MITx: Atomic and Optical Physics I
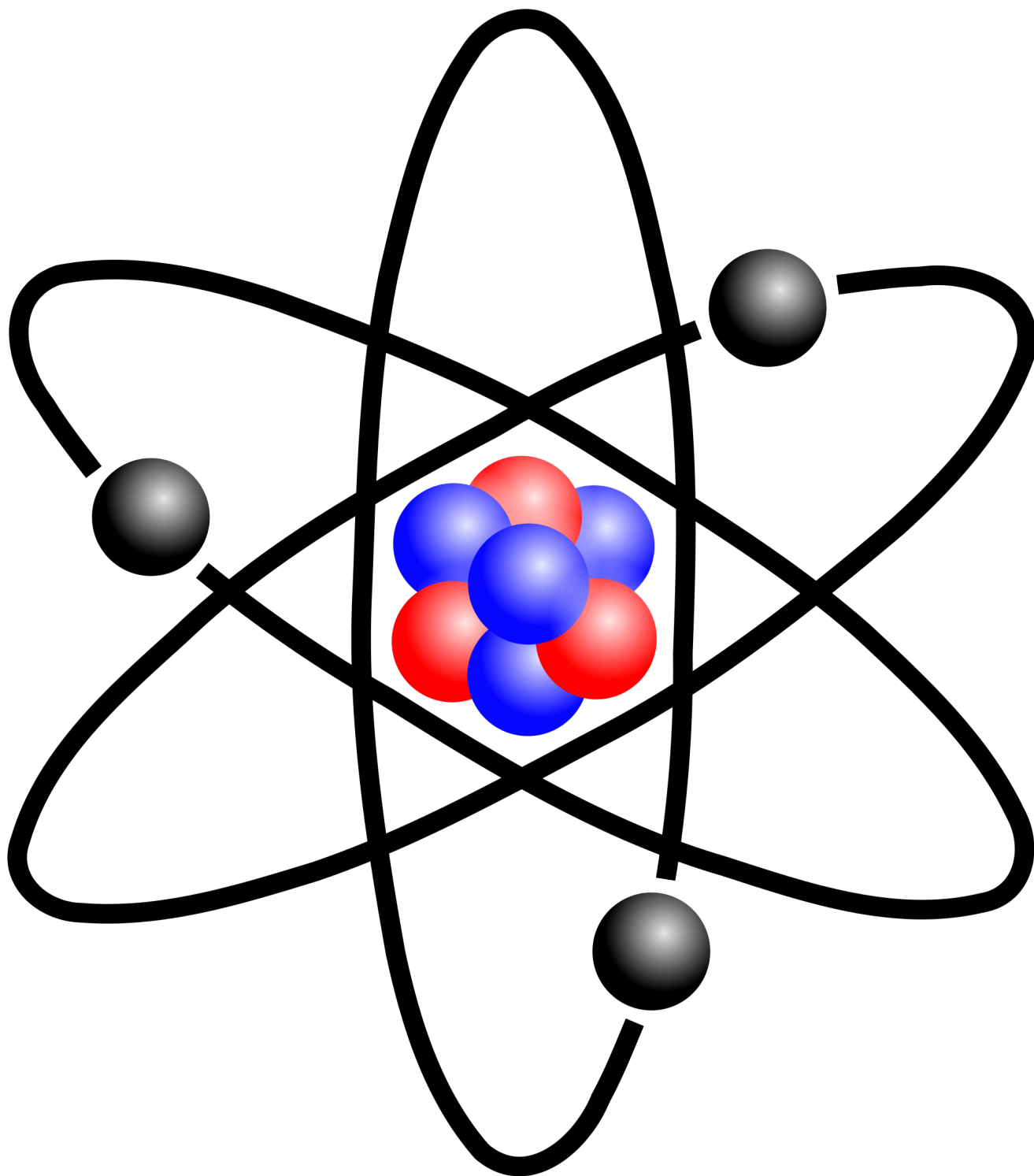
by Prof. Wolfgang Ketterle

LaTeX notes for the MITx: 8.421 Atomic and Optical Physics I MOOC

by Piotr 'Kabat' Kabacinski

Part 1: Resonance

Week 1: Classical Resonances

1 Resonances - an overview

1.1 Introduction to resonance

- Resonance - any periodic variation of some variable. When you drive a system with a variable frequency, you observe a peak at resonant frequency.

- Atomic Physics is interested with every single possible aspect of resonance. Resonance is the language physicists talk to atoms with.

- Oscillators are characterized by the sharpness of the resonance (Q - quality factor) which is a ratio of the frequency width of the resonance and its resonant frequency. Q is the number of oscillations that can be observed before the oscillation decays away.

