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THREE-LEVEL IDENTICAL ATOMS IN ONE AND TWO-MODE QUANTUM FIELDS I: INTERNAL ELECTRIC DIPOLE AND QUADRUPOLE COUPLING IN SINGLE ATOM BY SINGLE MODE

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Abstract. We consider a single atom from the system of identical non-overlapping atoms coupled to the one and two-mode electromagnetic quantum fields. Each atom is assumed to have only three levels, either $|1>, |2>$ and $|3>$ and under the following conditions: (i) all the atom-photon interactions are electric dipole or electric quadrupole nature; (ii) only three atomic levels are included in the interaction; (iii) one or two quantized laser modes interact with this three-level system; (iv) each of these modes interacts with only one couple of levels; (v) so, from three possible couples of levels, only two of them interact directly. Levels of the third couple interact only by means of an intermediate level.

Keywords and phrases: Three-level quantum system, electromagnetic field, creation and annihilation operators, eigenstate, ground eigenvalue.

AMS subject classification (2000): 68Q05.

1. Three-level atom plus one mode

Consider a system of one three-level atom and one mode of the electromagnetic field. These two are coupled by the dipole/quadrupole interaction with the rotating wave approximation (RWA), and the system is described by the Hamiltonian

$$H = H_A + H_F + H', \tag{1}$$

where the free atomic part H_A and the free field part H_F are

$$H_A = \sum_{j=1}^{3} \hbar\omega_j b_j^+ b_j \tag{2}$$

and

$$H_F = \hbar\omega a^+ a. \tag{3}$$

Above $\hbar\omega_j$, $j = 1, 2, 3$ is the j-th atomic level energy, ω is the single mode laser frequency, b_j^+ and b_j are the creation and annihilation operators of an electron at level j, while a^+ and a are those of a photon in the mode. b_j, b_j^+ obey Fermion commutation rules, and a^+a a Boson commutation rules [1]:

$$\{b_j, b_j^+\} = \delta_{ij}, \ \ \{b_j, b_j\} = 0 = \{b_j^+, \widehat{b}_j^+\}, \ \ [a, a^+] = 1, [b_i, \widehat{a}] = 0, \ \ \text{etc.} \tag{4}$$

We assume that due to above mentioned couple restriction direct dipole (or quadrupole) transitions are allowed between atomic levels $|1>$ and $|2>$ and between $|2>$ and $|3>$, and forbidden between levels $|1>$ and $|3>$.

We express the laser field operators in terms of the annihilation and creation operators a, and a^+ the laser field mode which has the wave vector $\mathbf{k}$, frequency $\omega = ck$ and polarization $\widehat{\mathbf{p}}$. Thus we write the laser field operator at position R in the form

$$E(R) = i\hbar\sqrt{\frac{2\pi\omega}{\hbar V}}\widehat{p}(ae^{ikR} - a^+e^{-ikR}). \tag{5}$$

Here $\mathbf{R}$ is not an operator. So in such an approximation atom has only electronic levels.

2. Dipole and quadrupole transitions

We assume that atomic levels $|i>$ and $|j>$ are connected by an electric multipole transition of order m, i.e. that the first non-vanishing multipole transition moment between the levels of atom is that of $q^{(m)}$[2],

$$q^{(m)} = q_{12}b_1^+b_2 + q_{21}b_2^+b_1 + q_{23}b_2^+b_3 + q_{32}b_3^+b_2 \tag{6}$$

where $q_{ij} \equiv < i|q^{(m)}|j >$ is a tensor of order m. It is assumed for simplicity that the atom has no permanent multipole moment of order m in either $|1>$, $|2>$ and $|3>$ (see fig. 4.1). The interaction Hamiltonian $\widehat{H}'$ is the tensor product [2]

$$\widehat{H}' = -\frac{1}{m!}q^{(m)}\nabla^{m-1}E(R) \tag{7}$$

can be written in the normally ordered form according to (5) and (6), after the RWA the $\widehat{H}'$ is given, depending on the three possible types of the atomic level configurations, by [1]

