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Abstract
We analyze the possibility of tomographic reconstruction of a system of three-level atoms in both non-degenerate and degenerate cases. In the non-degenerate case (when both transitions can be accessed independently) a complete reconstruction is possible. In the degenerate case (when both transitions are excited simultaneously), the complete reconstruction is achievable only for a single atom in the Ξ configuration. For multiple Ξ atoms, or even a single atom in the Λ configuration, only partial reconstruction is possible. Examples of one- and two-atom cases are explicitly considered.

PACS number: 03.65.Wj

1. Introduction

Quantum tomography is now an accepted technique to reconstruct the state of a quantum system [1]. Recent applications include the reconstruction of numerous physical systems, such as a radiation field [2], trapped ions and molecular vibrational states [3–5], spin [6, 7] and some other systems [8, 9].

The main idea behind quantum tomography is to use population measurements of the 'rotated' density matrix of the system. Explicitly, if ρ is the density matrix, a tomogram $\omega(\psi, \kappa)$ is defined by

$$\omega(\psi, \kappa) \equiv \langle \psi | U(\kappa) \rho U^{-1}(\kappa) | \psi \rangle \tag{1}$$

where

$$\rho(\kappa) \equiv U(\kappa) \rho U^{-1}(\kappa) \tag{2}$$

is the density matrix rotated by the unitary transformation U and κ stands for all the parameters required to uniquely specify U. By varying the input parameters κ, one obtains a complete collection of different observables (called a *quorum*), from which a characterization of the initial quantum state of the system can be obtained [10].

Every tomographic scheme is centered on the possibility of inverting equation (1). This inversion and the corresponding reconstruction of ρ from $\omega(\psi, \kappa)$ can always be

mathematically achieved [11, 12] when a Lie group $\mathfrak{G}$ acts irreducibly in the Hilbert space appropriate for the description of the quantum system under investigation. Experimental success depends on whether or not all the requirements element in $\mathfrak{G}$ can be practically implemented.

The objective of this paper is to study the possible tomographic reconstruction of the density matrix describing a collection of three-level atoms. Several approaches have already been proposed to reconstruct the state of a general three-level system (qutrit). In [13–15], the reconstruction of the quantum state of a three-level optical system is implemented for a frequency- and estimating quantum states and measuring fourth-order field moments. The use of non-orthogonal measurements as a way to reconstruct the state of a system (provided those measurements span the Hilbert space) as well as a detailed example of reconstruction for one- and two-qutrit systems, is considered in [7].

Even though one technically may require only a finite number of different experimental set-ups for complete tomographic reconstruction of atomic states, we will focus on the so-called redundant reconstruction, which implies a continuous set of measurements 'blanketing' all the parameter space. We justify this redundancy on the grounds that the reconstruction of a many-atom system would, in practice, require a large number of such discrete measurements.

Our strategy is to investigate tomographic reconstruction of the atomic state by probing atoms through the application of a carefully selected sequence of dispersive and resonant electromagnetic pulses.

Once an initial pulse of classical light has created a state of collective excitation in an ensemble of cold atoms, another pulse converts the atomic excitations into field excitations generating, for different atomic configurations, photons in a well-defined spatial and temporal mode [16]. The total number of such photons is determined by photoelectric detection so that a probability of detecting a given number of photons can be directly related to a tomogram [17].

In this work, our analysis will focus on two of three fundamentally different atomic configurations. They are the so-called Λ and Ξ configurations, distinguished by the presence of transition degeneracies from the generic *non-degenerate* configuration.

In section 3, we discuss this non-degenerate case, where transition frequencies are essentially different for distinct atomic transitions and where each transition can be independently interrogated by a pulse of the appropriate frequency. In this case, the density matrix can be completely reconstructed.

In sections 4 and 5, the systems under consideration contain atomic transitions having the same frequency; it is *not* possible to interrogate every transition individually. We will consider these cases at length and highlight the differences between the (global) symmetries pertinent to the description of these inequivalent degenerate atomic configurations. We will show, for these cases, that the density matrix cannot in general be completely reconstructed and that the partial information extracted from the measurements in the case of Λ and Ξ atoms is essentially different.

2. $\mathfrak{u}(3), \mathfrak{su}(3)$ and three-level atoms

Our Hamiltonian governing the evolution of a collection of A three-level atoms in a classical field has the form

$$\hat{H} = \hat{H}_0 + \hat{H}_{12} + \hat{H}_{23} \qquad (3)$$

where $\hat{H}_0$ is the free atomic Hamiltonian, and $\hat{H}_{ij}$ is the interaction term between levels i and j. Throughout this work, we will assume the ordering $E_1 \leqslant E_2 \leqslant E_3$ of individual atomic levels.

The terms in equation (3) are most transparently analyzed by introducing a set $\{\hat{S}_{ij}; i, j = 1, 2, 3\}$ of collective transition operators that satisfy the standard commutation relations of the $\mathfrak{u}(3)$ algebra:

$$[\hat{S}_{ij}, \hat{S}_{kl}] = \delta_{jk}\hat{S}_{il} - \delta_{il}\hat{S}_{kj}. \tag{4}$$

Thus, the Hilbert space for our systems naturally decomposes into a sum of subspaces invariant under the action of the Lie group $\mathfrak{U}(3)$.

