time evolution

In a previous lecture we characterized the time evolution of closed quantum systems as *unitary*, $|\psi(t)\rangle = U(t,0)\,|\psi(0)\rangle$ and the state evolution as given by Schrödinger equation:

$$i\hbar\frac{d|\psi\rangle}{dt} = \mathcal{H}|\psi\rangle$$

Equivalently, we can find a differential equation for the dynamics of the propagator:

$$i\hbar\frac{\partial U}{\partial t} = \mathcal{H}U$$

This equation is valid also when the Hamiltonian is time-dependent.
As the Hamiltonian represents the energy of the system, its *spectral representation* is defined in terms of the energy eigenvalues ϵ_k, with corresponding eigenvectors $|k\rangle$: $\mathcal{H} = \sum_k \epsilon_k |k\rangle\langle k|$. The evolution operator is then: $U = \sum_k e^{-i\epsilon_k t}|k\rangle\langle k|$. The eigenvalues of U are therefore simply $e^{-i\epsilon_k t}$, and it is common to talk in terms of eigenphases $\varphi_k(t) = \epsilon_k t$. If the Hamiltonian is time-independent we have also $U^\dagger = U(-t)$, it is possible to obtain an effective inversion of the time arrow.

? Question: What is the evolution of an energy eigenvector $|k\rangle$?
First consider the infinitesimal evolution: $|k(t+dt)\rangle = U(t+dt,t)\,|k(t)\rangle = (\mathbb{1} - i\mathcal{H}dt)\,|k(t)\rangle = (1 - i\epsilon_k dt)\,|k(t)\rangle$. Thus we have the differential equation for the energy eigenket: $\frac{d|k\rangle}{dt} = -i\epsilon_k\,|k\rangle$, so that $|k(t)\rangle = e^{-i\epsilon_k t}\,|k(0)\rangle$.
We can also use the spectral decomposition of U: $|k(t)\rangle = U(t,0)\,|k(0)\rangle = (\sum_h e^{-i\epsilon_h t}\,|h\rangle\,\langle h|)\,|k(0)\rangle = e^{-i\epsilon_k t}\,|k(0)\rangle$. □

Notice that if a system is in a state given by an eigenvector of the Hamiltonian, then the system does not evolve. This is because the state will only acquire a global phase that, as seen, does not change its properties. Of course, superposition of energy eigenkets do evolve.

5.1 The Schrödinger and Heisenberg pictures

Until now we described the dynamics of quantum mechanics by looking at the time evolution of the state vectors. This approach to quantum dynamics is called the Schrödinger picture. We can easily see that the evolution of the

state vector leads to an evolution for the expectation values of the observables (which are the relevant physical quantities we are interested in and have access to).
From the evolution law for a state, $|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$, we obtain the following relation, when expressing the state in the Hamiltonian eigenbasis:

$$|\psi\rangle = \sum_k c_k |\epsilon_k\rangle \to |\psi'\rangle = e^{-i\mathcal{H}t}|\psi\rangle = \sum_k c_k e^{-i\epsilon_k t} |\epsilon_k\rangle$$

Then the expectation value of an observable A evolves as:

$$\langle A\rangle = \sum_{k,j} c_k^* c_j \langle\epsilon_k| A |\epsilon_j\rangle \;\to\; \sum_{k,j} c_k^* c_j \langle\epsilon_k| A |\epsilon_j\rangle e^{-i(\epsilon_j-\epsilon_k)t}$$

Quite generally, we can also write $\langle A(t)\rangle = \langle\psi(t)| A |\psi(t)\rangle = \langle(U\psi)| A |U\psi\rangle$. By the associative property we then write $\langle A(t)\rangle = \langle\psi|(U^\dagger A U)|\psi\rangle$.
It would than seem natural to define an "evolved" observable $A(t) = U^\dagger A U$, from which we can obtain expectation values considering states that are fixed in time, $|\psi\rangle$. This is an approach known as **Heisenberg picture**.
Observables in the Heisenberg picture are defined in terms of observables in the Schrödinger picture as

$$A^H(t) = U^\dagger(t) A^S U(t), \quad A^H(0) = A^S$$

The state kets coincide at $t = 0$: $|\psi\rangle_H = |\psi(t=0)\rangle_S$ and they remain independent of time. Analogously to the Schrödinger equation we can define the Heisenberg equation of motion for the observables:

$$\frac{dA^H}{dt} = -i[A^H, \mathcal{H}]$$

? Question: Derive the Heisenberg equation from the Schrödinger equation.
$\frac{dA^H}{dt} = \frac{d(U^\dagger A^S U)}{dt} = \frac{\partial U^\dagger}{\partial t} A^S U + U^\dagger A^S \frac{\partial U}{\partial t} = i(U^\dagger\mathcal{H})A^S U + U^\dagger A^S(-i\mathcal{H}U)$. Inserting the identity $\mathbb{1} = UU^\dagger$ we have $= i(U^\dagger\mathcal{H}UU^\dagger A^S U - U^\dagger A^S U U^\dagger \mathcal{H} U)$. We define $\mathcal{H}^H = U^\dagger\mathcal{H}U$. Then we obtain $\frac{dA^H}{dt} = -i[A^H, \mathcal{H}^H]$. U and $\mathcal{H}$ always commute for time-independent $\mathcal{H}$, thus $\mathcal{H}^H = \mathcal{H}$. □

