Two level systems and Einstein A and B coefficients

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We have been exclusively studying harmonic oscillators, which are always in the *correspondence limit* displaying only mundane quantum effects [1]. The average value of the generalized position and momentum follows the classical equations of motion and quantum mechanical features manifest themselves in higher moments like the variance of those basic quantities. To see more direct and interesting quantum effects it requires non-linear components, that is, anharmonic oscillators. We will learn how anharmonic oscillators are treated as two level systems and how they behave when they are coupled to the omnipresent Ohmic envionment.

I. TWO LEVEL SYSTEMS

A. Anharmonic potential and energy-level spacing [2]

Let us begin by examining energy-level spacings for systems with anharmonic potentials. Imagine a particle with mass m moving under a 1-dimensional potential $U(x) = A|x|^k$. Since the energy is given by

$$E = \frac{m}{2}\dot{x}^2 + U(x), \tag{1}$$

we have

$$\frac{dx}{dt} = \sqrt{\frac{2}{m}\left(E - U(x)\right)}. \tag{2}$$

Integration of Eq. (2) leads to

$$t = \sqrt{\frac{m}{2}} \int \frac{dx}{\sqrt{E - U(x)}} + const. \tag{3}$$

From Eq. (3) the oscillation period for the particle trapped in the potential $U(x) = A|x|^k$ can be found to be

$$\begin{aligned} T &= 4\sqrt{\frac{m}{2}} \int_0^{\left(\frac{E}{A}\right)^{\frac{1}{k}}} \frac{dx}{\sqrt{E - Ax^k}} \\ &= 2\sqrt{2m} A^{-\frac{1}{k}} E^{\frac{1}{k}-\frac{1}{2}} \int_0^1 \frac{dy}{\sqrt{1 - y^k}} \\ &\propto E^{\frac{1}{k}-\frac{1}{2}}, \end{aligned} \tag{4}$$

where the upper limit of the integral $\left(\frac{E}{A}\right)^{\frac{1}{k}}$ in the first line comes from the turning-point condition $E = Ax^k$. We thus recognize the peculiarity of the harmonic potential ($k = 2$), that is, $T = const.$, or rather

$$\Delta E = \hbar\omega = \hbar\frac{2\pi}{T} = const. \tag{5}$$

On the other hand, the oscillation periods for anharmonic potentials depend on their energies. For instance, the oscillation period for a potential $U(x) = -A|x|^{-1}$ responsible associated with the *inverse square law* $F(x) = A|x|^{-2}$ is $T \propto (-E)^{-\frac{3}{2}}$ (note that the minus sign before E coming from the fact that the E is *negative* for the case of $k < 0$),

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that for a triangular potential $U(x) = A|x|$ is $T \propto E^{\frac{1}{2}}$, and that for the infinitely deep wall potential $U(x) = \left(\frac{x}{l}\right)^{\infty}$ is $T \propto E^{-\frac{1}{2}}$. These findings lead to

$$\begin{cases} \Delta E_{inv} = \hbar\omega = \hbar\frac{2\pi}{T} \propto (-E)^{\frac{3}{2}} & \text{for } U(x) = -A|x|^{-1} \\ \Delta E_{tri} = \hbar\omega = \hbar\frac{2\pi}{T} \propto E^{-\frac{1}{2}} & \text{for } U(x) = A|x| \\ \Delta E_{wall} = \hbar\omega = \hbar\frac{2\pi}{T} \propto E^{\frac{1}{2}} & \text{for } U(x) = \left(\frac{x}{l}\right)^{\infty}. \end{cases} \tag{6}$$

B. Bohr's atom [3, 4]

A very basic non-linear component in the microscopic world is an atom. Now let us see how does Bohr's atom exemplify the anharmonic quantum paradigm. Suppose that an electron is orbiting the atomic nucleus in a circle. The radius r is determined by the balance between the *centrifugal force* $m_e\boldsymbol{\Omega}\times(\boldsymbol{r}\times\boldsymbol{\Omega}) = \frac{m_e v^2}{r}\boldsymbol{e_r}$ and the *inverse-square-law Coulomb force* $\frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2}\boldsymbol{e_r}$, that is,

$$\frac{m_e v^2}{r} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2}. \tag{7}$$

The total energy is given by

$$E = \underbrace{\frac{1}{2}m_e v^2}_{\text{Kinetic energy:T}} + \underbrace{-\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}}_{\text{Potential energy:U}}. \tag{8}$$

Since, from the *virial theorem* [2], the average kinetic energy $\bar{T}$ can be obtained by

$$2\bar{T} = k\bar{U} \tag{9}$$

for the potential $U(r) = -Ar^k$, we have

$$\begin{aligned} \bar{T} &\equiv \frac{1}{2}m_e\bar{v^2} \\ &= (-1)\frac{\bar{U}}{2} \equiv \frac{1}{4\pi\epsilon_0}\frac{e^2}{2\bar{r}}, \end{aligned} \tag{10}$$

whose validity can also be checked by Eq. (7). The average total energy can then be written as

$$\bar{E} = \bar{T} + \bar{U} = \frac{\bar{U}}{2} = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{2r}. \tag{11}$$

Now the *quantization of the angular momentum* imposes

$$m_e v r = n\hbar. \tag{12}$$

Using Eqs. (7) and (12) the *quantized radius* is obtained as

$$r_n = \frac{\hbar^2}{\frac{e^2}{4\pi\epsilon_0}m_e}n^2 = a_0 n^2, \tag{13}$$

where

$$a_0 = \frac{\hbar^2}{\frac{e^2}{4\pi\epsilon_0}m_e} \sim 0.53 \times 10^{-10}\ \text{m} \tag{14}$$

is the *Bohr radius*, a typical length scale in atomic physics, which is made up of fundamental constants. Plugging Eq. (13) into Eq. (11) leads to the famous Bohr formula:

$$E = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{2a_0}\frac{1}{n^2} = -\frac{Ry}{n^2}, \tag{15}$$

where

$$Ry \equiv 2\pi\hbar c R_\infty = \frac{1}{4\pi\epsilon_0}\frac{e^2}{2a_0} = \frac{e^4 m_e}{8(2\pi\hbar)^2\epsilon_0^2} \sim 13.6 \text{ eV} \tag{16}$$

is the *Rydberg characteristic energy*, a typical energy scale in atomic physics, which is again made up of fundamental constants.