We further assume that the A atoms are indistinguishable and their states are fully symmetric under permutation of the particle indices. Hence, the possible states of our system belong to a single unitariy irreducible representation of $\mathfrak{U}(3)$ having dimension $\frac{1}{2}(A+1)(A+2)$ and denoted by $(A, 0)$ in mathematics. The dimension of the Hilbert space is given by the number of ways of distributing A bosons in three modes.

If we introduce the atomic basis

$$\{|n_1 n_2 n_3\rangle, n_1, n_2, n_3 \geqslant 0, n_1 + n_2 + n_3 = A\}, \tag{5}$$

where n_j denotes the population in the jth atomic level, the matrix elements of $\hat{S}_{ij}$ can be easily evaluated using the Schwinger realization:

$$\hat{S}_{ij} \mapsto a_i^\dagger a_j. \tag{6}$$

In the one-atom case, this yields

$$\hat{S}_{ij}|j\rangle = |i\rangle, \tag{7}$$

where the following identification

$$|100\rangle \leftrightarrow |1\rangle, \qquad |010\rangle \leftrightarrow |2\rangle, \qquad |001\rangle \leftrightarrow |3\rangle, \tag{8}$$

has been made.

In terms of $\hat{S}_{ij}$'s, the Hamiltonian of equation (3) takes the form

$$\hat{H}_0 = \sum_{i=1}^{3} E_i \hat{S}_{ii}, \tag{9}$$

$$\hat{H}_{12} = g_1(e^{i\omega_1 t}\hat{S}_{12} + e^{-i\omega_1 t}\hat{S}_{21}), \tag{10}$$

$$\hat{H}_{23} = g_2(e^{i\omega_2 t}\hat{S}_{23} + e^{-i\omega_2 t}\hat{S}_{32}), \tag{11}$$

where ω_1 and ω_2 are frequencies of the external fields and g_1 and g_2 are coupling constants, chosen to be real for simplicity.

The operator

$$\hat{N} = \sum_{i=1}^{3} \hat{S}_{ii} \tag{12}$$

commutes with all other operators in the $\mathfrak{u}(3)$ algebra. This operator is proportional to the unit operator when acting on occupational states of the form $|n_1 n_2 n_3\rangle$,

$$\hat{N}|n_1 n_2 n_3\rangle = A|n_1 n_2 n_3\rangle. \tag{13}$$

Removing $\hat{N}$ reduces $\mathfrak{u}(3)$ to $\mathfrak{su}(3)$. Thus, the possible evolutions generated by the Hamiltonian $\hat{H}$ are, up to an unimportant global phase, finite $\mathfrak{SU}(3)$ transformations.
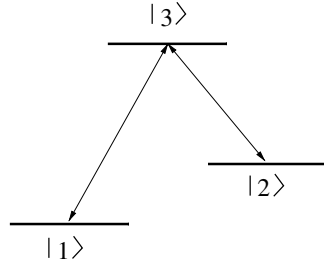
Figure 1. A typical level scheme for the non-degenerate case.

3. The non-degenerate case

The non-degeneracy condition is understood to imply that the atomic transition frequencies $(E_3 - E_2)$ and $(E_2 - E_1)$ are sufficiently distinct to satisfy

$$(E_3 - E_2) - (E_2 - E_1) \gg g_1, \qquad (E_3 - E_2) - (E_2 - E_1) \gg g_2. \qquad (14)$$

In this manner, each transition can be interrogated separately by an external field. A typical non-degenerate system is illustrated in figure 1.

For tomographic purposes, the level pairs $(1 \leftrightarrow 2), (2 \leftrightarrow 3)$ and their respective transitions, if taken in respective isolation, could be considered as independent two-level subsystems. However the full system must be treated as a three-level system under $\mathfrak{SU}(3)$ evolution.

In the rotating frame, the Hamiltonian of equation (3) takes the form

$$\hat{H}_{int} = \Delta_{23}\hat{S}_{33} - \Delta_{12}\hat{S}_{11} + g_{12}(\hat{S}_{12} + \hat{S}_{21}) + g_{23}(\hat{S}_{23} + \hat{S}_{32}), \qquad (15)$$

where

$$\Delta_{12} \equiv E_2 - E_1 - \omega_1, \qquad \Delta_{23} \equiv E_3 - E_2 - \omega_2. \qquad (16)$$

Because the frequencies ω_1 and ω_2 of the external field are adjustable parameters, two types of field pulses can be applied to our system. The first type is characterized by $\Delta_{ij} \approx 0$ and thus resonant; it stimulates the corresponding atomic transitions. The second type is characterized by $\Delta_{ij} \gg g_{ij}$ and is thus far-off resonant (dispersive); this kind of pulse leads to some phase shift.

The corresponding resonant and dispersive evolution operators have the form

$$U_{ij}^R(\beta_{ij}) = \exp[-\mathrm{i}\beta_{ij}(\hat{S}_{ij} + \hat{S}_{ji})], \qquad i \neq j, \qquad (17)$$

$$U_{11}^D(\phi_{12}) = \exp[\mathrm{i}\phi_{12}\hat{S}_{11}], \qquad (18)$$

$$U_{33}^D(\phi_{23}) = \exp[\mathrm{i}\phi_{23}\hat{S}_{33}], \qquad (19)$$

where $\beta_{ij} = g_{ij}t_{ij}$ and $\phi_{ij} = \left(\Delta_{ij} + g_{ij}^2/\Delta_{ij}\right)\tau_{ij}$. Here, t_{ij}, τ_{ij} are time intervals, not necessarily equal. It should be noted, that for short interaction times τ_{ij} satisfying $g^2\tau_{ij}/\Delta_{ij} \ll 1$ and $g^2\tau_{ij} \ll \Delta_{ij}^2$, the second term in the expression for ϕ_{ij} can be obviously neglected. However, for long interaction times, $\exp(-\mathrm{i}\Delta_{ij}\tau_{ij})$ becomes strongly oscillating and the measurements should be carried out in stroboscopic times, $\tau_{ij} = 2\pi n/\Delta_{ij}$.