5.2 Interaction Picture

We now consider yet another "picture" that simplifies the description of the system evolution in some special cases. In particular, we consider a system with an Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + V$$

where $\mathcal{H}_0$ is a "solvable" Hamiltonian (of which we already know the eigen-decomposition, so that it is easy to calculate e.g. $U_0 = e^{-i\mathcal{H}_0 t}$) and V is a perturbation that drives an interesting (although unknown) dynamics. In the so-called interaction picture the state is represented by

$$|\psi\rangle_I = U_0(t)^\dagger |\psi\rangle_S = e^{i\mathcal{H}_0 t}|\psi\rangle_S$$

where the subscript I, S indicate the interaction and Schrödinger picture respectively. For the observable operators we can define the corresponding interaction picture operators as:

$$A_I(t) = U_0^\dagger A_S U_0 \;\to\; V_I(t) = U_0^\dagger V U_0$$

We can now derive the differential equation governing the evolution of the state in the interaction picture (we now drop the subscript S for the usual Schrödinger picture):

$$i\frac{\partial|\psi\rangle_I}{\partial t} = i\frac{\partial(U_0^\dagger|\psi\rangle)}{\partial t} = i(\frac{\partial U^\dagger}{\partial t}|\psi\rangle + U_0^\dagger\frac{\partial|\psi\rangle}{\partial t}) = -U_0^\dagger\mathcal{H}_0|\psi\rangle + U_0^\dagger(\mathcal{H}_0+V)|\psi\rangle = U_0^\dagger V|\psi\rangle.$$

Inserting the identity $\mathbb{1} = U_0 U_0^\dagger$, we obtain

$$i\frac{\partial|\psi\rangle_I}{\partial t} = U_0^\dagger V U_0 U_0^\dagger|\psi\rangle = V_I|\psi\rangle_I.$$

This is a Schrödinger -like equation for the vector in the interaction picture, evolving under the action of the operator V_I only. However, in contrast to the usual Schrödinger picture, even the observables in the interaction picture evolve in time. From their definition $A_I(t) = U_0^\dagger A_S U_0$, we have the differential equation $\frac{dA_I}{dt} = i[\mathcal{H}_0, A_I]$, which is an Heisenberg-like equation for the observable, with the total Hamiltonian replaced by $\mathcal{H}_0$. The interaction picture is thus an intermediate picture between the two other pictures.

	S	**H**	**I**
$\|\psi\rangle$	✓	×	✓
A	×	✓	✓

Table 1: Time dependence of states and operators in the three pictures

5.2.1 Dyson Time-ordering operator

If we now want to solve the state-vector differential equation in terms of a propagator $|\psi(t)\rangle_I = U_I(t)\,|\psi\rangle_I$, we encounter the problem that the operator V_I is usually time-dependent since $V_I(t) = U_0^\dagger V U_0$, thus in general $U_I \neq e^{-iV_I t}$. We can still write an equation for the propagator in the interaction picture

$$i\frac{dU_I}{dt} = V_I(t)U_I$$

with initial condition $U_I(0) = \mathbb{1}$. When V_I is time dependent and $V_I(t)$ does not commute at different time, it is no longer possible to find a simple explicit expression for $U_I(t)$. Indeed we could be tempted to write $U_I(t) = e^{-i\int_0^t V_I(t')dt'}$. However in general

$$e^A e^B \neq e^{A+B} \quad \text{if} \quad [A,B] \neq 0,$$

thus for example, although we know that $U_I(t)$ can be written as $U_I(t,0) = U_I(t,t^\star)U_I(t^\star,0)$ $(\forall 0 < t^\star < t)$ we have that $e^{-i\int_0^{t^\star} V_I(t')dt' - i\int_{t^\star}^t V_I(t')dt'} \neq e^{-i\int_{t^\star}^t V_I(t')dt'} e^{-i\int_0^{t^\star} V_I(t')dt'}$. Thus we cannot find an explicit solution in terms of an integral.
We can however find approximate solutions or formal solution to the evolution.
The differential equation is equivalent to the integral equation

$$U_I(t) = \mathbb{1} - i\int_0^t V_I(t')U_I(t')dt'$$

By iterating, we can find a formal solution to this equation :

$$U_I(t) = \mathbb{1} - i\int_0^t dt' V_I(t') + (-i)^2 \int_0^t dt' \int_0^{t'} dt' V_I(t')V_I(t'') + \dots$$

$$+(-i)^n \int_0^t dt' \dots \int_0^{t^{(n-1)}} dt^{(n)} V_I(t') \dots V_I(t^{(n)}) + \dots$$

This series is called the *Dyson* series.
Note that in the expansion the operators are time-ordered, so that in the product the operators at earlier times are at the left of operators at later times. We then define an operator $\mathcal{T}$ such that when applied to a product of two operators it will return their time-ordered product:

$$\mathcal{T}(A(t)B(t')) = \begin{cases} A(t)B(t'), & \text{if } t < t' \\ B(t')A(t), & \text{if } t' < t \end{cases}$$

Now we can rewrite the expression above in a more compact way. We replace the limits of each intervals so that they span the whole duration $\{0, t\}$ and we divide by $n!$ to take into account that we integrate over a larger interval. Then we can write the products of integrals as powers and use the time-ordering operator to take this change into account. We then have:

$$U_I(t) = \mathcal{T}\left\{\sum_{n=0}^{\infty} \frac{(-i)^n}{n!}\left(\int_0^t dt' V_I(t')\right)^n\right\}$$

where we recognize the expression for an exponential

$$U_I(t) = \mathcal{T}\left\{\exp\left(-i\int_0^t dt' V_I(t')\right)\right\}$$

Note that the time-ordering operator is essential for this expression to be correct.

? Question: Prove that $\int_0^t dt' \ldots \int_0^{t^{(n-1)}} dt^{(n)} V_I(t') \ldots V_I(t^{(n)}) = \frac{1}{n!}\mathcal{T}\left\{(\int_0^t dt' V_I(t'))^n\right\}$ for $n = 2$.