- In Atomic Physics oscillators are characterized by extremely high Q factors

  - optical oscillators: 10^{15} Hz (light frequency) $\Rightarrow Q = 10^6$ (with doppler broadening), $Q = 10^{15}$ (without doppler broadening, eg. atom in optical lattice in metastable levels)
  - mechanical oscillators: eg. quartz $Q = 10^4$ - 10^6
  - micromechanical oscillators: $Q = 10^5$ (eg. whispering gallery mode can have $Q = 10^9$, where light circulates around the circle of the mushroom-like structure)
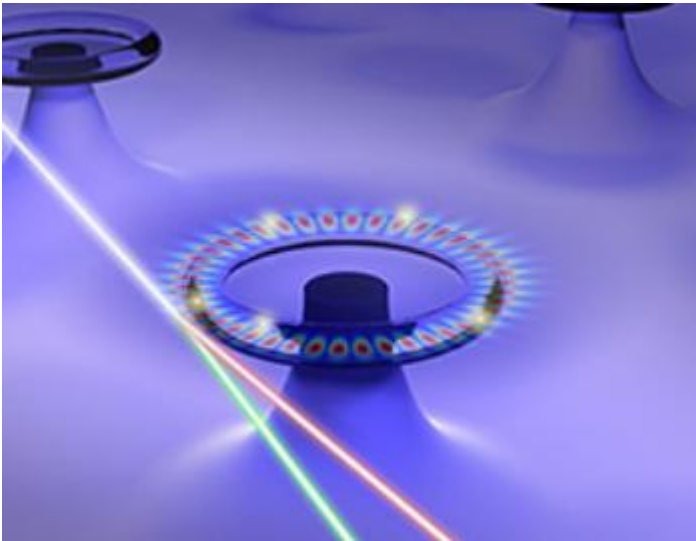
  - astronomical oscillators: earth rotation: $Q = 10^7$, neutron star: $Q = 10^{10}$

- "Useful" resonances are reproducible and connected by theory to fundamental constants.

- Rydberg constant ($R = 1.097... * 10^7 m^{-1}$) is the most accurately known constant in physics because it can be directly measured by performing spectroscopy experiments with hydrogen. Measuring fundamental constants more accurately is very important in understanding the world.

- Typical resonance lineshape is lorentzian which is proportional to $\text{Im}\left(\frac{1}{\omega_0 - \omega + i * \frac{\gamma}{2}}\right)$. For lorentzian: $\gamma =$FWHM and $Q = \frac{\omega_0}{\gamma}$.

1.2 Angular frequency units

- All parameters should be measured in angular frequency units which are technically $\frac{rad}{s}$, sometimes we use s^{-1}. Frequencies (not angular) are measured in Hz.

- Good manner is to write angular frequency as $\omega_0 = 2\pi * 1\text{MHz} = 6.28 * 10^6 s^{-1}$, *NEVER* $6.28 * 10^6$ Hz.

- Units for γ (temporal decay rate, inverse of dumping time) are s^{-1} (*NOT* Hz).

2 Resonance widths and uncertainty relations

2.1 How precisely can you measure frequencies?

- Some of the most accurate experiments in physics are done by measuring frequency.

- For oscillator oscillating for time Δt with finite width of frequency spectrum $\Delta\omega$: $\Delta\omega\Delta t \geq \frac{1}{2}$

2.2 Heisenberg limits on quantum and classical systems

- Heisenberg uncertainty relation is about single measurement on a single quantum system. To increase accuracy of the measurement it can be repeated many times or can be done on a system with many photons.

- Using nonlinear process it can be achieved for a single quantum system and a single photon utilizing many energy levels at the same time and jumping many levels at the same time. Precision of such an experiment is better by $\frac{1}{n}$ times, where n is the number of energy levels.

2.3 Frequency measurement example: atomic clocks

- Cesium atom fountain clock, $\omega = 2\pi * 10\text{GHz}$, interrogation time $\Delta t = 1\text{s}$ has fractional linewidth $\frac{\Delta\omega}{\omega} = 10^{-11}$. Accuracy of the best cesium fountains is now 10^{-16}.

- Strontium optical clock - extremely narrow transition. Accuracy $6 * 10^{-18}$!

3 Harmonic oscillators and two-level systems

3.1 Harmonic oscillators vs. two-level systems

- Two-level system is a system with 2 levels. Harmonic oscillator is a system with infinite number of equidistant levels.

- When some energy is put into the second state of HO, some small energy also goes into every higher level. In two-level system there are no higher levels than second one, so nothing can go higher.

- Quantum system can be described as a harmonic oscillator for weak excitation (when there is small energy in excited state).

- Two-level system can be saturated (harmonic oscillator can never be saturated). When the second energy level is full adding more energy can't go higher. If a two-level system is not saturated, it behaves like a harmonic oscillator so it behaves completely classical.

3.2 Rotating systems vs. 2-level systems

- Precessing gyroscope has a bound on amplitude. Motion of classical magnetic moments provides a model which captures almost all features of the quantum mechanical two-level system (except for projection, quantum measurement).