For a complete reconstruction of the density matrix in the absence of degeneracy, it suffices to measure the probability of detecting zero photons (i.e. zero fluorescence condition) in the

irradiated field. This corresponds to the detection the atoms in the ground state, $|A00\rangle$. It is worth noting here that, in the non-redundant scheme when only a finite number of different pulses have to be applied, the measurement of nonzero photons are required [17].

It is possible, by combining operations in equations (17)–(19), to obtain a element of the group $\mathfrak{U}(3)$ sufficiently general for our purpose. This is best seen by first observing that an element of $\mathfrak{SU}(3)$ is parameterized by eight real numbers and can be conveniently factorized [18] into a product of $\mathfrak{SU}(2)$ subgroup transformations:

$$\bar{U}(\alpha_1, \beta_1, \gamma_1, \alpha_2, \beta_2, \alpha_3, \beta_3, \gamma_3) = R_{23}(\alpha_1, \beta_1, \gamma_1) \cdot R_{12}(\alpha_2, \beta_2, \alpha_2) \cdot R_{23}(\alpha_3, \beta_3, \gamma_3). \tag{20}$$

The action of such a group element on basis states of an irreducible representation is given in [18].

The notation

$$n \equiv (n_1 n_2 n_3), \qquad I = I_{23} \equiv \tfrac{1}{2}(n_2 + n_3), \tag{21}$$

will be a useful shorthand throughout this paper. In particular, we note that

$$\langle \nu | R_{23}(\alpha, \beta, \gamma) | n \rangle \equiv \langle \nu_1 \nu_2 \nu_3 | R_{23}(\alpha, \beta, \gamma) | n_1 n_2 n_3 \rangle = \mathcal{D}^{I_{23}}_{M_\nu, M_n}(\Omega),$$

$$\langle \nu | R_{12}(\alpha, \beta, \gamma) | n \rangle \equiv \langle \nu_1 \nu_2 \nu_3 | R_{12}(\alpha, \beta, \gamma) | n_1 n_2 n_3 \rangle = \mathcal{D}^{I_{12}}_{m_\nu, m_n}(\Omega), \tag{22}$$

where $\mathcal{D}^J_{MM'}$ an $\mathfrak{SU}(2)$ Wigner $\mathcal{D}$-function and

$$I_{12} = \tfrac{1}{2}(n_1 + n_2), \qquad M_n = \tfrac{1}{2}(n_2 - n_3), \qquad m_n = \tfrac{1}{2}(n_1 - n_2). \tag{23}$$

More generally, the definition of states for the irrep (λ, μ) and $\mathfrak{SU}(3)$ elements between those states can be found in [18]. Specialized results are collected in appendix A. In particular, some formulae in this section implicitly depend on matrix elements of states in irreps of the type $(A, 0)$, $(0, A)$ and (σ, σ). The notation of $\mathfrak{SU}(3)\mathcal{D}$ functions conforms to that of [18] and uses the pair (λ, μ) with the labels n, I to unambiguously distinguish the $\mathfrak{SU}(3)\mathcal{D}$ functions. For occupational states, n, I are given by equation (21).

Because the state $|A00\rangle$ is, up to a global phase, unchanged by the action of dispersive pulses and operations of the form R_{23}, it is enough to consider a sequence of pulses of the form:

$$U(\varphi_{23}, \beta_{23}, \varphi_{12}, \beta_{12}) = U^D_{33}(-\varphi_{23}) U^R_{23}(\beta_{23}) U^D_{11}(\varphi_{12}) U^R_{12}(\beta_{12}). \tag{24}$$

In the single-atom case, the evolution operator equation (24) is a 3×3 matrix explicitly given by

$$U(\varphi_{23}, \beta_{23}, \varphi_{12}, \beta_{12})$$
$$= \begin{pmatrix} e^{i\varphi_{12}} \cos(\beta_{12}) & -i\, e^{i\varphi_{12}} \sin(\beta_{12}) & 0 \\ -i \cos(\beta_{23}) \sin(\beta_{12}) & \cos(\beta_{12}) \cos(\beta_{23}) & -i \sin(\beta_{23}) \\ -e^{-i\varphi_{23}} \sin(\beta_{12}) \sin(\beta_{23}) & -i\, e^{-i\varphi_{23}} \cos(\beta_{12}) \sin(\beta_{23}) & e^{-i\varphi_{23}} \cos(\beta_{23}) \end{pmatrix}. \tag{25}$$