Let us now see the anharmonic nature of Bohr's atom. For $n \gg 1$ the energy spacing ΔE_n between E_{n+1} and E_n is given by

$$\begin{aligned}
\Delta E_n = E_{n+1} - E_n &= -Ry\left(\left(\frac{1}{n+1}\right)^2 - \left(\frac{1}{n}\right)^2\right) \\
&\sim \frac{2Ry}{n^2(n+2)} \\
&\sim \frac{2Ry}{n^3}\left(= \frac{\partial E}{\partial n}\right) \\
&= \frac{2Ry}{\left(-\frac{Ry}{E_n}\right)^{\frac{3}{2}}} \propto (-E_n)^{\frac{3}{2}},
\end{aligned} \tag{17}$$

which agrees with the general classical result Eq. (6) for the potential associated with the inverse-square-law force.

We shall now introduce one more useful constant, the *fine-structure constant*:

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} = \frac{e^2}{2\epsilon_0 hc} = \frac{1}{2}\left(\frac{1}{\frac{h}{e^2}}\right)\left(\frac{1}{c\epsilon_0}\right) = \frac{1}{2}\frac{Z_{vac}}{R_k} \sim \frac{1}{137}, \tag{18}$$

where

$$R_k = \frac{h}{e^2} \sim 25.8 \text{ k}\Omega \tag{19}$$

$$Z_{vac} = \frac{1}{c\epsilon_0} = \sqrt{\frac{\mu_0}{\epsilon_0}} \sim 377 \text{ k}\Omega \tag{20}$$

are the *impedance quantum* (or the *von Klitzing constant*) and the *impedance of vacuum*, respectively. With the fine-structure constant α, the Bohr radius a_0 and the Rydberg characteristic energy Ry can be rewritten as more meaningful forms whose dimensions manifest themselves with fundamental constants:

$$a_0 = \frac{1}{\alpha}\frac{\hbar}{m_e c} \tag{21}$$

$$Ry = \frac{\alpha^2}{2} m_e c^2. \tag{22}$$

C. Quantum description of two level systems

1. Pauli operators

The system with anharmonic potential can be treated as the *two level system* by exploiting the fact that each energy spacing is unique thus by choosing two *distinct* energy levels $|0\rangle$ and $|1\rangle$, which are the energy eigenstates with energies $\hbar\omega_0$ and $\hbar\omega_1 > \hbar\omega_0$, respectively. The useful operators for the two level systems are the Pauli operators

$$\hat{\sigma}_0 = |0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{23}$$

$$\hat{\sigma}_x = |1\rangle\langle 0| + |0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{24}$$

$$\hat{\sigma}_y = -i|1\rangle\langle 0| + i|0\rangle\langle 1| = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{25}$$

$$\hat{\sigma}_z = -|0\rangle\langle 0| + |1\rangle\langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{26}$$

which satisfy the angular momentum commutation relation ($SU(2)$ algebra)

$$[\frac{\hat{\sigma}_i}{2}, \frac{\hat{\sigma}_j}{2}] = i\epsilon_{ijk}\frac{\hat{\sigma}_k}{2}, \tag{27}$$

where ϵ_{ijk} is the *structure constant* of $SU(2)$. Thus $\frac{\hat{\sigma}_x}{2}$, $\frac{\hat{\sigma}_y}{2}$, and $\frac{\hat{\sigma}_z}{2}$ form the *spin-$\frac{1}{2}$-representation* of $SU(2)$ algebra. We shall also define here the raising and lowering operators as

$$\hat{J}^+ = \frac{1}{\sqrt{2}}\left(\frac{\hat{\sigma}_x}{2} + i\frac{\hat{\sigma}_y}{2}\right) \tag{28}$$

$$\hat{J}^- = \frac{1}{\sqrt{2}}\left(\frac{\hat{\sigma}_x}{2} - i\frac{\hat{\sigma}_y}{2}\right), \tag{29}$$

respectively. Then we have the following relation:

$$\left[\hat{J}^+, \hat{J}^-\right] = \hat{J}_3, \tag{30}$$

and

$$\left[\hat{J}^-, \hat{J}^+\right] = -\hat{J}_3, \tag{31}$$

where $\hat{J}_3 = \frac{\hat{\sigma}_z}{2}$.

The Hamiltonian of an electron in Coulomb potential $U(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$ can be, within the *two-level-system approxiamtion*, written in terms of Pauli operators:

$$\begin{aligned} H_a &= \frac{\boldsymbol{p}^2}{2m_e} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} \\ &\simeq \hbar\omega_0|0\rangle\langle 0| + \hbar\omega_1|1\rangle\langle 1| \\ &= \hbar\underbrace{\left(\frac{\omega_1+\omega_0}{2}\right)}_{\Omega_A}\hat{\sigma}_0 + \hbar\underbrace{\left(\frac{\omega_1-\omega_0}{2}\right)}_{\frac{\Omega_0}{2}}\hat{\sigma}_z \\ &= \hbar\Omega_A\hat{\sigma}_0 + \hbar\frac{\Omega_0}{2}\hat{\sigma}_z. \end{aligned} \tag{32}$$