5.2.2 Some useful approximate formulas

Besides the formal solution found above and the Dyson series formula, there are other approximate formulas that can help in calculating approximations to the time evolution propagator.

A. Baker-Campbell-Hausdorff formula

The Baker-Campbell-Hausdorff formula gives an expression for $C = \log(e^A e^B)$, when A, B do not commute. That is, we want C such that $e^C = e^A e^B$. We have[10]

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] - [B, [A, B]]) - \frac{1}{24}[B, [A, [A, B]]] \ldots$$

The Hadamard series is the solution to $f(s) = e^{sA} B e^{-sA}$. To find this, differentiate the equation:

$$f'(s) = e^{sA} A B e^{-sA} - e^{sA} B A e^{-sA} = e^{sA}[A, B]e^{-sA}$$

$$f''(s) = e^{sA} A[A, B]e^{-sA} - e^{sA}[A, B]A e^{-sA} = e^{sA}[A, [A, B]]e^{-sA}$$

$$f'''(s) = e^{sA}[A, [A, [A, B]]]e^{-sA}$$

etc. and then construct the Taylor series for $f(s)$:

$$f(s) = f(0) + sf'(0) + \frac{1}{2}s^2 f''(0) + \frac{1}{3!}s^3 f''(0) + ...$$

to obtain

$$e^{sA} B e^{-sA} = B + [A, B]s + \frac{1}{2}[A, [A, B]]s^2 + \frac{1}{3!}[A, [A, [A, B]]]s^3 + \ldots$$

With $s = it$ and $A = \mathcal{H}$, this formula can be useful in calculating the evolution of an operator (either in the Heisenberg or interaction representation or for the density operator).

[10] See e.g. wikipedia for more terms and mathworld for calculating the series.

B. Suzuki-Trotter expansion

Another useful approximation is the Suzuki-Trotter expansion[11]. To first order this reads:

$$e^{A+B} = \lim_{n\to\infty}(e^{A/n}e^{B/n})^n$$

Suzuki-Trotter expansion of the second order:

$$e^{A+B} = \lim_{n\to\infty}(e^{A/(2n)}e^{B/n}e^{A/(2n)})^n$$

In general we can approximate the evolution under a time-varying Hamiltonian by a piecewise constant Hamiltonian in small enough time intervals:

$$U(t,t_0) = U(t,t_{n-1})\dots U(t_2,t_1)U(t_1,t_0), \qquad t_0 < t_1 < t_2 < \cdots < t_{n-1} < t,$$

where we usually take $t_k - t_{k-1} = \delta t$ and consider the Hamiltonian $\mathcal{H}$ to be constant during each of the small time interval δt.

C. Magnus expansion

The Magnus expansion is a perturbative solution to the exponential of a time-varying operator (for example the propagator of a time-varying Hamiltonian). The idea is to define an effective time-independent Hamiltonian by taking: $U = \mathcal{T}e^{-i\int_0^t dt'\mathcal{H}(t')} \equiv e^{-it\overline{H}}$. The effective Hamiltonian is then expanded in a series of terms of increasing order in time $\overline{H} = \overline{H}^{(0)} + \overline{H}^{(1)} + \overline{H}^{(2)} + \dots$, so that

$$U = \exp\{-it[\overline{H}^{(0)} + \overline{H}^{(1)} + \overline{H}^{(2)} + \dots]\}$$

where the terms can be found by expanding $\mathcal{T}e^{-i\int_0^t dt'\mathcal{H}(t')}$ and equating terms of the same time power. In order to keep the time order, commutators are then introduced. The lowest order terms are

$$\begin{aligned}
\overline{H}^{(0)} &= \tfrac{1}{t}\int_0^t H(t')dt' \\
\overline{H}^{(1)} &= -\tfrac{i}{2t}\int_0^t dt'\int_0^{t'} dt''[H(t'),H(t'')] \\
\overline{H}^{(2)} &= \tfrac{1}{6t}\int_0^t dt'\int_0^{t'} dt''\int_0^{t''} dt'''\{[[H(t'),H(t'')],H(t''')] + [[H(t'''),H(t'')],H(t')]\}
\end{aligned}$$

The convergence of the expansion is ensured only if $\|\mathcal{H}\|t \ll 1$.

[11] See: M. Suzuki, *Generalized Trotter's formula and systematic approximants of exponential operators and inner derivations with applications to many-body problems*, Comm. Math. Phys. **51**, 183-190 (1976)

5.3 Spin-$\frac{1}{2}$ precession

We consider the semi-classical problem of a spin-1/2 particle in a classical magnetic field. To each spin with spin angular momentum $\mathbf{J}$ is associated a magnetic moment $\mu = \gamma \mathbf{S}$ where γ is called the gyromagnetic ratio, a property of each spin-carrying particle (nucleus, electron, etc.). The energy of the system in an external mangetic field is (classically) given by $\mu \cdot \mathbf{B}$, where B is of course the field. Thus, the system Hamiltonian is simply $\mathcal{H} = \gamma B_z S_z = \omega S_z$, where we take the z axis to point along the external field for simplicity and we defined the Larmor frequency for the given system.
If the spin is initially in the state $|0\rangle$, the system does not evolve (as it is an eigenstate of the Hamiltonian). If instead it is prepared in a superposition state, it will undergo an evolution.

$$|\psi_0\rangle = \alpha_0|0\rangle + \beta_0|1\rangle \rightarrow |\psi(t)\rangle = \alpha(t)|0\rangle + \beta(t)|1\rangle$$