$$H' = H'_\Xi \equiv \xi ab_2^+b_1 + \xi^*a^+b_1^+b_2 + \eta ab_3^+b_2 + \eta^*a^+b_2^+b_3 \quad (\Xi - \text{type}), \tag{8}$$

$$H' = H'_\Lambda \equiv \xi ab_2^+b_1 + \xi^*a^+b_1^+b_2 + \eta a^+b_3^+b_2 + \eta^*ab_2^+b_3 \quad (\Lambda - \text{type}), \tag{9}$$

$$H' = H'_V \equiv \xi a^+b_2^+b_1 + \xi^*ab_1^+b_2 + \eta ab_3^+b_2 + \eta^*a^+b_2^+b_3 \quad (V - \text{type}), \tag{10}$$

where

$$\xi_D = \left(\frac{2\pi\omega}{\hbar V}\right)^{\frac{1}{2}} q_{12}\widehat{p}e^{ikR}, \quad \eta_D = \left(\frac{2\pi\omega}{\hbar V}\right)^{\frac{1}{2}} q_{23}\widehat{p}e^{ikR}, \tag{11}$$

are electric dipole coupling constants and

$$\xi_Q = i\left(\frac{2\pi\omega^3}{\hbar Vc^2}\right)^{\frac{1}{2}} q_{12}\widehat{k}\widehat{p}e^{ikR}, \quad \eta_D = i\left(\frac{2\pi\omega^3}{\hbar Vc^2}\right)^{\frac{1}{2}} q_{23}\widehat{k}\widehat{p}e^{ikR}, \tag{12}$$

are electric quadrupole coupling constants where $k = kk$. After RWA in (4.8) the following terms are neglected, for Ξ-type: $ab_2^+b_1$, $\widehat{a}b_1^+b_2$, $ab_2^+b_3$, $a^+b_3^+b_2$; for Λ-type: $a^+b_2^+b_1$, $ab_1^+b_2$, $ab_3^+b_2$, $a^+b_2^+b_3$; and for V-type: $ab_2^+b_1$, $a^+b_1^+b_2$, $a^+b_3^+b_2$, $ab_2^+b_3$. So ξ and η are coupling constants (see fig. 1). Although it is always possible to make ξ and η real and positive, if desired, by choosing the relative phases of the state vectors properly, we treat ξ and η as complex here.

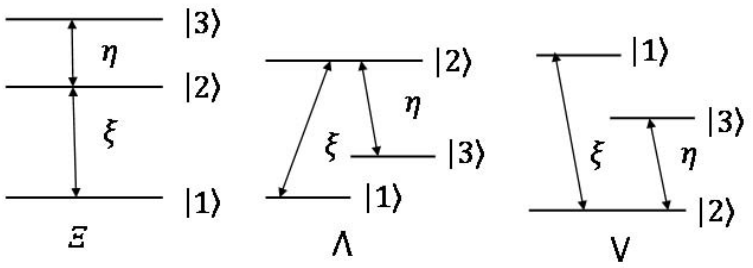

Fig. 1. The three possible energy level configurations for a three-level atom. The arrows indicate the transitions where ξ and η are defined.

The Hamiltonian eq. (7) has two obvious constant operators of motion [1]: One is the total electron number operator P_E

$$P_E = b_1^+ b_1 + b_2^+ b_2 + b_3^+ b_3 \tag{13}$$

and the other is the so-called excitation number operator $\widehat{N}$ given for each atom type by

$$N = a^+ a + b_3^+ b_3 - b_1^+ b_1 + I \ \ (\Xi - \text{type}), \tag{14}$$

$$N = a^+ a + b_2^+ b_2 \ \ \ (\Lambda - \text{type}), \tag{15}$$

$$N = a^+ a - b_2^+ b_2 + I \ \ \ (V - type). \tag{16}$$

N is a sum of the photon number operator and the "atomic excitation" number operator. In eqs. (14) and (16) a unit operator I is added so that the eigenvalues of N start at zero, which corresponds to no photons and the lowest atomic state.