4 Classical magnetic moment in a uniform field

4.1 Magnetic resonance

- Gyromagnetic ratio (γ) is a ratio between magnetic moment and angular momentum ($\boldsymbol{\mu} = \gamma \mathbf{L}$). From that we can find that derivative of angular momentum is given by: $\dot{\mathbf{L}} = \gamma \mathbf{L} \times \mathbf{B}$. Solution of that equation is a pure precession of $\mathbf{L}$ around $\mathbf{B}$. Precession around the $\mathbf{B}$ is happening at the constant tipping angle with an angular frequency called Larmor frequency $\Omega_L = -\gamma B$.
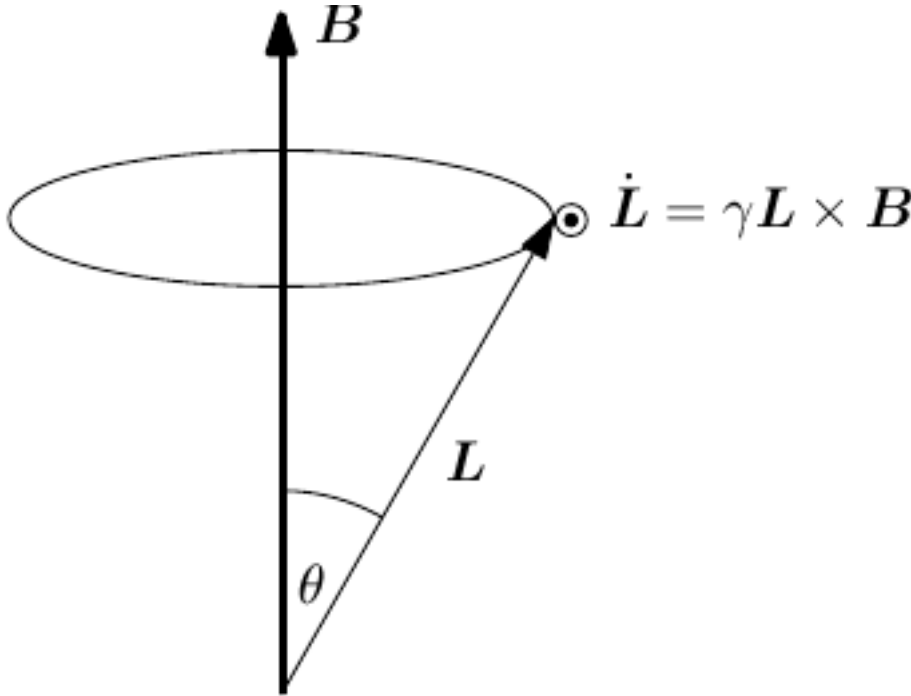
- For an electron $\gamma_e = 2\pi * 2.8\text{MHz/G}$. For classical charge distribution (of particles with the same charge to mass ratio as electrons) gyromagnetic ratio is a half of that: $\gamma = 2\pi * \mu_B$ (where $\mu_B = 1.4\text{MHz/G}$ and is called Bohr magneton).

- Proton is heavier than the electron ($\frac{m_p}{m_e} = 1836.153$) and therefore $\gamma_P = 2\pi * 4.2\text{kHz/G}$.

- The magnetic moment of the electron is 1 Bohr magneton.

- Precession frequency of a system depends on energy difference of two neighbouring energy levels.

4.2 Rotating coordinate transform for equations of motion of a classical magnetic moment

- Going into rotating frame is useful to solve certain problems.

- Rotating vector $\mathbf{A}$ which rotates with a constant angular frequency $\boldsymbol{\Omega}$ is described by: $\dot{\mathbf{A}} = \boldsymbol{\Omega} \times \mathbf{A}$.

- When we view the system in a coordinate system rotating at $\boldsymbol{\Omega}$ then derivatives of the vector $\mathbf{A}$ in rotating and inertial frames are related by: $\dot{\mathbf{A}}_{\mathbf{in}} = \dot{\mathbf{A}}_{\mathbf{rot}} + \boldsymbol{\Omega} \times \mathbf{A}_{\mathbf{in}}$. From that follow two special cases:

  - If $\mathbf{A}$ is constant in the rotating system then: $\dot{\mathbf{A}}_{\mathbf{in}} = \boldsymbol{\Omega} \times \mathbf{A}_{\mathbf{in}}$.
  - If rotating frame is not rotating ($\boldsymbol{\Omega} = 0$) then: $\dot{\mathbf{A}}_{\mathbf{in}} = \dot{\mathbf{A}}_{\mathbf{rot}}$.

- From above there can be derived an operator equation for transforming a vector from inertial to rotating frame: $\left(\frac{d}{dt}\right)_{\text{rot}} = \left(\frac{d}{dt}\right)_{\text{in}} - \boldsymbol{\Omega} \times ()_{\text{in}}$.

- We can apply this operator equation to angular momentum vector $\mathbf{L}$ and we get:
  $\dot{\mathbf{L}}_{\mathbf{rot}} = \gamma \mathbf{L}_{\mathbf{in}} \times (\mathbf{B} + \mathbf{B}_{\mathbf{fict}})$, where $\mathbf{B}_{\mathbf{fict}} = \frac{\Omega}{\gamma}$.

- If we choose the rotating frequency to be Larmor frequency $\boldsymbol{\Omega} = \boldsymbol{\Omega}_{\mathbf{L}} = -\gamma\mathbf{B}$ then our effective magnetic field $\mathbf{B}_{\mathbf{eff}} = \mathbf{B} + \mathbf{B}_{\mathbf{fict}} = 0$ and because in that situation there is no magnetic field, we know that angular momentum $\mathbf{L}$ is constant in the rotating frame. To get the knowledge what happens in the real frame the answer has to be 'rotated back'.