$U(\varphi_{23}, \beta_{23}, \varphi_{12}, \beta_{12})$ can be more easily analyzed in the factorized form

$$U(\varphi_{23}, \beta_{23}, \varphi_{12}, \beta_{12}) = e^{-\frac{1}{3}i(\varphi_{12} - \varphi_{23})} \bar{U}, \tag{26}$$

where

$$\bar{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -i\, e^{i(\chi - \varphi_{12})} \cos(\beta_{23}) & e^{i(2\chi - \varphi_{12})} \sin(\beta_{23}) \\ 0 & -e^{-i(2\chi - \varphi_{12})} \sin(\beta_{23}) & i\, e^{-i(\chi - \varphi_{12})} \cos(\beta_{23}) \end{pmatrix}$$
$$\times \begin{pmatrix} e^{i\chi} \cos(\beta_{12}) & -\sin(\beta_{12}) & 0 \\ \sin(\beta_{12}) & e^{-i\chi} \cos(\beta_{12}) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & i\, e^{i\chi} & 0 \\ 0 & 0 & -i\, e^{-i\chi} \end{pmatrix}, \tag{27}$$

and

$$\chi = \tfrac{1}{3}(2\varphi_{12} + \varphi_{23}). \tag{28}$$

Clearly, the matrix $U(\varphi_{23}, \beta_{23}, \varphi_{12}, \beta_{12})$ of equation (26) is an element of $\mathfrak{U}(3)$ whereas $\bar{U}$ of equation (27) is an $\mathfrak{SU}(3)$ transformation. Comparing with the parametrization of [18], we have the correspondences

$$\begin{aligned}
&\alpha_1 \to -\varphi_{23} - \tfrac{1}{2}\pi, &&\beta_1 \to 2\beta_{23}, &&\gamma_1 \to \tfrac{3}{2}\pi + \tfrac{2}{3}\varphi_{12} + \tfrac{1}{3}\varphi_{23} \\
&\alpha_2 \to -\tfrac{2}{3}\varphi_{12} - \tfrac{1}{3}\varphi_{23}, &&\beta_2 \to 2\beta_{12}, && \\
&\alpha_3 \to -\tfrac{4}{3}\varphi_{12} - \tfrac{2}{3}\varphi_{23} - \pi, &&\beta_3 = 0, &&\gamma_3 = 0.
\end{aligned} \tag{29}$$

Note that, although $\bar{U}$ is not the most general $\mathfrak{SU}(3)$, it can be multiplied on the right by a transformation of the form

$$R_{12}(\bar{\alpha}_2, 0, \bar{\alpha}_2)\, R_{23}(\bar{\alpha}_3, \bar{\beta}_3, \bar{\gamma}_3) =$$
$$\times \begin{pmatrix} e^{-i\bar{\alpha}_2} & 0 & 0 \\ 0 & e^{\frac{i}{2}i(2\bar{\alpha}_2 - \bar{\alpha}_3 - \bar{\gamma}_3)} \cos\left(\frac{\bar{\beta}_3}{2}\right) & -e^{\frac{i}{2}(2\bar{\alpha}_2 - \bar{\alpha}_3 + \bar{\gamma}_3)} \sin\left(\frac{\bar{\beta}_3}{2}\right) \\ 0 & e^{\frac{i}{2}(\bar{\alpha}_3 - \bar{\gamma}_3)} \sin\left(\frac{\bar{\beta}_3}{2}\right) & e^{\frac{i}{2}(\bar{\alpha}_3 + \bar{\gamma}_3)} \cos\left(\frac{\bar{\beta}_3}{2}\right) \end{pmatrix} \tag{30}$$

without affecting the dynamics of the $|100\rangle$ state. Thus, $\bar{U}$ is equivalent to a general transformation when acting on $|100\rangle$.

Expanding the density matrix in the occupational basis:

$$\rho = \sum_{n\nu} |n\rangle\langle\nu|\rho_{n,\nu}, \tag{31}$$

and introducing the shorthand $\tau = (\varphi_{23}, \beta_{23}, \varphi_{12}, \beta_{12})$, we rapidly obtain

$$\begin{aligned}
\omega(\tau) &= \sum_{n\nu} \langle A00|\bar{U}(\tau)|n\rangle\langle\nu|\bar{U}^{\dagger}(\tau)|A00\rangle\rho_{n,\nu} \\
&= \sum_{n\nu} (-1)^{\nu_2} \mathcal{D}^{(A,0)}_{(A00)0,nI}(\tau)\mathcal{D}^{(0,A)}_{(0AA)0,\nu^*I'}(\tau)\rho_{n,\nu},
\end{aligned} \tag{32}$$

where

$$\mathcal{D}^{(\lambda,\mu)}_{n_1\bar{I}_1,n_2 I_2}(\tau) \equiv \langle(\lambda,\mu)n_1 I_1|U(\tau)|(\lambda,\mu)n_2 I_2\rangle \tag{33}$$

is an $\mathfrak{SU}(3)$ Wigner-function for the irrep (λ,μ). Further notational details and properties of these functions (in particular equation (A.4)) can be found in appendix A.

Products of $\mathfrak{SU}(2)\mathcal{D}$-functions can be decomposed into sums of $\mathcal{D}$-functions multiplied by products of $\mathfrak{SU}(2)$ Clebsch–Gordan coefficients. The same holds for products of $\mathfrak{SU}(3)\mathcal{D}$-functions provided that we use $\mathfrak{SU}(3)$ Clebsch–Gordan technology. Thus, given that $\mathfrak{SU}(3)$-coupling $(A,0) \otimes (0,A)$ decomposes in the direct sum [19]

$$(A,0) \otimes (0,A) = (A,A) \oplus (A-1,A-1) \oplus \cdots \oplus (0,0),$$
$$= \bigoplus_{\lambda=0}^{A}(\lambda,\lambda), \tag{34}$$