We separate H into two parts H_I and H_{II}, in which H_I consists of N and P_E only. Thus both H_I an H_{II} are constants of motion:

$$H = H_I + H_I I, \tag{17}$$

and

$$[H_I, H_I I] = 0, \tag{18}$$

where for Ξ-type:

$$H_I = \hbar\omega(N - I) + \hbar\omega_2 P_E, \ \ H_{II} = -\hbar\Delta_l b_1^+ b_1 - \Delta_r b_3^+ b_3 + H'_\Xi \tag{19}$$

for Λ-type:

$$H_I = \hbar\omega N + \hbar(\omega_2 - \omega)P_E, \ \ \ H_{II} = -\hbar\triangle_l b_1^+ b_1 - \hbar\triangle_r b_3^+ b_3 + H'_\Xi \tag{20}$$

and for V-type:

$$H_I = \hbar\omega(N - I) + \hbar(\omega_2 + \omega)P_E, H_{II} = \hbar\Delta_l b_1^+ b_1 + \hbar\Delta_r b_3^+ b_3 + \widehat{H}'_V. \tag{21}$$

We have defined the detuning parameters Δ_l and Δ_r by

$$\Delta_l \equiv |\omega_{12}| - \omega, \Delta_r \equiv |\omega_{23}| - \omega, \tag{22}$$

with $\omega_{ij}| = \omega_i - \omega_j,$, where l and r stands for "left" and "right", respectively as in fig. 2. The separation given in eq. (17), with eq. (18) as a consequence, was first noted by Walls for Ξ-type [7]. Note that the separation of H into H_I and H_{II} shown in eq. (17) and eqs. (18) is not unique. H_{II} as chosen in eqs. (18), however, provides the maximum symmetry to the resultant expressions [1].

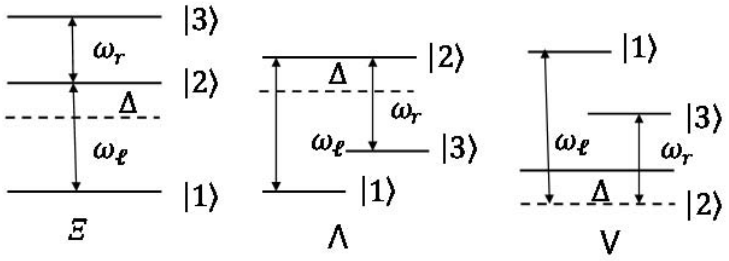

Fig. 2. The atomic level diagrams under the two-photon resonance condition. Two mode case. Mode l couples with the dipole d_{12} and mode r couples with the dipole d_{23}.

Due to eq. (18) the time translation operator $U(t) \equiv \exp(-iHt)$ factors:

$$U(t) = U_I(t)U_{II}(t) \tag{23}$$

with

$$U_I(t) = \exp(-iH_I t), U_{II}(t) = \exp(-iH_{II}t) \tag{24}$$

$U(t)$ was calculated by Yoon and Eberly [1] in terms of a matrix representation with a set of properly ordered Fock states as its basis. A Fock state $|n_1^A, n_2^A, n_3^A; n^F >$ is a common eigenstate of P_E and N and hence of H_I, where $n_j^A, j = 1, 2, 3$ is the electron occupation number at the jth atomic level, and n^F is the photon occupation number in the mode. We restrict ourselves to the one-electron case: $P_E = n_1^A + n_2^A + n_3^A = 1$ for a while. An excitation number N, which is an eigenvalue of N, is a non-negative integer, $N = 0, 1, 2....$ For a given excitation number N there exist three corresponding eigenstates $|j >^{(N)}$ in general. Take the Ξ-type for example: $|j >^{(N)}$ are then given by

$$\begin{aligned} |1>^{(N)} &\equiv |1,0,0;N> \equiv |1;N> \\ |2>^{(N)} &\equiv |0,1,0;N-1> \equiv |2;N-1> \\ |3>^{(N)} &\equiv |0,0,1;N-1> \equiv |3;N-2> \end{aligned} \tag{25}$$