- For classical charge distribution (of electrons) forming magnetic moment, Larmor frequency at which magnetic moment of the distribution is precessing is: $\Omega_L = \frac{e}{2m}B$. Frequency of the cyclotron motion for free electron in a magnetic field is twice that: $\Omega_{cyclotron} = \frac{e}{m}B$.

4.3   Rotating magnetic field on resonance

- We put a magnetic moment in a time-dependent field: $\mathbf{B}(t) = B_1(\hat{e}_x cos\Omega_L t - \hat{e}_y sin\Omega_L t) + B_0 \hat{e}_z$
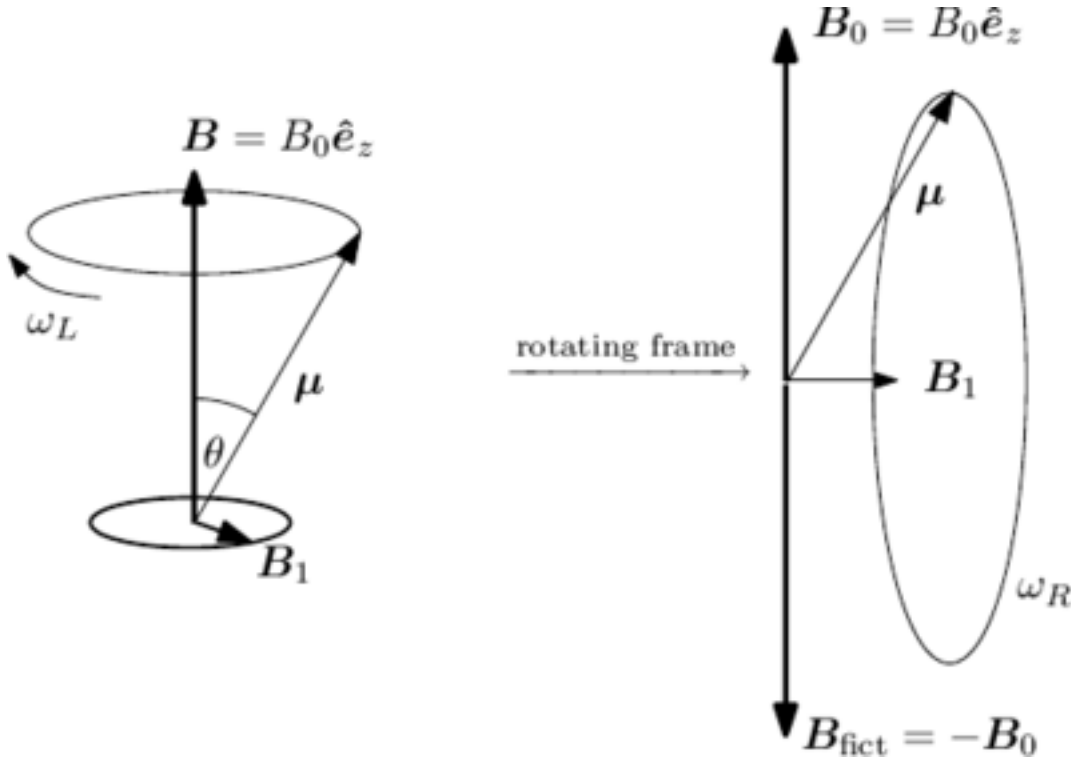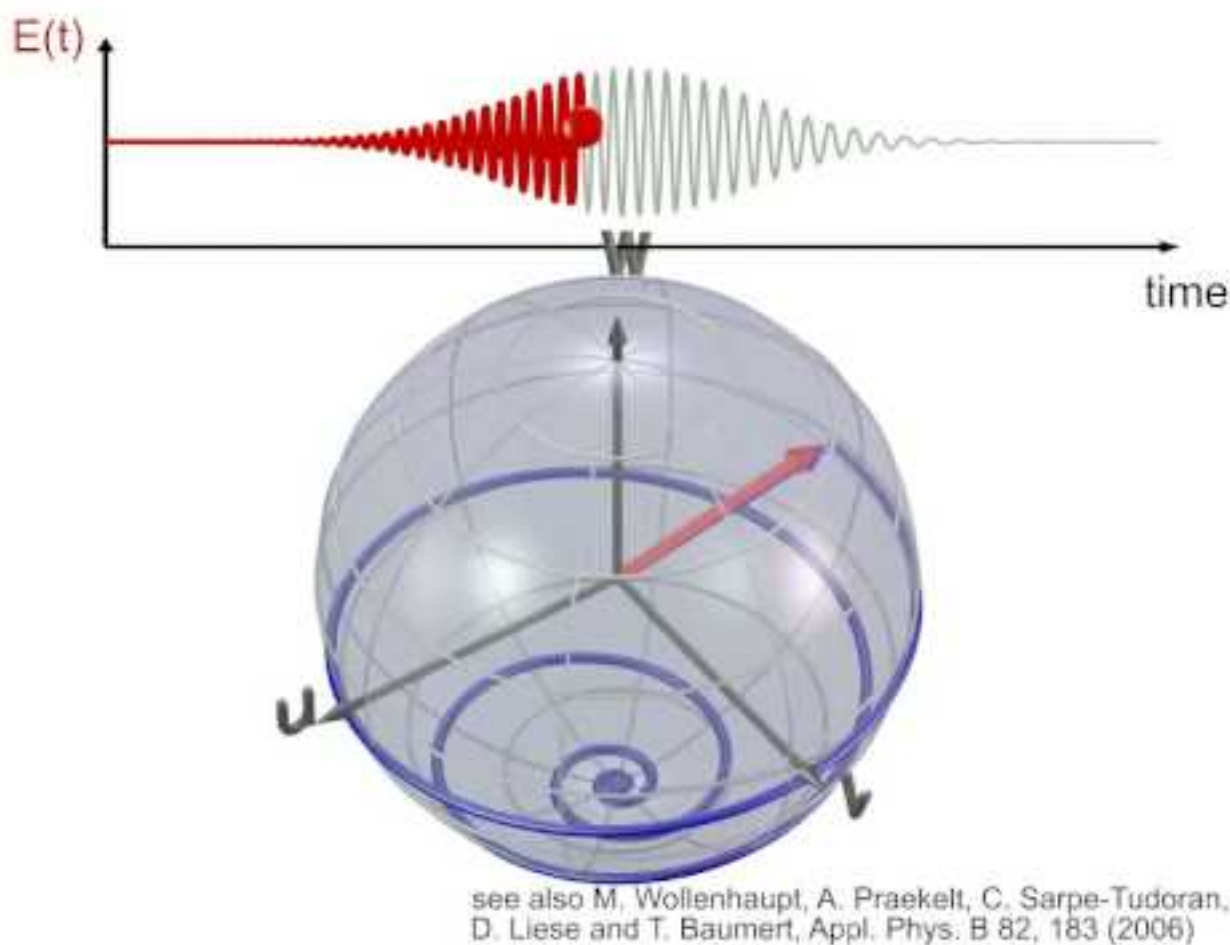