we have

$$\begin{aligned}
\mathcal{D}^{(A,0)}_{(A00)0,nI}(\tau)\mathcal{D}^{(0,A)}_{(0AA)0,\nu^*I'}(\tau) &= \sum_{\lambda,J} \mathcal{D}^{(\lambda,\lambda)}_{(\lambda\lambda\lambda)0,N^{(\lambda)}J}(\tau) \left\langle \begin{array}{cc|c} (A,0) & (0,A) & (\lambda,\lambda) \\ (A00)0 & (0AA)0 & (\lambda\lambda\lambda)0 \end{array} \right\rangle \\
&\quad \times \left\langle \begin{array}{cc|c} (A,0) & (0,A) & (\lambda,\lambda) \\ nI & \nu^*I' & N^{(\lambda)}J \end{array} \right\rangle,
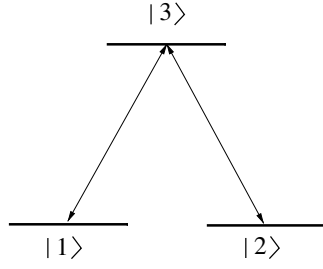\end{aligned} \tag{35}$$

Figure 2. Schematic representation of a single atom in a Λ configuration.

where

$$N^{(\lambda)} = (n_1 + \nu_1^* - (A - \lambda), n_2 + \nu_2^* - (A - \lambda), n_3 + \nu_3^* - (A - \lambda)), \tag{36}$$

and where

$$\left\langle \begin{array}{cc|c} (A, 0) & (0, A) & (\lambda, \lambda) \\ n_1 I_1 & n_2 I_2 & N^{(\lambda)} I_3 \end{array} \right\rangle \tag{37}$$

is the $\mathfrak{SU}(3)$ Clebsch–Gordan coefficient for the coupling of $|(A, 0)n_1 I_1\rangle$ and $|(0, A)n_2 I_2\rangle$ to $|(\lambda, \lambda)N^{(\lambda)} I_3\rangle$. The appearance of extra factors of $(A - \lambda)$ in the construction of $N^{(\lambda)}$ is discussed in equation (B.10) of appendix B.

Inserting equation (35) in equation (32) yields

$$\omega(\tau) = \sum_{n\nu\lambda J} (-1)^{\nu_2} \rho_{n,\nu} \mathcal{D}^{(\lambda,\lambda)}_{(\lambda\lambda\lambda)0, N^{(\lambda)}J}(\tau)$$
$$\times \left\langle \begin{array}{cc|c} (A, 0) & (0, A) & (\lambda, \lambda) \\ (A00)0 & (0AA)0 & (\lambda\lambda\lambda)0 \end{array} \right\rangle \left\langle \begin{array}{cc|c} (A, 0) & (0, A) & (\lambda, \lambda) \\ nI & \nu^*I' & N^{(\lambda)}J \end{array} \right\rangle. \tag{38}$$

After some straightforward manipulations detailed in appendix C, we obtain the final expression

$$(-1)^{\nu_2} \rho_{n,\nu} = \sum_{\mu J} \frac{(\mu + 1)^3}{1024\pi^5} \left\langle \begin{array}{cc|c} (A, 0) & (0, A) & (\mu, \mu) \\ (A00)0 & (0AA)0 & (\mu\mu\mu)0 \end{array} \right\rangle^{-1}$$
$$\times \left\langle \begin{array}{cc|c} (A, 0) & (0, A) & (\mu, \mu) \\ nI & \nu^*I' & N^{(\mu)}J \end{array} \right\rangle \int d\Omega \, \mathcal{D}^{(\mu,\mu)*}_{(\mu\mu\mu)0, N^{(\mu)}J}(\tau)\omega(\tau). \tag{39}$$

As there is no restriction on n or ν^*, equation (39) shows that, in the non-degenerate case, the density matrix can be completely reconstructed.

4. Degenerate Λ-type atomic systems

Let us turn our attention to the case of a degenerate Λ-type system. A typical Λ atom is schematically illustrated in figure 2.

In the single-atom case, the allowed transitions are $|1\rangle \leftrightarrow |3\rangle$, $|2\rangle \leftrightarrow |3\rangle$. The degeneracy condition is

$$E_3 - E_1 = E_3 - E_2. \tag{40}$$

In the multi-atom case, the only atomic configuration that can be unambiguously identified by photon counting is when every atom is excited, i.e. when the system of A atoms is in the state $|00A\rangle$.
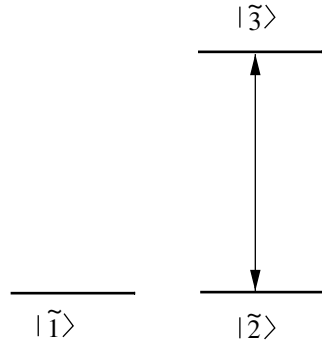
$$|\tilde{3}\rangle$$

$$|\tilde{1}\rangle \qquad\qquad |\tilde{2}\rangle$$

Figure 3. The basis states resulting from the transformation T_{12}.

4.1. The evolution

In the rotating frame, the interaction Hamiltonian has the form

$$\hat{H}_\Lambda = \Delta S_{33} + g(S_{13} + S_{23}) + g(S_{31} + S_{32}), \tag{41}$$

where $\Delta = E_3 - E_1 - \omega$ and $g_1 = g_2 = g$ for simplicity.