Figure 3 shows the diagrams for the states corresponding to eq. (25). For an arbitrary type of atom, the $|j >^{(N)}$ are given by

$$|j >^{(N)} = b_j^{(N)} |0,0,0;N-\mu_j>, j = 1,2,3. \tag{26}$$

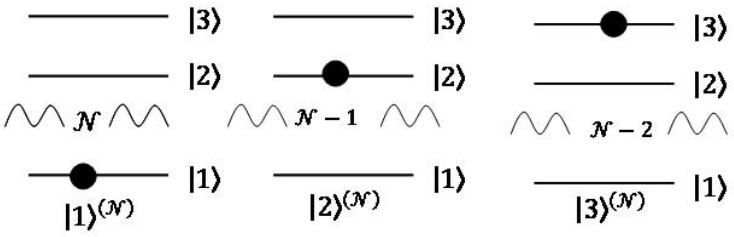

Fig. 3. The diagrammatic representations for the three basis states in the N-subspace for one mode Ξ-type. One photon is absorbed by the atom for an electron to transfer into the next higher level.

In eqn.(26) (μ_1, μ_2, μ_3) are "configuration parameters" defined to be $(0, 1, 2)$ for Ξ-type, $(0, 1, 0)$ for Λ-type and $(1, 0, 1)$ for V-type atoms, respectively. In case $N = 1$ or 0, some of the $N - \mu_j$, are negative, and then the corresponding state $|j>^{(N)}$ just be eliminated. (For example $N = 1$ of Ξ-type has only two eigenstates $|1>^{(1)}$ and $|2>^{(1)}$ while $N = 0$ of the same type has only one eigenstate $|1>^{(0)}$). We can order these states as [1]

$$...|1>^{(N)}, |2>^{(N)}, |3>^{(N)}, |1>^{(N+1)}, |2>^{(N+1)}, |3>^{(N+1)}, ... \tag{27}$$

and use them as the basis. With this basis the matrix representation of the Hamiltonian is block diagonal, each block a 3×3 submatrix (except for $N = 0$ in V- and A-types and for $N = 0, 1$ in S-type where a submatrix is 1×1 or 2×2). Hence in order to calculate $U(t)$ we only have to work in a three-dimensional subspace labeled by an excitation number N, the (N)-subspace, with its basis $|j>^{(N)}$ given by eq. (26). This is the natural generalization of the block form first noted by Jaynes in the two-level one-mode case [1].

In the (N)-subspace the matrix representations of H_I and H_{II} are [1]

$$H_I^{(N)} = (\omega N + const)I \tag{28}$$

and

$$H_{II}^{(N)} = \begin{pmatrix} -\Delta_l \mu_{21} & \xi_N^* & 0 \\ \xi_n & 0 & \eta_N^* \\ 0 & \eta_N & \Delta_r \mu_{32} \end{pmatrix}, \tag{29}$$

where$I$ is a 3×3 unit matrix, $\mu_{ij} = \mu_i - \mu_j$, $\xi_N \equiv \sqrt{\xi}$ and $\eta_N \equiv \sqrt{N}$ for Λ- and V-types, whereas $\eta_N \equiv \eta\sqrt{N-1}$ for Ξ-type. In case of exact two-photon resonance, $H_{II}^{(N)}$ in eq. (29) becomes

$$H_{II}^{(N)} = \begin{pmatrix} -\Delta & \xi_N^* & 0 \\ \xi_n & 0 & \eta_N^* \\ 0 & \eta_N & \Delta \end{pmatrix}, \tag{30}$$

where Δ the detuning parameter from the intermediate atomic level 2, is

$$\Delta = \Delta_l = -\Delta_r, \text{ for } \Xi - \text{type}, \tag{31}$$

$$\Delta = \Delta_l = \Delta_r, \text{ for } \Lambda - \text{type}, \tag{32}$$

$$\Delta = -\Delta_l = -\Delta_r, \text{ for } \Xi - \text{type}. \tag{33}$$

Figure 2 shows the corresponding diagrams for the three types. Note that levels 1 and 3 are degenerate with each other in Λ- and V-type systems in the one mode case.