From now on, we shall neglect the first term since $\hat{\sigma_0}$ commutes other Pauli operator and thus does not contribute to the dynamics. Thus we have

$$H_a = \hbar\Omega_0\hat{J}_3 \tag{33}$$

II. EINSTEIN A AND B COEFFICIENTS

A. Master equation [5]

Let us now treat the *nonlinear* LCR circuit from the viewpoint of Hamiltonian formalism. We shall assume the total Hamiltonian to be

$$H = H_a + H_b + H_I, \tag{34}$$

where H_a, H_b, and H_I are the Hamiltonians of the nonlinear LC circuit (the two level system), the transmission line (the Ohmic environment), and their interaction (capacitive coupling), and are respectively given by

$$
\begin{aligned}
H_a &= \hbar\Omega_0 \hat{J}_3 && (35)\\
H_b &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \hbar\omega \hat{c}^\dagger(\omega)\hat{c}(\omega) && (36)\\
H_I &= -i\hbar \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left(f(\omega)\hat{J}^+\hat{c}(\omega) - f^*(\omega)\hat{J}^-\hat{c}^\dagger(\omega) \right) \\
&= -i\hbar \left[\hat{J}^+ \underbrace{\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega)\hat{c}(\omega)}_{R^-} - \hat{J}^- \underbrace{\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f^*(\omega)\hat{c}^\dagger(\omega)}_{R^+} \right] \\
&= -i\hbar \left[\hat{J}^+ R^- - \hat{J}^- R^+ \right]. && (37)
\end{aligned}
$$

Note that these are compared to the Eqs. (1), (2), (3), and (4) in *note 2015-12-07*, where we treated an LCR circuit. We recognize the following replacements,

$$
\begin{aligned}
\hat{a} &\leftrightarrow \hat{J}^- && (38)\\
\hat{a}^\dagger &\leftrightarrow \hat{J}^+, && (39)
\end{aligned}
$$

but otherwise the same. This fact allows us to derive (through the same argument as for deriving Eq. (45) in *note 2015-12-07*) the master equation for the nonlinear LCR circuit as

$$
\begin{aligned}
\frac{\partial\rho(t)}{\partial t} &= -\frac{i}{\hbar}\left[\hbar(\Omega_0 + \Delta + \Delta')\hat{J}_3, \rho(t)\right] + \frac{\Gamma' + \Gamma}{2}\left(2\hat{J}^-\rho(t)\hat{J}^+ - \hat{J}^+\hat{J}^-\rho(t) - \rho(t)\hat{J}^+\hat{J}^-\right) \\
&\quad + \frac{\Gamma'}{2}\left(2\hat{J}^+\rho(t)\hat{J}^- - \hat{J}^-\hat{J}^+\rho(t) - \rho(t)\hat{J}^-\hat{J}^+\right), && (40)
\end{aligned}
$$

where $\rho(t)$ is the reduced density operator of the the nonlinear LCR circuit and

$$
\begin{aligned}
\Gamma &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} |f(\omega)|^2 \delta(\Omega_0 - \omega) = |f(\Omega_0)|^2 && (41)\\
\Gamma' &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} |f(\omega)|^2 \langle n(\Omega_0)\rangle \delta(\Omega_0 - \omega) = |f(\Omega_0)|^2 \langle n(\Omega_0)\rangle = \Gamma\langle n(\Omega_0)\rangle && (42)
\end{aligned}
$$

are the dissipation rates and

$$
\begin{aligned}
\Delta &= \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{|f(\omega)|^2}{\Omega_0 - \omega} && (43)\\
\Delta' &= \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{|f(\omega)|^2 \langle n(\Omega_0)\rangle}{\Omega_0 - \omega} && (44)
\end{aligned}
$$

are the radiative shifts. The equation assumes the Lindblad form and can be rewritten as in terms of the Lindblad superoperator as

$$
\frac{\partial\rho(t)}{\partial t} = -\frac{i}{\hbar}\left[\hbar(\Omega_0 + \Delta + \Delta')\hat{J}_3, \rho(t)\right] + \frac{1}{2}\mathcal{L}_D\left[\sqrt{\Gamma' + \Gamma}\hat{J}^-\right]\rho(t) + \frac{1}{2}\mathcal{L}_D\left[\sqrt{\Gamma'}\hat{J}^+\right]\rho(t). \quad (45)
$$

Note the presence of Δ', which is absent in the master equation for the damped harmonic oscillators (Eq. (45) or (46) in *note 2015-12-07*). The survival of Δ' can be traced back to the commutation relation, Eq. (30), where the commutator is *operator-valued*. This is in fact the manifestation of the *saturation phenomenon* of two level system and the energies of the system suffer *radiative shifts*.

B. Einstein equations [5]

Let us now evaluate the master equation (40) in the basis of the Eigenstate of H_a, that is, $|0\rangle$ and $|1\rangle$.

$$\begin{aligned}\frac{d\rho_{00}(t)}{dt} &= \frac{\Gamma+\Gamma'}{2}\Big(2\langle 0|\hat{J}^-\rho(t)\hat{J}^+|0\rangle - \langle 0|\hat{J}^+\hat{J}^-\rho(t)|0\rangle - \langle 0|\rho(t)\hat{J}^+\hat{J}^-|0\rangle\Big) \\ &\qquad + \frac{\Gamma'}{2}\Big(2\langle 0|\hat{J}^+\rho(t)\hat{J}^-|0\rangle - \langle 0|\hat{J}^-\hat{J}^+\rho(t)|0\rangle - \langle 0|\rho(t)\hat{J}^-\hat{J}^+|0\rangle\Big) \\ &= -\underbrace{\Gamma_\uparrow}_{\Gamma'}\rho_{00}(t) + \underbrace{\Gamma_\downarrow}_{\Gamma+\Gamma'}\rho_{11}(t) \qquad (46)\\ \frac{d\rho_{11}(t)}{dt} &= \frac{\Gamma+\Gamma'}{2}\Big(2\langle 1|\hat{J}^-\rho(t)\hat{J}^+|1\rangle - \langle 1|\hat{J}^+\hat{J}^-\rho(t)|1\rangle - \langle 1|\rho(t)\hat{J}^+\hat{J}^-|1\rangle\Big) \\ &\qquad + \frac{\Gamma'}{2}\Big(2\langle 1|\hat{J}^+\rho(t)\hat{J}^-|1\rangle - \langle 1|\hat{J}^-\hat{J}^+\rho(t)|1\rangle - \langle 1|\rho(t)\hat{J}^-\hat{J}^+|1\rangle\Big) \\ &= -\underbrace{\Gamma_\downarrow}_{\Gamma+\Gamma'}\rho_{11}(t) + \underbrace{\Gamma_\uparrow}_{\Gamma'}\rho_{00}(t). \qquad (47)\end{aligned}$$