In the single-atom case, $\hat{H}_\Lambda$ can be represented as the following 3×3 matrix:

$$\hat{H}_\Lambda = \begin{pmatrix} 0 & 0 & g \\ 0 & 0 & g \\ g & g & \Delta \end{pmatrix}. \tag{42}$$

A simple basis transformation

$$|1\rangle \mapsto |\tilde{1}\rangle = \tfrac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right), \qquad |2\rangle \mapsto |\tilde{2}\rangle = \tfrac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right), \qquad |3\rangle \mapsto |\tilde{3}\rangle, \tag{43}$$

given by the constant matrix

$$T_{12} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{44}$$

transforms equation (42) to the block diagonal form

$$\hat{H}_\Lambda \mapsto \hat{H}_T = T_{12}^{-1}\hat{H}_\Lambda T_{12} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \sqrt{2}g \\ 0 & \sqrt{2}g & \Delta \end{pmatrix}. \tag{45}$$

The effect T_{12} on basis states is illustrated in figure 3; T_{12} produces a *dark state* $|\tilde{1}\rangle$ completely decoupled from the remaining doublet. In view of this we can expect, on general grounds, that a complete reconstruction will not be possible as our Hamiltonian $\hat{H}_\Lambda$ cannot possibly probe the dark state $|\tilde{1}\rangle$.

Using the basis $\{|\tilde{1}\rangle, |\tilde{2}\rangle, |\tilde{3}\rangle\}$, the resonant pulses, with $\Delta = 0$, are of the form

$$\tilde{U}_\Lambda^R(\sqrt{2}gt) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\sqrt{2}gt) & \mathrm{i}\sin(\sqrt{2}gt) \\ 0 & \mathrm{i}\sin(\sqrt{2}gt) & \cos(\sqrt{2}gt) \end{pmatrix}. \tag{46}$$

In the same basis, the dispersive pulses, with $\Delta \gg g$, are described in the stroboscopic approximation by the effective evolution operator

$$\tilde{U}_\Lambda^D(2g^2 t/\Delta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{2ig^2 t/\Delta} & 0 \\ 0 & 0 & e^{-2ig^2 t/\Delta} \end{pmatrix}. \tag{47}$$

In the two-dimensional subspace spanned by $|\tilde{2}\rangle$ and $|\tilde{3}\rangle$, the operators $\tilde{U}_\Lambda^R$ and $\tilde{U}_\Lambda^D$ correspond to $\mathfrak{SU}(2)$ rotations about the $\hat{x}$ and $\hat{z}$ axes, respectively:

$$\tilde{U}_\Lambda^R(\alpha) \mapsto R_{23}^x(\alpha), \qquad \tilde{U}_\Lambda^D(\beta) \mapsto R_{23}^z(\beta), \tag{48}$$

in an obvious notation. A sufficiently general sequence of pulses can thus be written as

$$\tilde{U}_\Lambda(\tilde{\Omega}) = R_{23}^z(\alpha) \cdot R_{23}^x(\beta) \cdot R_{23}^z(\gamma),$$
$$= R_{23}^z\left(\alpha + \frac{\pi}{2}\right) \cdot R_{23}^y(\beta) \cdot R_{23}^z\left(\gamma - \frac{\pi}{2}\right) = R_{23}(\tilde{\Omega}). \tag{49}$$

For the one-atom case, the 3×3 matrix representation for this evolution has the form

$$\tilde{U}_\Lambda(\tilde{\Omega}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & * & * \\ 0 & * & * \end{pmatrix} \tag{50}$$

where $*$ indicates a nonzero entry. The block diagonal form of $\tilde{U}$ is explicit. It shows that, for a system containing one or more than one atom, there will always be at least one subspace which cannot be reached in the course of evolution of $|00A\rangle$; such decoupled subspaces are an obstruction to complete reconstruction.

To illustrate this, we expand the density matrix for an A-atom system in the basis $\{|\tilde{n}_1\tilde{n}_2\tilde{n}_3\rangle\}$ of occupation of the states $|\tilde{1}\rangle$, $|\tilde{2}\rangle$ and $|\tilde{3}\rangle$:

$$\tilde{\rho} = \sum_{\tilde{n}_1\tilde{n}_2\tilde{n}_3\tilde{v}_1\tilde{v}_2\tilde{v}_3} |\tilde{n}_1\tilde{n}_2\tilde{n}_3\rangle\langle\tilde{v}_1\tilde{v}_2\tilde{v}_3|\tilde{\rho}_{(\tilde{n}_1\tilde{n}_2\tilde{n}_3),(\tilde{v}_1\tilde{v}_2\tilde{v}_3)}. \tag{51}$$

Using the shorthand $\tilde{n}$ for the triplet $\tilde{n}_1\tilde{n}_2\tilde{n}_3$, we can write the tomogram as

$$\omega(\tilde{\Omega}) = \sum_{\tilde{n}\tilde{v}} \langle 00A|R_{23}(\tilde{\Omega})|\tilde{n}_1\tilde{n}_2\tilde{n}_3\rangle\langle\tilde{v}_1\tilde{v}_2\tilde{v}_3|R_{23}(\tilde{\Omega})|00A\rangle\tilde{\rho}_{(\tilde{n}_1\tilde{n}_2\tilde{n}_3),(\tilde{v}_1\tilde{v}_2\tilde{v}_3)}. \tag{52}$$