The eigenvalues of $H_{II}^{(N)}$ in eq. (36) are

$$E^{(N)} = -\frac{\Delta}{2} f_N \text{ and } E_0^{(N)} = -\Delta, \tag{34}$$

where

$$f_N = \sqrt{\frac{\Delta^2}{4} + g_n^2} \tag{35}$$

with $g_N = \sqrt{|\xi_N|^2 + |\eta_N|^2}$.

Thus the diagonalization matrix is given by

$$V^{(N)} = \begin{pmatrix} \frac{\xi_N^*}{\lambda_N} & \frac{\xi_N^{*\prime}}{\lambda_N} & \frac{\eta_N^*}{g_N} \\ \frac{h_N}{\lambda_N} & -\frac{h'_N}{\lambda'_N} & 0 \\ \frac{\eta_N}{\lambda_N} & \frac{\eta_N}{\lambda'_N} & -\frac{\xi_N^*}{g_N} \end{pmatrix}, \tag{36}$$

which is unitary. Here is defined h_N, h'_N, λ_N and λ'_N by

$$h_N = f_N + \frac{\Delta}{2}, h'_N = f_N - \frac{\Delta}{2}, \lambda_N = \sqrt{2 f_N h_N}, \lambda'_N = \sqrt{2 f_N h'_N}.$$

$V^{(N)}$ diagonalizes $H_{II}^{(N)}$:

$$V^{(N)+} H_{II}^{(N)} V^{(N)} = \begin{pmatrix} E_+^{(N)} & 0 & 0 \\ 0 & E_-^{(N)} & 0 \\ 0 & 0 & E_0^{(N)} \end{pmatrix}, \tag{37}$$

Equation (37) and the unitarity of $V^{(N)}$ lead to the following matrix representation of $U_{II}(t)$ in the (N)-subspace:

$$U_{II}^{(N)}(t) = \begin{pmatrix} |\overline{\eta}_N|^2 e^{i\Delta t/2} + |\overline{\xi}_N|^2 x_N(t) & \overline{\xi}_N^* y_N(t) & \overline{\xi}_N^* \overline{\eta}_N^* (-e^{i\Delta t/2} + x_N(t)) \\ \overline{\xi}_N y_N(t) & x_N^* & \overline{\eta}_N^* y_N(t) \\ \overline{\xi}_N \overline{\eta}_N (-e^{i\Delta t/2} + x_N(t)) & \overline{\xi}_N y_N(t) & |\overline{\xi}_N|^2 e^{i\Delta t/2} + |\overline{\eta}_N|^2 x_N(t) \end{pmatrix}, \tag{38}$$

with following abbreviations $\overline{\xi}_N = \frac{\xi_n}{g_n}$, $\overline{\eta}_N = \frac{\eta_N}{g_N}$, $x_N(t) = \frac{1}{2} f_N (h_N e^{i f_N t} + h'_N e^{-i f_N t})$ and $y_N(t) = \frac{g_N}{2 f_N} (e^{i f_N t} + e^{-i f_N t}) = -i \frac{g_N}{2 f_N} \sin(f_N t)$.

The operator $U_I^{(N)}$, on the other hand, is just a phase factor: $U_I^{(N)}(t) = e^{-i(\omega N + const.)t} \times I$. In the case $N = 0$ (and also $N = 1$ for the Ξ-type) the

dimensionality of the corresponding subspace is less than three. $H_{II}^{(N)}$ and $U_{II}^{(N)}$ in this case, are given as the appropriate smaller matrices.

3. Control of three-level system

The paper [5] (see also [6]) is devoted to an optimal control problem for a three-level quantum system. A reduction of a quantum system to the first three eigenstates is described by a three-dimensional bilinear control system. The problem of optimal transfer of the system between eigenstates corresponding to the first and the third eigenvalues is stated as an optimal control problem with a quadratic cost. The problem is transformed to a sub-Riemannian problem on the spheres S^2 and S^5 (the real and complex cases). In these cases, the problem is lifted to a right-invariant sub-Riemannian problem on the Lie groups $SO(3)$ and $SU(3)$. Application of the *Pontryagin Maximum Principle* on Lie groups and other techniques of sub-Riemannian geometry yields a complete description of optimal controls and trajectories.