- In the frame rotating with Larmor frequency we have: $\mathbf{B}_{\mathbf{eff}}(t) = \mathbf{B}(t) - \frac{\Omega_L}{\gamma}\hat{e}_z = B_1\hat{e}_{x'}$, where $\hat{e}_{x'} = \hat{e}_x cos(\Omega_L t) - \hat{e}_y sin(\Omega_L t)$. Therefore in the rotating frame we have a static field of value B_1, and we know that in the static magnetic field magnetic moment is just precessing around the field vector with the Rabi frequency $\omega_R = \gamma B_1$.

- If we start with the magnetic moment aligned with the z-axis (at $t = 0$ $\mu = \mu\hat{e}_z$), after half a Rabi cycle the magnetic moment will be inverted (at $t = \frac{\pi}{\omega_R}$ $\mu = -\mu\hat{e}_z$). This is called π pulse, because it rotates a spin by π or we can call it a 'spin flip'.

- For the off-resonant case, the field in the z direction will not be canceled and the resulting field $\mathbf{B}_{\mathbf{eff}}$ is a sum of the field in the z direction and the rotating field. The magnetic moment precesses at generalized Rabi frequency: $\Omega_R = \gamma B_{eff} = \sqrt{\omega_R^2 + (\omega_L - \omega)^2} = \sqrt{\omega_R^2}$. Therefore the generalized Rabi frequency is the resonant Rabi frequency added in quadrature with the detuning from resonance. When the rotating field is at frequency lower or higher than the Larmor frequency, oscillation frequency of the magnetic moment will be larger than the resonant Rabi frequency. Driving the system off-resonance, the spin will never fully invert.

- Classical magnetic moment time dependence while in a magnetic field rotating at the generalized Rabi frequency: $\mu_z(t) = \mu \left(1 - 2\frac{\omega_R^2}{\Omega_R^2} \sin^2 \frac{\Omega_R t}{2}\right)$. This result is correct in quantum-mechanical treatment and the spin flip probability is: $P = \frac{\omega_R^2}{\Omega_R^2} \sin^2 \frac{\Omega_R t}{2}$.

4.4 Rapid adiabatic passage

- Rapid (compared to decoherence and relaxation processes) adiabatic passage is a technique for inverting spins by slowly (compared to the Larmor frequency) sweeping the frequency of the drive field across the resonance. As the frequency of the rotating field is increased, the effective field changes its position from pointing up to pointing in the x-direction on resonance to pointing down after the process. As the precession around the effective magnetic field is at small angle and is happening fast compared to the frequency change, the magnetic moment is moved down together with the field and after the process is complete, the magnetic moment points downwards.

see also M. Wollenhaupt, A. Praekelt, C. Sarpe-Tudoran, D. Liese and T. Baumert, Appl. Phys. B 82, 183 (2006)

[Visualization of a spin flip with chirped femtosecond laser pulses](#)

- Adiabaticity condition is: $|\dot{\omega}| \ll \omega_R^2$.