These are the celebrated *Einstein equations*. We thus identify Γ as *Einstein A coefficient*, which represents the spontaneous emission rate, and Γ as *Einstein B coefficient*, which is proportional to the thermal photon population $\langle n(\Omega_0)\rangle$ and represents both the absorption and the stimulated emission rates. In the steady state, we have

$$\frac{\rho_{11}}{\rho_{00}} = \frac{\Gamma'}{\Gamma+\Gamma'} = \frac{\langle n(\Omega_0)\rangle}{\langle n(\Omega_0)\rangle+1} = \frac{\left(\frac{1}{e^{\frac{\hbar\Omega_0}{k_{\rm B}T}}-1}\right)}{\left(\frac{1}{e^{\frac{\hbar\Omega_0}{k_{\rm B}T}}-1}\right)+1} = e^{-\frac{\hbar\Omega_0}{k_{\rm B}T}} = e^{-\frac{\hbar\Omega_0}{k_{\rm B}T}}, \qquad (48)$$

that is, two level system reaches the thermodynamic equilibrium.

Now we see that any systems (harmonic oscillators, anharmonic oscillators, and two level systems) undergo the non-unitay evolution even when the environment is in a vacuum state. This is due to the seemingly unavoidable vacuum fluctuation, which leads to the existance of the spontaneous emission with the rate Γ. Is this Einstein A coefficinet Γ fundamentally limit our ability to manipulate quantum systems? Let us now inspect the Einstein A coefficinet Γ a little bit more hoping we could find ways in which the omnipresent envionmental effect can be counteracted.

C. Dipole operator

It is time for us to face up to the reality: Our surrounding world is 3-dimensional in space. It requires us to consider the envionment as 3-dimensinal and the resultant Bosonic modes live in (3+1)-dimensional world. To make the complicated 3-dimensinal analysis simple, it is better to remember some group-theoretic arguments and discuss from the viewpoint of symmetry of the environment, which is assumed to be isotropic.

1. *Irreducible tensor operators [6, 7]*

Although the spin-$\frac{1}{2}$-representation with Pauli operators is the simplest for $SU(2)$ algebra, the electric dipole operator $\boldsymbol{d}$, which acts a major rule in spontaneous emission, is in fact a *polar vector* operator having odd parity. By appreciating the characteristic symmetry property of the polar vector, the electric dipole moment $\boldsymbol{d}$ should be given in terms of the *irreducible spin-1 tensor operators*. Let us define the spin-1 raising and lowering operators by

$$\hat{J}_+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \qquad (49)$$

and

$$\hat{J}_- = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad (50)$$

respectively. We then find the following relation for the $SU(2)$ algebra

$$\left[\hat{J}_+, \hat{J}_-\right] = \hat{J}_3, \tag{51}$$

and

$$\left[\hat{J}_-, \hat{J}_+\right] = -\hat{J}_3, \tag{52}$$

where

$$\hat{J}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{53}$$

is called the *Cartan generator*. With these operators let us define $\hat{J}_x$ and $\hat{J}_y$ as

$$\hat{J}_x = \frac{1}{\sqrt{2}}\left(\hat{J}_+ + \hat{J}_-\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{54}$$

and

$$\hat{J}_y = \frac{1}{\sqrt{2}}\left(\hat{J}_+ + \hat{J}_-\right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \tag{55}$$

respectively. We then find the following *spin-1-representation* of $SU(2)$ algebra:

$$[\hat{J}_i, \hat{J}_j] = i\epsilon_{ijk}\hat{J}_k. \tag{56}$$

Here $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ are called the *adjoint representation* of $SU(2)$ algebra and "+1" and "-1" in the right hand side of Eqs. (51) and (52) is called *root*.

The vector operator $\hat{\boldsymbol{r}} = (\hat{r}_1, \hat{r}_2, \hat{r}_3)$ transform under $SU(2)$ group as the *irreducible spin-1 tensor operator* T^1_q with angular momentum, 1, and magnetic quantum number, $q = -1$, 0, and 1. T^1_q is defined as

$$\left[\hat{J}_3, T^1_q\right] = q\, T^1_q \tag{57}$$

$$\left[\hat{J}_\pm, T^1_q\right] = \sqrt{\frac{2 - q(q \pm 1)}{2}}\, T^1_{q\pm1}, \tag{58}$$

which can be viewed as an operator extension of the more familiar definition of angular momentum eigenstates

$$\begin{aligned} \hat{J}_z|1, q\rangle &= q\, |1, q\rangle \\ \hat{J}_\pm|1, q\rangle &= \sqrt{\frac{2 - q(q \pm 1)}{2}}\, |1, q \pm 1\rangle. \end{aligned} \tag{59}$$

Here the Cartesian vector components $(\hat{r}_1, \hat{r}_2, \hat{r}_3)$ and the components of the irreducible spin-1 tensor operator (T^1_{-1}, T^1_0, T^1_1) are related as

$$T^1_0 = \hat{r}_3 \tag{60}$$

$$T^1_{\pm1} = \mp\frac{1}{\sqrt{2}}\left(\hat{r}_1 \pm i\hat{r}_2\right). \tag{61}$$

Note here that the factors $\sqrt{2}$ in the denominators in Eqs. (58) and (59) are coming from our definition of the raising and lowering operators, Eqs. (49) and (50), and are missing in some other literatures.