As the $R_{23}(\bar{\Omega})$ rotation does not affect the first atomic index and acts irreducibly as an $\mathfrak{SU}(2)$ rotation in each the subspace spanned by states having a common fixed $\tilde{n}_1$, we write

$$|\tilde{n}_1\tilde{n}_2\tilde{n}_3\rangle \to |\tilde{n}_1; Im\rangle, \qquad |\tilde{v}_1\tilde{v}_2\tilde{v}_3\rangle \to |\tilde{v}_1; I\mu\rangle, \tag{53}$$

where

$$I = \tfrac{1}{2}(\tilde{n}_2 + \tilde{n}_3) = \tfrac{1}{2}(\tilde{v}_2 + \tilde{v}_3), \qquad m = \tfrac{1}{2}(\tilde{n}_2 - \tilde{n}_3), \qquad \mu = \tfrac{1}{2}(\tilde{v}_2 - \tilde{v}_3). \tag{54}$$

Furthermore, the tomograms of equation (52) must have $\tilde{n}_1 = \tilde{v}_1 = 0$, so equation (54) leads to

$$\omega(\tilde{\Omega}) = \sum_{m\mu} \mathcal{D}_{-I,m}^I(\tilde{\Omega})\mathcal{D}_{-I,\mu}^{I*}(\tilde{\Omega})\tilde{\rho}_{(0;Im),(0;I\mu)}$$
$$= \sum_{m\mu L} (-1)^{-I-\mu} C_{II,I-I}^{L0} C_{Im,I-\mu}^{LM} \mathcal{D}_{0,M}^L(\tilde{\Omega})\tilde{\rho}_{(0;Im),(0;I\mu)}, \tag{55}$$

where $\tilde{\rho}_{(n_1n_2n_3),(v_1v_2v_3)} \to \tilde{\rho}_{(n_1;Im),(v_1;I\mu)}$ has been used to conform to the notation of equation (53), where $\mathcal{D}_{mm'}^I$ is the usual $\mathfrak{SU}(2)\mathcal{D}$ function and where $C_{L_1m_1,L_2m_2}^{LM}$ is an $\mathfrak{SU}(2)$ Clebsch–Gordan coefficient.

Table 1. Basis states for two atoms in the Λ configuration.

$|n_1 n_2 n_3\rangle$	$|\tilde{1}\rangle^{n_1} |2\rangle^{n_2} |3\rangle^{n_3}$	
$|002\rangle$	$|\tilde{3}\rangle|\tilde{3}\rangle$	$|0; 1, -1\rangle$
$|011\rangle$	$\frac{1}{\sqrt{2}}(|\tilde{2}\rangle|\tilde{3}\rangle + |\tilde{3}\rangle|\tilde{2}\rangle)$	$|0; 1, 0\rangle$
$|020\rangle$	$|\tilde{2}\rangle|\tilde{2}\rangle$	$|0; 1, 1\rangle$
$|101\rangle$	$\frac{1}{\sqrt{2}}(|\tilde{1}\rangle|\tilde{3}\rangle + |\tilde{3}\rangle|\tilde{1}\rangle)$	$\left|1; \frac{1}{2}, -\frac{1}{2}\right\rangle$
$|110\rangle$	$\frac{1}{\sqrt{2}}(|\tilde{1}\rangle|\tilde{2}\rangle + |\tilde{2}\rangle|\tilde{1}\rangle)$	$\left|1; \frac{1}{2}, \frac{1}{2}\right\rangle$
$|200\rangle$	$|\tilde{1}\rangle|\tilde{1}\rangle$	$|2; 0, 0\rangle$

Multiplying both sides of (55) by $\mathcal{D}_{0,M}^{L'*}(\tilde{\Omega})$, integrating over $\mathfrak{SU}(2)$ and using orthogonality of the Clebsch–Gordan coefficients rapidly gives the elements of the density matrix that can be reconstructed from the tomographic process as

$$\tilde{\rho}_{(0;Im),(0;I\mu)} = (-1)^{I+\mu} \sum_L \frac{2L+1}{8\pi^2} C_{Im,I-\mu}^{LM} \left(C_{II,I-I}^{L0} \right)^{-1} \int d\tilde{\Omega}\, \omega(\tilde{\Omega}) \mathcal{D}_{0,M}^{L*}(\tilde{\Omega}). \tag{56}$$

4.2. Reconstruction for state of one and two Λ-type atoms

In a system containing a single atom, the Hilbert space is spanned, in the notation of equation (53), by states of the form $|\tilde{n}_1; Im\rangle$, with

$$|\tilde{1}\rangle = |100\rangle, \qquad |\tilde{2}\rangle = \left|0; \frac{1}{2}\frac{1}{2}\right\rangle, \qquad |\tilde{3}\rangle = \left|0; \frac{1}{2}, -\frac{1}{2}\right\rangle. \tag{57}$$

Under the evolution $\tilde{U}_\Lambda(\tilde{\Omega}) = R_{23}(\tilde{\Omega})$, the initial state $\left|0; \frac{1}{2}, -\frac{1}{2}\right\rangle$ cannot reach the dark state so it is only possible to reconstruct element of ρ of the form $\rho_{(0;\frac{1}{2}m),(0;\frac{1}{2}m')}$, with $m, m' = \pm\frac{1}{2}$. The last diagonal element, $\rho_{(1;00),(1;00)}$ can be inferred from the normalization. None of the remaining four matrix elements can be determined by our scheme.