- It doesn't matter if we start with low frequency and sweep to high or start with high and sweep to low, the effect is the same.

- This technique is easier to use than π pulse because in π pulse you have to be exactly at resonance, and with RAP you just sweep across it.

- Similar process is used in magnetic trap experiments (quadrupole traps).

Week 2: Quantized Spin in a Magnetic Field

5 Equation of motion for the expectation value

### 5.1 Quantized spin in a magnetic field

- Everything we have learned about classical magnetic moment exactly applies to quantum version.

- Hamiltonian for an atom in a magnetic field: $H = -\mu \mathbf{B_0} = -\gamma \mathbf{L_z} B_0$.

- Heisenberg equation of motion for any operator: $\frac{d\hat{O}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{O}]$.

- Using the above equation and the hamiltonian we get simple equation of motion for the system: $\frac{d\hat{\mu}}{dt} = \gamma \hat{\mu} \times \mathbf{B}$. It looks exactly as a classical result and is valid for any value of spin.

- Any two-level system can be regarded as spin $\frac{1}{2}$ system and it just precesses (unless magnetic field is very strong).

- Valid for a system of N two-level systems $\Rightarrow$ Dicke superradiance.

  Superradiance is a phenomenon of collective emission of an ensemble of excited atoms or ions, first considered by Dicke. It is similar to superfluorescence, but it starts with the coherent excitation of the ensemble, usually with an optical pulse. This coherence (i.e. a well-defined phase relationship between the excitation amplitudes of lower and upper electronic states) leads to a macroscopic dipole moment. The maximum intensity of the emitted light scales with the square of the number of atoms, because each atom contributes a certain amount to the emission amplitude, and the intensity is proportional to the square of the amplitude. As the number of photons rises in a kind of chain reaction, Dicke later (in a patent application) described the phenomenon of superradiance as an optical bomb. Link to the Dicke's paper.

6 The two-level system: spin $\frac{1}{2}$

6.1 Two-level system - spin $\frac{1}{2}$ Rabi oscillations

- An electron in a magnetic field is in its ground state while being anti-aligned with the field (it has lower energy than when being aligned) because the electron has negative gyromagnetic ratio.

- Probability to find the system in the excited state at time t if it was in ground state at time $t = 0$ (Rabi transition probability): $P = \frac{\omega_R^2}{\Omega_R^2} \sin^2 \frac{\Omega_R t}{2}$.
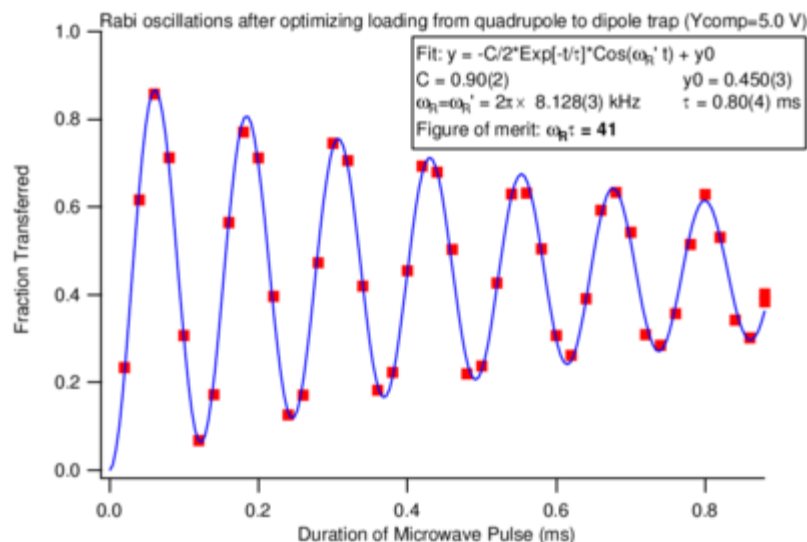
6.2 Two-level system Hamiltonian

- The famous 'dressed atom' Hamiltionian in the so called 'rotating wave approximation':

$$\hat{H} = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_R e^{-i\omega t} \\ \omega_R e^{i\omega t} & -\omega_0 \end{pmatrix}$$

  That expression is exact. Its eigenstates and eigenvalues provide a very elegant, very intuitive solution to the two-state problem. It describes two-level system + one mode of the e-m field with arbitrary amplitude.

- The Hamiltonian can be easily solved after the unitary transformation: $R = \begin{pmatrix} e^{\frac{i\omega t}{2}} & 0 \\ 0 & e^{-\frac{i\omega t}{2}} \end{pmatrix}$ which
  is a rotation operator and it makes the problem time independent. After the transformation we get
  a Hamiltonian: $\hat{H}' = \frac{\hbar}{2} \begin{pmatrix} \delta & \omega_R \\ \omega_R & \delta \end{pmatrix}$ (where $\delta = \omega_0 - \omega$ is a detuning) that can be easily solved and
  we get the same answer as before (Rabi transition probability).