2. Dipole operator [6, 7]

The electric dipole moment of Bohr's atom can be written in terms of vecotr operator $\hat{\boldsymbol{r}}$ as

$$\boldsymbol{d} = er_n\boldsymbol{r} = ea_0n^2\left(\hat{r}_1\boldsymbol{e}_x + \hat{r}_2\boldsymbol{e}_y + \hat{r}_3\boldsymbol{e}_z\right) \tag{62}$$

with the Cartesian basis $\{\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z\}$. More convenient form from the viewpoint of symmetry of polar vector can be given in terms of the irreducible spin-1 tensor operators, defined in Eqs. (57) and (58), as

$$\boldsymbol{d} = ea_0n^2\left(T^1_1\boldsymbol{e}^*_1 + T^1_0\boldsymbol{e}^*_0 + T^1_{-1}\boldsymbol{e}^*_{-1}\right), \tag{63}$$

where $\{\boldsymbol{e}_1, \boldsymbol{e}_0, \boldsymbol{e}_{-1}\}$ is the spherical basis, whose elements are given by

$$\boldsymbol{e}_1 = -\frac{1}{\sqrt{2}}\left(\boldsymbol{e}_x + i\boldsymbol{e}_y\right) \tag{64}$$

$$\boldsymbol{e}_0 = \boldsymbol{e}_z \tag{65}$$

$$\boldsymbol{e}_{-1} = \frac{1}{\sqrt{2}}\left(\boldsymbol{e}_x - i\boldsymbol{e}_y\right). \tag{66}$$

It can be recognized that to account the odd parity $\left(T^1_{-1}, T^1_0, T^1_1\right)$ should be identified as the *normalization-modified* spherical harmonics $\left(\sqrt{\frac{4\pi}{3}}Y_{1-1}(\theta,\phi), \sqrt{\frac{4\pi}{3}}Y_{10}(\theta,\phi), \sqrt{\frac{4\pi}{3}}Y_{11}(\theta,\phi)\right)$ [3].

This is in stark contrast to the *magnetic* dipole operator $\boldsymbol{\mu}_e$ for spin-$\frac{1}{2}$, which sometimes identified as two level systes. $\boldsymbol{\mu}_e$ can be written in terms of Pauli operators (irreducible spin-$\frac{1}{2}$ tensor operators) as

$$\boldsymbol{\mu}_e = g_e\mu_{\mathrm{B}}\left(\frac{\hat{\sigma}_x}{2}\boldsymbol{e}_x + \frac{\hat{\sigma}_y}{2}\boldsymbol{e}_y + \frac{\hat{\sigma}_z}{2}\boldsymbol{e}_z\right), \tag{67}$$

which has the even parity and is called an *axial vector*. Here $g_e \sim 2$ is the electron spin g-factor and μ_{B} is the Bohr magneton:

$$\mu_{\mathrm{B}} = \frac{e\hbar}{2m_e}. \tag{68}$$

D. Electric dipole Hamiltonian [8, 9]

We shall now survey the interaction Hamiltonian Eq. (37) once more equipped with better understanding of 3-dimensional structure of the problem with appropriate symmetry properties. The dynamics of an electron in Bohr's atom in an electromagnetic environment can be formally described by the *minimal-coupling Hamiltonian*

$$H = \frac{1}{2m_e}\left[\boldsymbol{p} + e\boldsymbol{A}(\boldsymbol{r})\right]^2 + U(r) + H_R. \tag{69}$$

Under the assumption that an electron confined within a volume far smaller than the wavelength of the field (*long-wavelength approximation*) we can get more user-friendly *electric-dipole Hamiltonian*,

$$H' = \underbrace{\frac{\boldsymbol{p}^2}{2m_e} + U(r)}_{\text{Atomic part: } H_a} + \underbrace{H_{dip}}_{\text{Dipole selfenergy}} + \underbrace{\left(-\boldsymbol{d}\cdot\frac{\boldsymbol{D}'(0)}{\epsilon_0}\right)}_{\text{Interaction part: } H_{el}} + \underbrace{H_R}_{\text{Free field part}}, \tag{70}$$

from the minimal-coupling Hamiltonian Eq. (69) by performing a canonical transformation, the so-called *Power-Zienau-Woolley* transformation. Here $\boldsymbol{d}$ is the electric dipole moment defined by Eq. (63) for Bohr's atom. The *displacement* $\boldsymbol{D}'(r)$ after the transformation is related to the *transverse* electric field $\boldsymbol{E}_\perp(\boldsymbol{r})$ before the transformation as

$$\frac{\boldsymbol{D}'(r)}{\epsilon_0} = \boldsymbol{E}_\perp(\boldsymbol{r}). \tag{71}$$

Thus the interaction Hamiltonian represents the electric-dipole interaction

$$H_{el} = -\boldsymbol{d}\cdot\boldsymbol{E}_\perp(0). \tag{72}$$

Note that the atomic part H_a and the dipole self energy H_{dip} degenerate into Eq. (35) within the two level approximation.

More heuristic approach to the electric dipole interaction Hamiltonian Eq. (72) goes as follow [7]. The starting point is again the minimal-coupling Hamiltonian Eq. (69). By expanding the first term we have

$$H = \frac{\boldsymbol{p}^2}{2m_e} + \frac{e}{2m_e}\left(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p}\right) + \frac{e^2}{2m_e}\boldsymbol{A}^2 + U(r) + H_R. \tag{73}$$