? Question: What are the functions $\alpha(t),\ \beta(t)$?
1. As $|0\rangle,\ |1\rangle$ are eigenstates of the Hamiltonian with eigenvalues $\pm\omega/2$, we know that their evolution is just a phase $e^{\pm i\omega t/2}$, so that $\alpha(t) = \alpha_0 e^{-i\omega t/2}$ and $\beta(t) = \beta_0 e^{+i\omega t/2}$.
2. $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$, with $U = e^{-i\mathcal{H}t} = e^{-i\omega S_z t} = \mathbb{1}\cos(\omega t/2) - i\sin(\omega t/2)\,2S_z$. Then $U(t)|0\rangle = (\cos\omega t/2 - i\sin\omega t/2)|0\rangle = e^{-i\omega t/2}|0\rangle$ and we find the same result. □

? Question: What is the probability of finding the spin back to its initial state?
Let's write the initial state as $|\psi\rangle_0 = \cos(\vartheta/2)|0\rangle + e^{i\varphi/2}\sin(\vartheta/2)|1\rangle$. Then the evolution is $e^{i\omega t/2}\cos(\vartheta/2)|0\rangle + e^{i(\omega t+\varphi)/2}\sin(\vartheta/2)|1\rangle$ and the probability $p = \cos^2(\omega t/2) + \cos\vartheta^2\sin^2(\omega t/2)$ In particular, for $\vartheta = \pi/4$ we have $\cos^2(\omega t/2)$ (notice that this is an eigenstate of the S_x operator). □

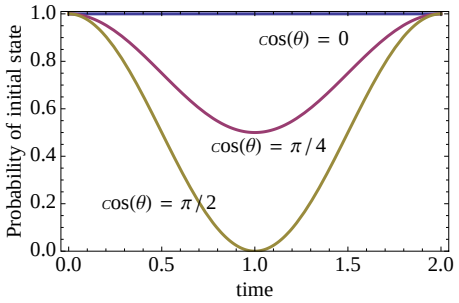

Fig. 4: Spin precession: probability of being in the initial state

? Question: What is the evolution of the magnetization in the x direction?
We want to calculate $\langle S_x(t)\rangle$. We can use the Heisenberg picture, and calculate $U^\dagger S_x U = S_x\cos(\omega t) - S_y\sin(\omega t)$. Thus we see that the periodicity is $T = \frac{2\pi}{\omega}$ while it was $\frac{4\pi}{\omega}$ for the spin state (spinor behavior). Then we know that $\langle S_x\rangle = \cos(\varphi/2)\sin(\vartheta)$ and $\langle S_y\rangle = \sin(\varphi/2)\sin(\vartheta)$ from which we find $\langle S_x(t)\rangle = \cos(\varphi/2 + \omega t)\sin(\vartheta)$ □

Nuclear Magnetic Resonance

The evolution of the magnetization is what is usually detected in NMR. The precession of the spin in a large static magnetic field creates an oscillating magnetic field that in turns generate a current/voltage in a pickup coil. Fourier-transform of the signal gives spectroscopic information regarding the Larmor frequency; local modification of the magnetic field (due e.g. to electronic field) induces a variation on the Larmor frequency of each nuclear spin in a molecule, thus providing a way to investigate the structure of the molecule itself. Before we can have a full vision of a (simple) NMR experiment, we still need to answer the question on how we first prepare the spin in a superposition state (e.g. in a S_x eigenstate). We will be able to answer this question in a minute.

5.4 Examples: Resonance of a Two-Level System

We have looked at the precession of the spin at the Larmor frequency, which happens if the spin is initially in a superposition state. However, the question remained on how we rotate initially the spin away from its equilibrium state pointing along the large external magnetic field. Consider then a more general problem in which we add a (small) time-dependent magnetic field along the transverse direction (e.g. x-axis):

$$\vec{B}(t) = B_z\hat{z} + 2B_1\cos(\omega t)\hat{x} = B_z\hat{z} + B_1\left[(\cos(\omega t)\hat{x} + \sin(\omega t)\hat{y}) + (\cos(\omega t)\hat{x} - \sin(\omega t)\hat{y})\right],$$

where B_1 is the strength of the radio-frequency (for nuclei) or microwave (for electron) field.
The Hamiltonian of the system $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1(t) + \mathcal{H}_1'(t)$ is then:

$$\mathcal{H} = \frac{\omega_0}{2}\sigma_z + \frac{\omega_1}{2}\left[\cos(\omega t)\sigma_x + \sin(\omega t)\sigma_y\right] + \frac{\omega_1}{2}\left[\cos(\omega t)\sigma_x - \sin(\omega t)\sigma_y\right],$$

where we defined the rf frequency ω_1. We already know the eigenstates of $\mathcal{H}_0$ ($|0\rangle$ and $|1\rangle$). Thus we use the interaction picture to simplify the Hamiltonian, with $U_0 = e^{-i\omega\sigma_z/2}$ defining a frame rotating about the z-axis at a frequency ω: this is the so-called *rotating frame*. Remembering that $U_0\sigma_x U_0^\dagger = \cos(\omega t)\sigma_x + \sin(\omega t)\sigma_y$, it's easy to see that the perturbation Hamiltonian in the interaction frame is $\mathcal{H}_{1I} = U_0^\dagger\mathcal{H}_1 U_0 = \frac{\omega_1}{2}\sigma_x$. We also have $\mathcal{H}_{1I}' = U_0^\dagger\mathcal{H}_1' U_0 = \frac{\omega_1}{2}\left(\cos(2\omega t)\sigma_x - \sin(2\omega t)\sigma_y\right)$. Under the assumptions that $\omega_1 \ll \omega$, this is a small, fast oscillating term, that quickly averages out during the evolution of the system and thus can be neglected. This approximation is called the *rotating wave approximation* (RWA). Under the RWA, the Hamiltonian in the rotating frame simplifies to