7 Rapid adiabatic passage - quantum treatment

7.1 Rapid adiabatic passage and Landau-Zener transitions

- We can use previous results to make a graph. The dashed line comes from the basic Hamiltonian and the curves are caused by the driving Hamiltonian.
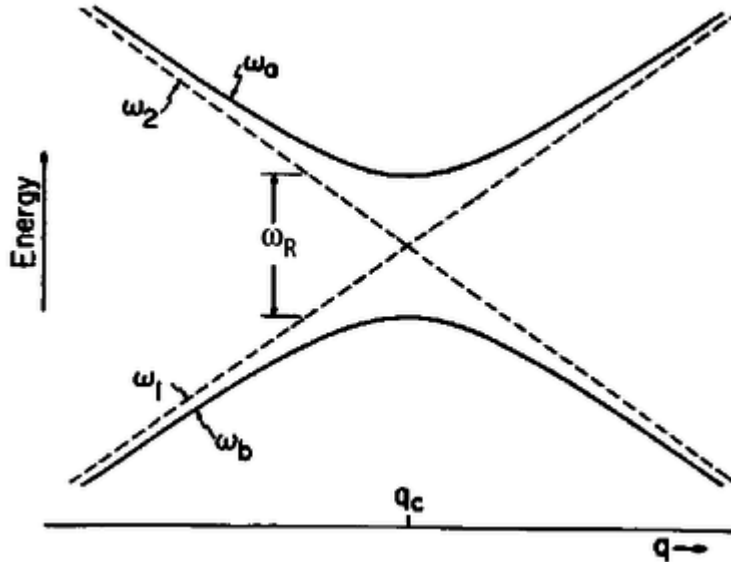
- When we sweep the frequency ω at a rate $\dot{\omega}$ through the resonance (change δ) we realize Landau-Zener problem of a sweep through the avoided crossing which is a quantum mechanical description of rapid adiabatic passage. Probability of a jump at the crossing that happens when the sweep is sufficiently rapid is: $P = e^{-2\pi\Gamma}$ where $\Gamma = \frac{1}{4}\frac{\omega_R^2}{\dot{\omega}}$ is the Landau-Zener parameter. Adiabaticity requires that $\frac{\omega_R^2}{\dot{\omega}} \gg 1$. The process is coherent.

Week 3: Resonance and Decoherence Processes

8 Resonance in a QM System: Density Matrix Formalism

8.1 Density matrices - review

- We cannot describe processes like decoherence or loss of particles with Shroedinger equation as it deals only with pure states. The exception is when you have two states and all what happens is a loss to some other levels. Then Hamiltonian description can be used but eigenvalues have to be replaced by complex numbers. For processes like spontaneous emission density matrix approach have to be used.

- If we have a time dependent wave function:

$$|\Psi(t)\rangle = \sum_n c_n(t) |\Psi_n\rangle$$

then we can define arbitrary operators by matrices: $A_{nm} = \langle \Psi_n | \hat{A} | \Psi_m \rangle$. Expectation value of the operator is:

$$\left\langle \hat{A} \right\rangle_t = \langle \Psi(t) | \hat{A} | \Psi(t) \rangle = \sum_{m,n} c^*{}_m(t) c_n(t) A_{nm} = \sum_{m,n} \rho_{nm}(t) A_{nm} = Tr(\hat{\rho}(t)\hat{A})$$

with $\hat{\rho}(t) = |\Psi(t)\rangle \langle \Psi(t)|$ and the matrix element given by: $\rho_{nm} = c^*_m(t) c_n(t)$. The diagonal matrix elements ρ_{nn} are called the populations and the off-diagonal matrix elements ρ_{mn} are called coherences.

When we include the probabilites of being in a certain state to the density matrix description we get:

$$\hat{\rho}(t) = \sum_i P_i |\Psi(t)\rangle \langle \Psi(t)|$$

$$\left\langle \hat{A} \right\rangle_t = Tr(\hat{\rho}(t)\hat{A})$$

and we have two averages here; one is quantum mechanical expectation value and the other one is ensemble average with probability P_i.

- Using the Shroedinger equation we can derive an equation for density matrix:

$$i\hbar\dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]$$

.

- Properties of the density matrix:
$$Tr(\hat{\rho}) = \sum_i P_i = 1$$

$$Tr(\hat{\rho}^2) = \sum_i P_i^2 \leq 1,$$

for pure states:
$$Tr(\hat{\rho}^2) = \sum_i P_i^2 = 1.$$

Density matrix operator is hermitian.

- We want to use the density matrix for non-unitary time evolution. This is often the situation for smaller system that is open for a bigger system, where we limit our description to a small part of a larger system.