Under the weak filed condition $|\boldsymbol{p}| \gg |e\boldsymbol{A}|$ the third term $\frac{e^2}{2m_e}\boldsymbol{A}^2$ can be neglected. The second term can be simplified to

$$\frac{e}{2m_e}\left(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p}\right) = \frac{e}{m_e}\boldsymbol{p}\cdot\boldsymbol{A} \tag{74}$$

by noticing the fact that

$$\begin{aligned}
\left[\boldsymbol{p}\cdot\boldsymbol{A}(\boldsymbol{r})\right]\psi(\boldsymbol{r}) &= -i\hbar\nabla\cdot\left(\boldsymbol{A}(\boldsymbol{r})\psi(\boldsymbol{r})\right) \\
&= -i\hbar\left(\underbrace{\nabla\cdot\boldsymbol{A}(\boldsymbol{r})}_{0:\ \text{Coulomb gauge}}\right)\psi(\boldsymbol{r}) + -i\hbar\boldsymbol{A}(\boldsymbol{r})\cdot\left(\nabla\psi(\boldsymbol{r})\right) \\
&= \left[\boldsymbol{A}(\boldsymbol{r})\cdot -i\hbar\nabla\right]\psi(\boldsymbol{r}) \\
&= \left[\boldsymbol{A}(\boldsymbol{r})\cdot\boldsymbol{p}\right]\psi(\boldsymbol{r}),
\end{aligned} \tag{75}$$

that is, $\boldsymbol{p}$ and $\boldsymbol{A}$ commute ($\boldsymbol{p}\cdot\boldsymbol{A} = \boldsymbol{A}\cdot\boldsymbol{p}$). Substituting

$$\boldsymbol{p} = m_e\frac{d\boldsymbol{r}}{dt} = m_e\frac{1}{i\hbar}\left[\boldsymbol{r}, H_a\right] \tag{76}$$

into Eq. (74) the transition probability from the upper state $|1\rangle$ to lower state $|0\rangle$ becomes

$$\begin{aligned}
\langle 0|\frac{e}{m_e}\boldsymbol{p}\cdot\boldsymbol{A}|1\rangle &= \frac{e}{i\hbar}\langle 0|\left[\boldsymbol{r}, H_a\right]\cdot\boldsymbol{A}|1\rangle \\
&= \frac{e}{i\hbar}\langle 0|\left(\boldsymbol{r}H_a - H_a\boldsymbol{r}\right)|1\rangle\cdot\boldsymbol{A} \\
&= \frac{e}{i\hbar}\left(\hbar\omega_1 - \hbar\omega_0\right)\langle 0|\boldsymbol{r}|1\rangle\cdot\boldsymbol{A} \\
&= \underbrace{e\langle 0|\boldsymbol{r}|1\rangle}_{\langle 0|\boldsymbol{d}|1\rangle}\cdot\underbrace{(-i\Omega_0)\boldsymbol{A}}_{\dot{\boldsymbol{A}}=-\boldsymbol{E}_\perp} \\
&= \langle 0|-\boldsymbol{d}\cdot\boldsymbol{E}_\perp|1\rangle.
\end{aligned} \tag{77}$$

Thus the second term $\frac{e}{m_e}\boldsymbol{p}\cdot\boldsymbol{A}$ in Eq. (73) is related to the the electric dipole Hamiltonian H_{el}.

E. From capacitive coupling Hamiltonian to electric dipole Hamiltonian

Comparing the capacitive cupling Hamiltonian H_I in Eq. (37) and its origin, Eq. (1) in *note 2015-12-14* with the electric dipole Hamiltonian H_{el} in Eq. (70), we find the following correspondance:

$$Q_s \ \leftrightarrow\ \boldsymbol{d} \tag{78}$$

$$V = \frac{q}{c} \ \leftrightarrow\ -\boldsymbol{E}_\perp = \frac{\boldsymbol{\Pi}}{\epsilon_0}, \tag{79}$$

where these relations are anticipated in Table II in *note 2015-11-16*. Let the relevant dipole moment which would interacts with the electric field Eq. (82) be along $\boldsymbol{e}_x$, that is,

$$\boldsymbol{d} = ea_0n^2\hat{r}_x\boldsymbol{e}_x = \mu_n\left(-T^1_1 + T^1_{-1}\right)\boldsymbol{e}_x, \tag{80}$$

where

$$\mu_n = \frac{ea_0n^2}{\sqrt{2}} \tag{81}$$

is the electric dipole moment of the transition $n \to n-1$ [4]. Suppose also initially that the polarization of the electric field is along x-axis. Then the transverse electric field $\boldsymbol{E}_\perp(0,t)$ can be given by

$$\boldsymbol{E}_\perp(0,t) = i\sum_k \sqrt{\frac{\hbar\omega_k}{2\epsilon_0 V}}\boldsymbol{e}_x \left(\hat{a}_k e^{-i\omega_k t} - \hat{a}_k^\dagger e^{i\omega_k t}\right). \tag{82}$$

This can be obtained at once when we exploit the analogy between $V = \frac{q}{c}$ and $\boldsymbol{E}_\perp = \frac{\Pi}{\epsilon_0}$, where $V = \frac{q}{c}$ is written as (see Eq. (29) in *note 2015-11-30*)

$$V(x,t) = -i\sum_k \sqrt{\frac{\hbar\omega_k}{2cL}} \left(\hat{a}_k e^{-i\omega_k t} - \hat{a}_k^\dagger e^{i\omega_k t}\right) \tag{83}$$

before taking the second continuum limit (remenber? c is the capacitance per unit length, not the speed of light!).

F. Einstein A coefficient [7]

Now that we have the proper interaction Hamiltonian H_{el} for the two level system coupled to the electromagnetic environment, we can see how the vacuum fluctuation or zero-point-fluctuation of the electromagnetic field causes the energy decay from the upper state $|1\rangle$ of the two level system to the lower state $|0\rangle$. The decay rate Γ_A from excited state to ground state is called Einstein's A coefficient, explicitly. The interaction-picture interaction Hamiltonian can then be given by

$$H_{el} = i\hbar\sum_k \sqrt{\frac{\omega_k}{2\hbar\epsilon_0 V}}\mu_n \left(-T^1_1 \hat{a}_k e^{i(\Omega_0-\omega_k)t} - T^1_{-1}\hat{a}_k^\dagger e^{-i(\Omega_0-\omega_k)t}\right). \tag{84}$$

Then, from Fermi's golden rule Eq. (41), we have the following expression of the Einsten A coefficient:

$$\Gamma_A = \sum_k \left(\frac{\omega_k}{2\hbar\epsilon_0 V}\mu_n^2\right) \left|\langle 0|T^1_{-1}|1\rangle\right|^2 \delta(\Omega_0 - \omega_k). \tag{85}$$