$$\mathcal{H}_I = \frac{\Delta\omega}{2}\sigma_z + \frac{\omega_1}{2}\sigma_x$$

where $\Delta\omega = \omega_0 - \omega$. Notice that if $\Delta\omega$ is large ($\gg \omega_1$), we expect that the eigenstates of the systems are still going to be close to the eigenstates of $\mathcal{H}_0$ and the small perturbation has almost no effect. Only when $\omega \approx \omega_0$ we will see a change: this is the resonance condition. In particular, for $\Delta\omega = 0$ the new Hamiltonian $\sim \sigma_x$ will cause a spin initially in, say, $|0\rangle$ to rotate away from the z axis and toward the y axis. This is how a "pulse" is generated e.g. in NMR or ESR pulsed spectroscopy. For example, if the B_1 field is turned on for a time $t_{\pi/2} = \pi/2\omega_1$ we prepare the state $|\psi\rangle = (|0\rangle - i|1\rangle)/\sqrt{2}$ that will then precess at the Larmor frequency, giving a spectroscopic signature in the recorded signal.
We want to study the Hamiltonian in the general case. Given the matrix representation

$$\mathcal{H}_I = \frac{1}{2}\begin{pmatrix} \Delta\omega & \omega_1 \\ \omega_1 & -\Delta\omega \end{pmatrix}$$

we can find the eigenvalues:

$$\omega_I = \pm\frac{\Delta\omega}{2}\sqrt{1 + (\omega_1/\Delta\omega)^2}.$$

There are two interesting limits, on resonance ($\Delta\omega = 0$) where $\omega_I = \omega_1$ and far off resonance ($\Delta\omega \gg \omega_1$) where $\omega_I \approx \Delta\omega \sim \omega_0$. The eigenstates are found (e.g. via a rotation of the Hamiltonian) to be

$$\begin{aligned} |+\rangle_I &= \cos\vartheta|0\rangle + \sin\vartheta|1\rangle \\ |-\rangle_I &= \cos\vartheta|1\rangle - \sin\vartheta|0\rangle, \end{aligned}$$

with

$$\sin\vartheta = \sqrt{\frac{\omega_I - \Delta\omega}{2\omega_I}}, \qquad \cos\vartheta = \sqrt{\frac{\omega_I + \Delta\omega}{2\omega_I}}$$

Consider the evolution of the state $|0\rangle$ under the rotating frame Hamiltonian. At time $t = 0$ the two frame coincide, so $|\psi\rangle_I = |\psi\rangle = |0\rangle$. The state then evolves as

$$|\psi(t)\rangle_I = \left[\cos\left(\frac{\Omega t}{2}\right) - i\frac{\Delta\omega}{\Omega}\sin\left(\frac{\Omega t}{2}\right)\right]|0\rangle - i\frac{\omega_1}{\Omega}\sin\left(\frac{\Omega t}{2}\right)|1\rangle$$

where we defined $\Omega = \sqrt{\Delta\omega^2 + \omega_1^2}$. The probability of *flipping* the spin (that is, of finding the spin in the $|1\rangle$ state) is then $p(1) = \frac{\omega_1^2}{\Delta\omega^2+\omega_1^2}\sin^2\left(\frac{\Omega t}{2}\right)$. Notice that only if $\Delta\omega = 0$ we can have perfect inversion (i.e. $p(1) = 1$ for $t = \pi/\omega_1$. Notice that we have defined all the evolutions as in the rotating frame.

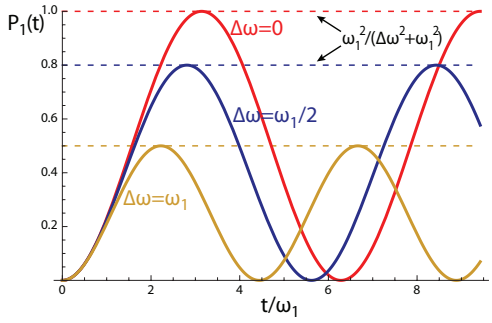

Fig. 5: **Rabi oscillation.** Probability of being in the $|1\rangle$ state for different values of the ratio $\omega_1/\Delta\omega$

5.4.1 Dressed states and AC Stark shift

This Hamiltonian is also used in Atomic physics to describe the ground and (one) excited levels coupled by an external e.m. field (for example in the visible spectrum). The evolution of an atom in an e.m. field (here we are considering a classical e.m. field, but we will see that we can also consider the quantized version) is usually described with the *dressed atom* picture. This picture (due to Cohen-Tannoudji) describes the atom as *dressed* by a cloud of virtual photons, with which it interacts.
This atomic TLS has (unperturbed) eigenstates $|e\rangle = |0\rangle$ and $|g\rangle = |1\rangle$ with energies $E_0 - E_1 = \Delta\omega$, which are coupled through an interaction $\omega_1/2$. When we consider the optical transition of an atom we usually call ω_1 the *Rabi* frequency.
The coupling mixes these states, giving two new eigenstates as seen before with energies $\pm\omega_I = \pm\frac{\Delta\omega}{2}\sqrt{1+(\omega_1/\Delta\omega)^2}$, which is called the effective Rabi frequency.