Description of physical picture. Assume that dynamics is governed by the time dependent Schrödinger equation (in a system of units such that $\hbar = 1$):

$$i\frac{d\psi(t)}{dt} = H\psi(t), \tag{39}$$

where $\psi(.) : \mathbb{R} \to \mathbb{C}^{\mathbb{Ж}}$ and:

$$H = \begin{pmatrix} E_1 & \Omega_1 & 0 \\ \Omega_1^* & E_2 & \Omega_2 \\ 0 & \Omega_2^* & E_3 \end{pmatrix}. \tag{40}$$

Let the controls $\Omega_1(.), \Omega_2(.)$, different from zero only in a fixed interval $[0, T]$, be connected to the physical parameters by $\Omega_j(t) = \mu_j F_j(t)/2$, $j = 1, 2$, with F_j the external pulsed field and μ_j are the couplings (intrinsic to the quantum system), restricted to couple only levels j and $j + 1$ by pairs.

This Hamiltonian is the sum of a "drift-term" H_0, plus a time dependent potential $V(t)$ (the control term, i.e., the lasers). The drift term is assumed to be diagonal with eigenvalues (energy levels) $... > E_3 > E_2 > E_1$. Then in this spectral resolution of H_0, the control term $V(t)$ is assumed to couple only the energy levels E_1, E_2 and E_2, E_3. The projected problem in the eigenspaces corresponding to E_1, E_2, E_3 is completely decoupled and is described by the Hamiltonian (40).

The problem is as follows:

Assume that for time $t \leq 0$ the state of the system lies in the eigenspace corresponding to the ground eigenvalue E_1. We want to determine suitable controls $\Omega_i(.)$, $i = 1, 2$, such that for time $t \geq T$, the system reaches the eigenspace corresponding to E_3, requiring that these controls minimize the cost (energy in the following):

$$J = \int_0^T \left(|\Omega_1(t)|^2 + |\Omega_2(t)|^2\right)\, dt. \tag{41}$$

The solution of this problem is the following theorem:

Theorem 1. *[5],[6] For the three-level problem with complex controls, optimality implies resonance. More precisely, controls* $\Omega_1(.), \Omega_2(.)$ *are optimal, if and only if they have the following form:*

$$\begin{cases} \Omega_1(t) = \cos(t/\sqrt{3})e^{i[(E_2-E_1)t+\varphi_1]}, \\ \Omega_2(t) = \sin(t/\sqrt{3})e^{i[(E_3-E_2)t+\varphi_2]}. \end{cases} \tag{42}$$

where φ_1, φ_2 *are two arbitrary phases. Here, the final time* T *is fixed in such a way that sub-Riemannian geodesics are parameterized by arclength, and it is given by* $T = \frac{\sqrt{3}}{2}\pi$.

For the Hamiltonians of type

$$H^{(L)} = \begin{pmatrix} 0 & e^{-i\delta\varphi}g_b t\hat{b} & 0 \\ e^{i\delta\varphi}g_b t\hat{b}^+ & 0 & g_a t\hat{a} \\ 0 & g_a t\hat{a}^+ & 0 \end{pmatrix},$$

$$H^{(\Lambda)} = \begin{pmatrix} 0 & -e^{-i\delta\varphi}g_b t\hat{b}^+ & 0 \\ -e^{i\delta\varphi}g_b t\hat{b} & 0 & g_a t\hat{a} \\ 0 & g_a t\hat{a}^+ & 0 \end{pmatrix},$$

and

$$H^{(V)} = \begin{pmatrix} 0 & e^{-i\delta\varphi}g_b t\hat{b} & 0 \\ e^{i\delta\varphi}g_b t\hat{b}^+ & 0 & -g_a t\hat{a}^+ \\ 0 & -g_a t\hat{a} & 0 \end{pmatrix}$$

the result analogical to this theorem is an open question (see [6], [7]).

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