Let us now take the second continuum limit. The task is to change $\sum_k$ into $\int \frac{d\omega}{2\pi}$ by properly counting the number of modes supported by the environment. The number of modes per unit volume $\rho(k)$ can be obtained by the following geometric argument. Suppose the spherical shell of radius k and thickness dk in the reciprocal space. Since there are 2 polarization modes in unit cell $\left(\frac{2\pi}{L}\right)^3$ in the reciprocal space associated with the real space of volume $V = L^3$ the following relation holds:

$$2 : \left(\frac{2\pi}{L}\right)^3 = V\rho(k)\frac{dk}{2\pi} : 4\pi k^2 dk, \tag{86}$$

and thus we have

$$\rho(k)\frac{dk}{2\pi} = \frac{k^2}{\pi^2}dk. \tag{87}$$

The *density of state* with respect to ω, $\rho(\omega)$, can then be given by

$$\rho(\omega)\frac{d\omega}{2\pi} = \frac{\omega^2}{\pi^2 c^3}d\omega. \tag{88}$$

Consequently the sum over k in Eq. (85) can be replaced by the integral over ω as

$$\begin{aligned}\frac{1}{V}\sum_k \delta\left(\Omega_0 - \omega_k\right) \xrightarrow{V\to\infty} & \int_{-\infty}^{\infty}\frac{dk}{2\pi}\rho(k)2\pi\delta\left(\Omega_0-\omega_k\right) = \int_{-\infty}^{\infty} dk\frac{2k^2}{\pi}\delta\left(\Omega_0-\omega_k\right) \\ = & \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\rho(\omega)2\pi\delta\left(\Omega_0-\omega\right) = \int_{-\infty}^{\infty} d\omega\frac{2\omega^2}{\pi c^3}\delta\left(\Omega_0-\omega\right) = \frac{2\Omega_0^2}{\pi c^3}.\end{aligned} \tag{89}$$

Note that this procedure of changing from sum to integral *implicitly* involved the *second continuum limit* $V \to \infty$ with

$$\hat{a}(\omega) = \frac{\hat{a}(k)}{\sqrt{c}} = \lim_{V\to\infty} \frac{\sqrt{V}\hat{a}_k}{\sqrt{c}}, \tag{90}$$

where $\hat{a}(\omega)$ and $\hat{a}^\dagger(\omega')$ satisfy the commutation relation

$$\left[\hat{a}(\omega), \hat{a}^\dagger(\omega')\right] = \left[\frac{\hat{a}(k)}{\sqrt{c}}, \frac{\hat{a}^\dagger(k')}{\sqrt{c}}\right] = \frac{2\pi}{c}\delta(k-k') = 2\pi\delta(\omega-\omega'). \tag{91}$$

Plugging those into Eq. (85), we have

$$\begin{aligned}\Gamma_A &= \frac{2V\Omega_0^2}{\pi c^3}\left(\frac{\Omega_0}{2\hbar\epsilon_0 V}\mu_n^2\right)\left|\langle 0|T^1_{-1}|1\rangle\right|^2 \\ &= \frac{\Omega_0^3}{\pi\hbar\epsilon_0 c^3}\mu_n^2\left|\langle 0|T^1_{-1}|1\rangle\right|^2. \end{aligned}\tag{92}$$

Let us look at the part $\mu_n^2\left|\langle 0|T^1_{-1}|1\rangle\right|^2$ more carefully. In terms of the irreducible tensor representation in Eq. (80) it can be rewritten in more informative form as

$$\mu_n^2|\langle 0|T^1_{-1}|1\rangle|^2 = \frac{1}{2J'+1}\sum_{M_J}\sum_{M'_J}\mu_n^2|\langle g,J,M_J|T^1_{-1}|e,J',M'_J\rangle|^2 \tag{93}$$

where the initial state is averaged over the excited state sub-levels and the final state is the sum over the possible ground state sub-levels;

$$|1\rangle = \frac{1}{2J'+1}\sum_{M_J}|e,J',M'_J\rangle \tag{94}$$

$$|0\rangle = \sum_{M'_J}|g,J,M_J\rangle. \tag{95}$$

From the *Wigner-Eckart theorem*, the matrix element in Eq. (93) can be rewritten in terms of the *Clebsch-Gordan coefficient* as

$$|\langle g,J,M_J|T^1_{-1}|e,J',M'_J\rangle|^2 = \frac{|\langle g,J||T^1||e,J'\rangle|^2}{2J+1}|\langle J',M'_J;1,-1|J,M_J\rangle|^2. \tag{96}$$

where $\langle g,J||T^1||e,J'\rangle$ is called the *reduced matrix element* of the tensor operator T^1, which is independent on the geometry of the system (independent on magnetic sub-levels M_J and M'_J). Using the following identity for the Clebsch-Gordan coefficient,

$$\begin{aligned}\sum_q\sum_{M_J}\sum_{M'_J}|\langle J',M'_J;1,q|J,M_J\rangle|^2 &= \sum_{M_J}\left(\sum_{M'_J}\sum_q|\langle J',M'_J;1,q|J,M_J\rangle|^2\right) \\ &= \sum_{M_J}1 = 2J+1, \end{aligned}\tag{97}$$

we have

$$\sum_{M_J}\sum_{M'_J}|\langle J',M'_J;1,-1|J,M_J\rangle|^2 = \frac{2J+1}{3}, \tag{98}$$

since the concerned space is isotropic the equality in choosing particular q out of three possible value $\{-1,0,1\}$ results. Plugging Eqs. (96) and (98) in Eq. (93) we have

$$\begin{aligned}\mu_n^2\left|\langle 0|T^1_{-1}|1\rangle\right|^2 &= \frac{1}{2J'+1}\mu_n^2\frac{|\langle g,J||T^1||e,J'\rangle|^2}{2J+1}\left(\frac{2J+1}{3}\right) \\ &= \frac{1}{3}\mu_n^2\underbrace{\frac{|\langle g,J||T^1||e,J'\rangle|^2}{2J'+1}}_{1\ :\ \text{for}\ J'=J+1} \\ &= \frac{1}{3}\mu_n^2 = \frac{1}{3}\left(\frac{ea_0n^2}{\sqrt{2}}\right)^2. \end{aligned}\tag{99}$$