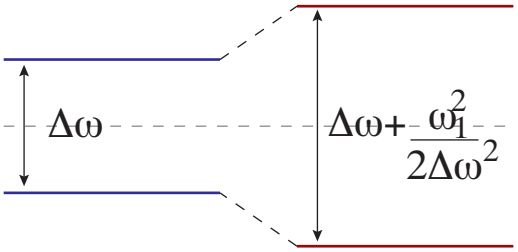

Fig. 6: Energy shift for small coupling perturbation

If the coupling is small, we can treat it as a perturbation, and the energies are just shifted by an amount $\delta E = \frac{\omega_1^2}{4\Delta\omega}$. That is, the new energies are $E_0' = \frac{\Delta\omega}{2}(1+\frac{\omega_1^2}{2\Delta\omega^2})$. This shift in the context of a two-level atom dressed by the e.m. field is called the *AC Stark shift*. It is a quadratic effect that can be seen also as arising (in a more general context) from second order perturbation theory.
The perturbed energies are shown in the following diagram. Here we explore the range of the eigenvalues $\pm\omega_I =$ found before, given a fixed value of the coupling ω_1 and a varying splitting $\Delta\omega$ between the two levels. In red are the two perturbed energies, while the dashed lines follow the unperturbed energies. For $\Delta\omega = 0$, in the absence of a coupling term, the two eigenstate are degenerate. The perturbation lifts this degeneracy, giving rise to an *avoided crossing*. The eigenstates are a complete mix of the unperturbed states, yet remain split in energy by the strength of interaction ω_1.

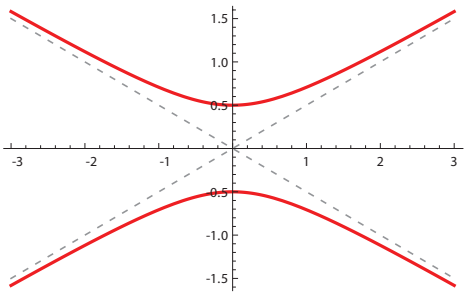

Fig. 7: Dressed atom energies as a function of the splitting $\Delta\omega$ showing the avoided crossing

5.5 The wave-function

We have so far considered systems associated to observables with a discrete spectrum. That is, the system can assume only a discrete number of states (for example 2, for the TLS) and the possible outcomes of an experiments are a discrete set of values. Although for the first part of the class this is all that we'll need, it's important to introduce as well systems with a continuous set of states, as they lead to the concept of a particle's wave function[12]. This is an essential concept in non-relativistic QM that you might has seen before (and probably as one of the very first topics in QM).

5.5.1 Position representation

The state $|\psi\rangle$ of a point-like particle is naturally expanded onto the basis made of the eigenstates of the particle's position vector operator $\mathbf{R}$. Of course the position of a point particle is a continuous variable (more precisely a vector whose components are the three commuting coordinate operators X, Y and Z). The rigorous mathematics definition of these continuous basis states is somewhat complex, so we will skip some of the details to instead obtain a practical description of the wave function. The basis states $|\mathbf{r}\rangle$ satisfy the relations generalizing the orthonormality conditions:

$$\langle \mathbf{r}|\,\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}'), \quad \int d^3\mathbf{r}\,|\mathbf{r}\rangle\,\langle\mathbf{r}| = \mathbb{1}$$

where $\delta(\mathbf{r}-\mathbf{r}')$ is the three-dimensional Dirac function. Developing $|\psi\rangle$ in the $|\mathbf{r}\rangle$ basis yields:

$$|\psi\rangle = \int d^3\mathbf{r}\,|\mathbf{r}\rangle\,\langle\mathbf{r}|\,\psi\rangle$$

where we define the wave function (in the position representation)

$$\psi(\mathbf{r}) = \langle\mathbf{r}|\,\psi\rangle$$

The shape of the wave function depends upon the physical situation under consideration. we may say that the wave function describes the state of the particle suspended, before measurement, in a continuous superposition of an infinite number of possible positions. Upon measurement of $\mathbf{R}$ performed with a linear precision δr, this superposition collapses into a small wave packet of volume $(\delta r)^3$ around a random position $\mathbf{r}$, with the probability $p(\mathbf{r}) = |\,\langle\mathbf{r}|\,\psi\rangle|^2(\delta r)^3$.

5.5.2 Momentum representation

The position representation is suited for measurements of the particle's position. If one is interested in the particle momentum $\mathbf{P}$ or velocity $\mathbf{V} = \mathbf{P}/m$ (where m is the particle mass) it is appropriate to choose the momentum

[12] For a nice introduction to these concepts, see S. Haroche, J.-M. Raimond, *Exploring the quantum: atoms, cavities and photons*, Oxford University Press (2006). In this section we follow their presentation closely.

representation and to expand $|\psi\rangle$ over the continuous basis of the momentum eigenstates $|\mathbf{p}\rangle$:

$$|\psi\rangle = \int d^3\mathbf{p}\, |\mathbf{p}\rangle \langle \mathbf{p}|\, \psi\rangle$$

where we define the wave function (in the position representation)

$$\widetilde{\psi}(\mathbf{p}) = \langle \mathbf{p}|\, \psi\rangle$$

A simple system could be describing a single particle with a well defined momentum. The state is then $|\psi\rangle = |\mathbf{p}\rangle$. In the momentum representation, we obtain the wave function $\widetilde{\psi}(\mathbf{p}) = \delta(\mathbf{p})$. We can as well describe this state in the position representation, $|\mathbf{p}\rangle = \int d^3\mathbf{r}\, |\mathbf{r}\rangle \langle \mathbf{r}|\, \mathbf{p}\rangle$. Following de Broglie's hypothesis which associates to a particle of momentum p a plane wave of wavelength $\lambda = h/p$, the momentum eigenstates are plane waves in the position representation

$$\psi_p(r) = \langle \mathbf{r}|\, \mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}.$$

We can take this as the definition itself of the momentum eigenstates; from this definition the well-known commutation relationship between position and momentum follow. Otherwise one could state the commutation relationship as an axiom and derive the form of the momentum eigenstates in the position representation.

? Question: Show how $[r_i, p_j] = i\hbar\delta_{ij} \;\Leftrightarrow\; \psi_p(r) = \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{(2\pi\hbar)^{3/2}}$

i)Hint: Show that the momentum generates translations in x and consider an infinitesimal translation.

ii)Hint: Show that $[P_x, f(x)] = -i\hbar\partial_x f(x)$.