8.2   Density matrices formalism for arbitrary two-level systems

- The most general Hamiltonian for the most general two-level system can be constructed from Pauli matrices and the identity matrix. By appropriately shifting the zero-point energy we can use only Pauli matrices and we get:

$$\hat{H} = \frac{\hbar}{2}(\omega_1\hat{\sigma}_x + \omega_2\hat{\sigma}_y + \omega_3\hat{\sigma}_z) = \frac{\hbar}{2}\boldsymbol{\omega}\cdot\hat{\boldsymbol{\sigma}}$$

- We describe two-level systems by density matrice which is also 2x2 matrix. The most general density matrix can also be expanded into those basic matrices. This time we can't throw away identity matrix because then there would be no trace and therefore no probability to find the particle.

$$\hat{\rho} = \frac{1}{2}(r_0\hat{\mathbb{I}} + r_1\hat{\sigma}_x + r_2\hat{\sigma}_y + r_3\hat{\sigma}_z) = \frac{1}{2}(\hat{\mathbb{I}} + \mathbf{r}\cdot\hat{\boldsymbol{\sigma}}),$$

  because $Tr(\hat{\rho}) = r_0 = 1$. Vector $\mathbf{r}$ is called the Bloch vector.

- We can insert those above formulas into the equation of motion to get:

$$\dot{\mathbf{r}} = \boldsymbol{\omega} \times \mathbf{r}$$

  This equation tells us that an arbitrary two-level system with an arbitrary Hamiltonian can be regarded as a system where we have a vector $\mathbf{r}$ which undergoes precession.

- Pure state will state pure forever, because: $Tr(\hat{\rho}^2) = \frac{1}{2}[r_0^2 + |\mathbf{r}|^2] = const$. This is because $r_0 = 1$ and from the equation of motion we get that the length of the vector is not changing. This does not describe loss of coherence (decoherence).

9   Relaxation and the Bloch Equations

9.1   Relaxation - the Bloch equations

- Everything has to come to thermal equilibrium if we will wait for ever. So after long time the density matrix will thermalize to: $\hat{\rho}^T = \frac{1}{Z}e^{-H_0/kT}$ where Z is a partition function. No matter with what density matrix we start there will be some relaxation process which will restore $\hat{\rho}$ to the thermal equilibrium $\hat{\rho} = \hat{\rho}^T$.

- We can add damping in a phenomenological way by adding a term which will damp the density matrix to the thermal equilibrium density matrix with equilibration time T_e:

$$\dot{\hat{\rho}} = \frac{1}{i\hbar}[\hat{H}, \hat{\rho}] - \text{''}\frac{\hat{\rho} - \hat{\rho}^T}{T_e}\text{,''}$$

  the added relaxation term will have no influence on the density matrix when it is in equilibrium.

- In many cases there are TWO relaxation times T_1 and T_2. T_1 is a damping time for population differences (described by r_3 component of the Bloch vector), it is the energy decay time. The off-diagonal components r_1 and r_2 correspond to coherences and they are only non-zero if you have two states populated with a well-defined relative phases. When the quantum mechanical system looses its memory of the phase, r_1 and r_2 components go to zero. Therefore the time T_2 is a time that describes the loss of coherence, the dephasing time. In general $T_2 < T_1$ (often by a lot).

- Using the times T_1 and T_2 we can now write the Bloch equations in a proper way:

$$\dot{r}_z = (\boldsymbol{\omega} \times \mathbf{r})_z - \frac{r_z - r_z^T}{T_1}$$

$$\dot{r}_{x,y} = (\boldsymbol{\omega} \times \mathbf{r})_{x,y} - \frac{r_{x,y} - r_{x,y}^T}{T_2}$$

- The addition of phenomenological decay times does not generalize the density matrix enough to cover situations where atoms (possibly state-selected) are added or lost to a system. This situation can be covered by the addition of further terms to $\dot{\rho}$. Thus a calculation on a resonance experiment in which state-selected atoms are added to a two-level system through a tube which also permits atoms to leave (e.g. a hydrogen maser) might look like:

$$\dot{\rho} = \frac{1}{i\hbar}[H, \rho] - \begin{pmatrix} (\rho_{11} - \rho_{11T})/T_1 & \rho_{12}/T_2 \\ \rho_{21}/T_2 & (\rho_{22} - \rho_{22T})/T_1 \end{pmatrix} + R \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} - \rho/T_{\text{escape}} - \rho/T_{\text{collision}}$$

where R is the rate of addition of state-selected atoms. The last two terms express effects of atom escape from the system and of collisions (e.g. spin exchange) that can't easily be incorporated in T_1 and T_2.

The terms representing addition or loss of atoms will not have zero trace, and consequently will not maintain $Tr(\hat{\rho}) = 1$. Physically this is reasonable for systems which gain or lose atoms; the application of the density matrix to this case shows its power to deal with complicated situations. In most applications of the above equation, one looks for a steady state solution (with $\dot{\rho} = 0$), so this does not cause problems.

- Every process which contributes to T_1 will also contribute to T_2 but there are lots of processes which only contribute to T_2. Therefore in general T_2 is much faster because many more process contribute to it. T_1 is the time to damp population and that is a damping of $|\Psi|^2$. T_2 is due to the damping of the phase and this is more of a time of the wavefuction itself (Ψ). So if the only process that is happening is eg. spontaneous emission T_1 can be faster than T_2 (when it is defined as above). With our definition of T_1 and T_2 more proper way of comparing the times is: $\frac{T_2}{2} \leq T_1$.