Plugging Eqs. (99) into the form of the decay rate Eq. (92) we have the famous Einstein A coefficient:

$$\Gamma_A = \frac{\mu_n^2 \Omega_0^3}{3\pi\hbar\epsilon_0 c^3}. \tag{100}$$

The Einstein A coefficient Eq. (100) tells us (1) the decay rate increases third power in ω_A, which indicates the general trend that the two level systems with wider energy gap decay faster than those with narrow gap (2) the larger the dipole moment μ is the faster the decay rate becomes.

G. Trivia

In this juncture let me introduce the *trivia* regarding the Einstein A coefficient Γ_A.

1. Classical electron oscillator [10]

First, the angular frequency Ω_0 of Bohr's atom for quantum number of $n = 1$ (the orbit radius of $r_1 = a_0$) becomes

$$\Omega_0 = \frac{\hbar}{m_e r_1^2} = \frac{\hbar}{m_e a_0^2} \tag{101}$$

thus

$$\mu_1 = \frac{e a_0}{\sqrt{2}} = e \underbrace{\sqrt{\frac{\hbar}{2 m_e \Omega_0}}}_{x_{\rm zpf}} = e x_{\rm zpf}, \tag{102}$$

where μ_1 is the dipole moment of *classical electron oscillator*, an electron in a *harmonic trap* with the trap angular frequency of Ω_0 and the its r.m.s. displacement is zero-point-fluctuation $x_{\rm zpf}$. The radiative decay rate of the classical electron oscillator can then be obtained by plugging μ_1 of Eq. (102) into μ_n in Eq. (100):

$$\Gamma_1 = \frac{\mu_1^2 \Omega_0^3}{3\pi\epsilon_0 \hbar c^3} = \frac{e^2 \Omega_0^2}{6\pi\epsilon_0 m_e c^3}, \tag{103}$$

which does not contain $\hbar$.

2. Oscillator strength [10]

Second, the dimensionless *oscillator strength* $\mathcal{F}_{ij}$ of the transition (with angular frequency ω) from level j down to level i characterized by $\Gamma_{i\to j}(\omega)$ can be defined as

$$\mathcal{F}_{ij} = \frac{\Gamma_{i\to j}(\omega)}{3\Gamma_1(\omega)}, \tag{104}$$

where $\Gamma_1(\omega)$ is the classical electron oscillator with angular frequency ω, that is,

$$\Gamma_1(\omega) = \frac{e^2 \omega^2}{6\pi\epsilon_0 m_e c^3}, \tag{105}$$

and the factor 3 in the denominator is to undo the average we have performed in Eq. (98). This quantifies the decay rate of an atom (or an artificial atom) by comparing it with that of the classical electron oscillator.

3. Larmor formula [4]

Finally, it is instructive to see the relation between the Einstein A coefficient and the *Larmor formula* of radiation power P_r emitted from the classical dipole:

$$\begin{aligned} \hbar\Omega_0\Gamma_A &= \hbar\Omega_0 \frac{\mu_n^2 \Omega_0^3}{3\pi\epsilon_0\hbar c^3} = \frac{\left(\frac{e a_0 n^2}{\sqrt{2}}\right)^2 \Omega_0^4}{3\pi\epsilon_0 c^3} = \frac{e^2}{6\pi\epsilon_0 c^3}\left(\Omega_0^4 a_0^2 n^4\right) \\ &= \frac{e^2}{6\pi\epsilon_0 c^3}\left(\Omega_0^2 r_n\right)^2 = \frac{e^2}{6\pi\epsilon_0 c^3}\left(\ddot{r}_n\right)^2 = P_r. \end{aligned} \tag{106}$$

III. PROBLEM

A. Magnetic dipole transitions [3]

1. From inductive coupling Hamiltonian to magnetic dipole Hamiltonian

Derive the magnetic dipole Hamiltonian

$$H_{mag} = i\hbar \sum_k \sqrt{\frac{\omega_k}{2\hbar c^2 \epsilon_0 V}} \mu_{\rm B} \left(\hat{J}^+ \hat{a}_k e^{i(\Omega_0 - \omega_k)t} - \hat{J}^- \hat{a}_k^\dagger e^{-i(\Omega_0 - \omega_k)t} \right), \tag{107}$$

from the inductive cupling Hamiltonian H_j given by Eq. (63) in *note 2015-11-30*, where $\hat{J}^+$ and $\hat{J}^-$ are defined in Eqs. (30) and (31), respectively. Here you can exploit the following correspondences (see Table II in *note 2015-11-16*):

$$\Phi_s \;\leftrightarrow\; \boldsymbol{\mu}_e \tag{108}$$

$$I = -\frac{1}{l}\frac{\partial}{\partial x}\varphi \;\leftrightarrow\; -\boldsymbol{B} = -\nabla \times \boldsymbol{A}. \tag{109}$$

where $\boldsymbol{\mu}_e$ is the magnetic dipole operator defined by Eq. (67).

2. Einstein A coefficient

Calculate the Einstein A coefficient $\Gamma_{Am}(\Omega_0)$ for the spin-$\frac{1}{2}$ with the excited energy of $\hbar\Omega_0$ due to magnetic dipole interaction with isotopic electromagnetic environment by repeating the procedure outlined in Sec. II F. Convince yourself that the ratio of $\Gamma_{Am}(\Omega_0)$ to $\Gamma_A(\Omega_0)$ is

$$\frac{\Gamma_{Am}(\omega)}{\Gamma_A(\omega)} \sim \alpha^2, \tag{110}$$

where α is the fine-structure constant given by Eq. (18).

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