1) We start from $\langle p_x|x\rangle = \frac{e^{-ip_x x/\hbar}}{(2\pi\hbar)^{1/2}}$. Then we have for any translation a

$$\langle p_x|x+a\rangle \propto e^{-ip_x(x+a)/\hbar} = e^{-ip_x a/\hbar}\langle p_x|x\rangle$$

We thus recognized p as the generator of translation and the corresponding propagator $U(a) = e^{-ip_x a/\hbar}$. In the Heisenberg picture, we can thus show $U(a)^\dagger x U(a) = x + a\mathbb{1}$, since $\forall|\psi\rangle$ we have

$$\langle\psi|U^\dagger(a)xU(a)|\psi\rangle = \langle\psi + a|\, x\, |\psi + a\rangle = \langle x\rangle + a.$$

Now we consider an infinitesimal translation δa. The propagator then becomes $U(\delta a) \approx \mathbb{1} - ip_x\delta a/\hbar$. Calculating again $U(\delta a)^\dagger x U(\delta a) = x + \delta a\mathbb{1}$, we obtain:

$$x + \delta a\mathbb{1} = (\mathbb{1} + ip_x\delta a/\hbar)x(\mathbb{1} - ip_x\delta a/\hbar) = x + \frac{i\delta a}{\hbar}(px - xp) + \frac{\delta a^2 p^2}{\hbar^2} = x - \frac{i\delta a}{\hbar}[x,p] + O(\delta a^2)$$

Neglecting terms in δa^2 we thus proved the commutation relationship $[x,p] = i\hbar\mathbb{1}$. □

2) Now we start from the commutation relationship $[x,p] = i\hbar$ and we calculate $[x^n, p]$. We start from the lower powers:

$$[x^2,p] = x[x,p] + [x,p]x = 2i\hbar x; \quad [x^3,p] = x[x^2,p] + [x,p]x^2 = 3i\hbar x^2; \quad [x^n,p] = ni\hbar x^{n-1}$$

Let's now consider any function of x and its commutator with p. Since by definition we can expand the function in a power series, it is easy to calculate the commutator:

$$[f(x),p] = \sum_n f^{(n)}(0)/n![x^n,p] = \sum_n f^{(n)}(0)\frac{n}{n!}i\hbar x^{n-1} = i\hbar\frac{\partial f(x)}{\partial x}$$

Notice that this is also true for the wave function: $[\hat{p}_x, \psi_p(x)] = -i\hbar\partial_x\psi_p(x) = \hat{p}\langle x|p\rangle - \langle x|p\rangle\hat{p} = p\psi_p(x)$ from which, solving the differential equation, $\langle p_x|x\rangle = \frac{e^{-ip_x x/\hbar}}{(2\pi\hbar)^{1/2}}$ (where the denominator is chosen to have a normalized function). □

5.5.3 Schrödinger equation for the wavefunction

We have studied already the law governing the evolution of a quantum system. We saw that the dynamics of the system is generated by the system Hamiltonian $\mathcal{H}$ (the observable corresponding to the total energy of the system), as described by Schrödinger equation:

$$\frac{i\hbar d|\psi\rangle}{dt} = \mathcal{H}|\psi\rangle$$

We can express this same equation in the position representation. We want to describe the evolution of a point particle in a potential $V(\mathbf{r})$ and with kinetic energy $T = \frac{P^2}{2m}$. The Hamiltonian of this simple system is thus given by $\mathcal{H} = V(\mathbf{r}) + \frac{p^2}{2m}$. By multiplying the Schrödinger equation with the bra $\langle r|$ we obtain:

$$\frac{i\hbar d\langle r|\psi\rangle}{dt} = i\hbar\partial_t\psi(r) = \langle r|\,\mathcal{H}|\psi\rangle = \langle r|\,V(r)|\psi\rangle + \langle r|\,\frac{P^2}{2m}|\psi\rangle$$

Using the relationship

$$\langle x|\,P_x^2|\psi\rangle = (P_x^2\psi)(x,t) = \left(-i\hbar\partial_x\right)^2\psi(x,t) = -\hbar^2\frac{\partial^2\psi(x,t)}{\partial x},$$

we obtain

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r},t) + V(\mathbf{r},t)\psi(\mathbf{r},t)$$

(where Δ is the Laplacian operator in 3D).

5.6 Feynman's path-integral

The formal solution of the Schrödinger equation above can be written as $|\psi(t)\rangle = U(t,0)\,|\psi(0)\rangle$. Using the position representation and the closure relation $\int d^3\mathbf{r}\,|\mathbf{r}\rangle\,\langle\mathbf{r}| = \mathbb{1}$ we can write

$$\psi(\mathbf{r},t) = \int d^3\mathbf{r}'\,\langle\mathbf{r}|\,U(t,0)\,|\mathbf{r}'\rangle\,\psi(\mathbf{r}',0),$$

where $U(t,0) = e^{-i\mathcal{H}t/\hbar}$ and the matrix element $\langle\mathbf{r}|\,U(t,0)\,|\mathbf{r}'\rangle$ is the Green function describing how a localized wave packet centered at $\mathbf{r}'$ at time $t = 0$ propagates at a later time in the potential $V(\mathbf{r})$. This equation represents the wave function of a single particle $\psi(r,t)$ as a sum of partial waves propagating from r' at time 0 to r at time t; it is thus the superposition of many different paths taken by the particle during its evolution. The probability of finding the particle at r results from a multiple-path interference process.
This picture of the wavefunction propagation can be used to give a qualitative introduction of Feynman's path-integral approach to quantum physics. We do not aim here for a rigorous derivation of that theory, only the main concepts will be presented[13].
We start by expressing the probability amplitude that a particle, initially prepared at point x_i, will pass a time t later at point x_f as the matrix element between the initial and the final state of the system's evolution operator: $\langle x_f|\,U(t,0)\,|x_i\rangle$. We expand this expression by slicing the time interval t into infinitesimal intervals δt and by introducing at each of these times a closure relationship on the position eigenstates:

$$\langle x_f|\,U(t,0)\,|x_i\rangle = \langle x_f|\,U(\delta t)^n\,|x_i\rangle =$$

$$\int dx_n..dx_k..dx_1\,\langle x_f|\,U(t,t-\delta t)\,|x_n\rangle\,\langle x_n|\ldots U(\delta t)\,|x_k\rangle\,\langle x_k|\ldots U(\delta t)\,|x_1\rangle\,\langle x_1|\,U(\delta t,0)\,|x_i\rangle$$

$$= \int dx_n..dx_1\,\langle x_k|\,U(\delta t)\,|x_{k-1}\rangle\ldots$$

[13] In this section we again closely follow the presentation in S. Haroche, J.-M. Raimond, *Exploring the quantum: atoms, cavities and photons*, Oxford University Press (2006)

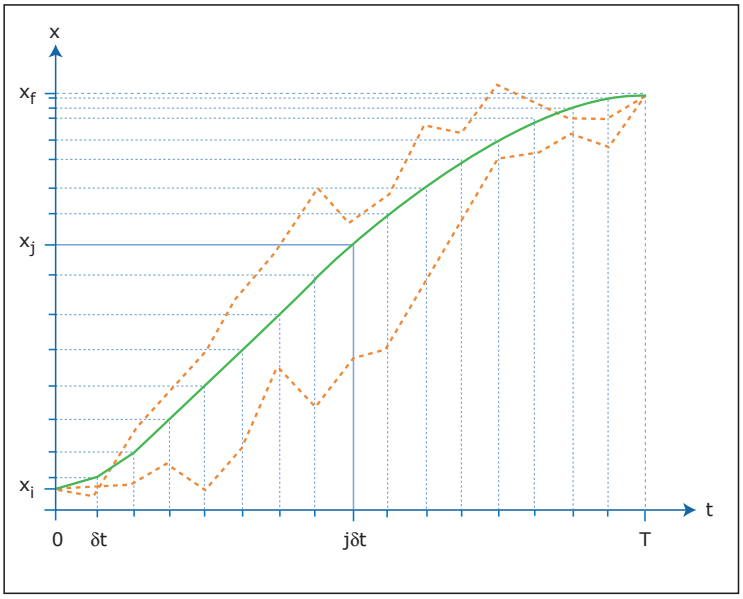

Image by MIT OpenCourseWare.

Fig. 8: Spacetime diagram of the propagation of a particle between two events. Taken from "Exploring the quantum", S. Haroche, J-M. Raimond.,

We then evaluate the amplitude $\langle x_k| U(\delta t) |x_{k-1}\rangle$ in the case $U(t) = e^{-it(p^2/2m+V)/\hbar}$. As δt is small, we can approximate it by the product of the two terms:
$U(t) = e^{-i\delta t(p^2/2m+V)/\hbar} \approx e^{-i\delta tV/\hbar}e^{-i\delta tp^2/2m\hbar} = e^{-i\delta tV/\hbar}e^{-i\delta tp^2/2m\hbar}\left(\int |p\rangle \langle p| \, dp\right)$ (where we introduced the closure expression for the momentum p). We thus obtain the integral

$$\langle x_k| U(\delta t) |x_{k-1}\rangle \approx e^{-i/\hbar V(x_k)\delta t} \int dp \; e^{i/\hbar p(x_k - x_{k-1})} e^{-i/\hbar(p^2/2m)\delta t},$$

where we used the fact $\langle x_k|p\rangle \propto e^{i/\hbar p x_k}$. The integral over p is just the Fourier transform of a Gaussian, yielding a Gaussian function of $x_k - x_{k-1}$. The probability amplitude is then

$$\langle x_f| U(t,0) |x_i\rangle \propto \int dx_1 dx_2 \dots dx_n e^{i/\hbar\delta t[\frac{1}{2}m(x_f - x_n)^2/\delta t^2 - V(x_n)]} \dots$$

$$= \int dx_1 dx_2 \dots dx_n e^{i/\hbar\delta t[mv_n^2/2 - V(x_n)]} \dots e^{i/\hbar\delta t[mv_i^2/2 - V(x_i)]}$$

where we introduced the velocity $v_k = (x_k - x_{k-1})/\delta t$. The probability amplitude for the system to go from x_i to x_f in time t is thus a sum of amplitudes one for each possible classical path - whose phase is the system's action $S = \int \mathcal{L} dt$ along the trajectory, where $\mathcal{L} = \frac{1}{2}mv^2 - V(x) = mv^2 - \mathcal{H}$ is the Lagrangian of the system. This phase is expressed in units of $\hbar$.
We have derived this important result by admitting the Schrödinger equation formalism of quantum mechanics. Feynman proceeded the other way around, postulating that a quantum system follows all the classical trajectories with amplitudes having a phase given by the classical action and has derived from there Schrödinger 's equation. At the classical limit $S/\hbar \gg 1$, the phase along a trajectory evolves very fast when the path is slightly modified, by changing for instance one of the x_j . The amplitudes of various neighboring paths thus interfere destructively, leaving only the contributions of the trajectories for which the phase, hence the action, is stationary. If the particles action in units of $\hbar$ is much larger than 1, the particle follows a classical ray. Suppressing the contributions to the amplitude coming from trajectories far from the classical one does not appreciably affect this amplitude.

22.51 Quantum Theory of Radiation Interactions

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