In the two-atom case, an even smaller proportion of matrix elements can be recovered. Using again the notation of equation (53), states of the irrep $(2, 0)$ are conveniently given, in the occupational, tensor product and $\mathfrak{SU}(2)$ basis $|\tilde{n}_1; \ell m\rangle$, in table 1.

The initial state $|002\rangle$ will not evolve out of the $I = 1$ subspace, so only matrix elements of the form $\rho_{(0;1m)(0;1m')}$ can be reconstructed using our scheme. These represent only nine of the possible 36 elements of the density matrix.

We conclude this section by noting that the situation obviously worsens (in the sense that a smaller and smaller proportions of the matrix elements can be recovered) as the number of atoms increases.

5. Degenerate Ξ-type atomic systems

Finally, we consider the case of the Ξ system. It is illustrated, for a single atom, in figure 4. For this configuration, the condition $E_2 - E_1 = E_3 - E_2$ holds.

5.1. The evolution

In the rotating frame, the Hamiltonian governing the evolution of a collection of A atoms in the Ξ configuration in an external field has the form ($g_1 = g_2 = g$)
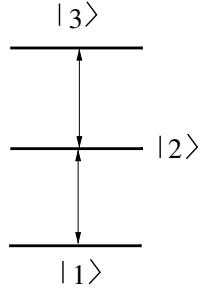
Figure 4. The Ξ configuration for a single atom.

$$\hat{H}_\Xi = \Delta(\hat{S}_{33} - \hat{S}_{11}) + g(\hat{S}_{12} + \hat{S}_{32} + \hat{S}_{21} + \hat{S}_{23}), \tag{58}$$

where $\Delta = \frac{1}{2}(E_3 - E_1) - \omega$.

Important insight into the nature of this Hamiltonian can be gained by noting that the operators $\hat{S}_{11} - \hat{S}_{33}$ and $\hat{S}_{12} + \hat{S}_{21} + \hat{S}_{23} + \hat{S}_{32}$ are, in fact, proportional to two of the three generators of the $\mathfrak{so}(3)$ subalgebra of $\mathfrak{su}(3)$:

$$\hat{S}_{11} - \hat{S}_{33} \mapsto \hat{L}_z, \qquad \hat{S}_{12} + \hat{S}_{21} + \hat{S}_{23} + \hat{S}_{32} \mapsto \sqrt{2}\hat{L}_x. \tag{59}$$

Thus, the possible evolutions are elements of the $\mathfrak{SO}(3)$ subgroup of $\mathfrak{SU}(3)$.

Clearly, a convenient sequence of pulse is given by

$$U_\Xi(\Omega) \equiv R^z(\alpha) \cdot R^x(\beta) \cdot R^z(\gamma),$$
$$= R^z(\alpha + \pi/2) \cdot R^y(\beta) \cdot R^z(\gamma - \pi/2). \tag{60}$$

Here, the resonant pulses are of the form

$$R^x(\beta) = \exp(-i\beta(\hat{S}_{12} + \hat{S}_{21} + \hat{S}_{32} + \hat{S}_{32})/\sqrt{2}) \tag{61}$$

while the dispersive pulses are generated by $\hat{S}_{11} - \hat{S}_{33}$.

It is important to note that, in the one-atom case, the exponentiation of $\hat{H}_\Xi$ in equation (58) produces an evolution that acts irreducibly on the non-degenerate states of the Hilbert space: in contrast with equation (49) of the Λ case, the 'rotations' R^x and R^z of the Ξ states are not restricted to a two-dimensional subspace of the whole Hilbert space.

To analyze the many-atom case, we start by observing that the state of the system for which every the atom is completely excited, $|00A\rangle$, is an eigenstate of $\hat{L}_z$ with eigenvalue $m = -A$ and is annihilated by $\hat{L}_-$. Here, $\hat{L}_- = (\hat{S}_{21} + \hat{S}_{32})/\sqrt{2}$ is constructed in the usual way: $\hat{L}_- = \hat{L}_x - i\hat{L}_y$. Thus, $|00A\rangle$ is the unique angular momentum state $|L, -L\rangle$, with $L = A$:

$$|00A\rangle \to |L = A, M = -A\rangle. \tag{62}$$

As this state contains the largest possible number of excitations, it can be uniquely identified through photon counting so that the corresponding tomogram is determined from the probability of detecting $2A$ photons in the irradiated field.

The general correspondence between the occupational basis states $|n_1 n_2 n_3\rangle$ is found in [20] and given by

$$|LM\rangle = \sqrt{\frac{2^{L+M}\left(\frac{1}{2}(A+L)\right)!(L+M)!(L-M)!(2L+1)}{\left(\frac{1}{2}(A-L)\right)!(A+L+1)!}}$$
$$\times \left((a_2^\dagger)^2 - 2a_1^\dagger a_3^\dagger\right)^{\frac{1}{2}(A-L)} \sum_p \frac{(a_1^\dagger)^p (a_2^\dagger)^{L+M-2p} (a_3^\dagger)^{p-M}}{2^p p!(p-M)!(L+M-p)!}|0\rangle. \tag{63}$$

Table 2. Angular momentum basis states as linear combinations of occupational number states for one and two atoms in the Ξ configuration.

A	L	M	$|LM\rangle$
1	1	1	$a_1^\dagger|0\rangle$
		0	$a_2^\dagger|0\rangle$
		-1	$a_3^\dagger|0\rangle$
2	2	2	$\frac{1}{\sqrt{2}}\left(a_1^\dagger\right)^2|0\rangle$
		1	$a_2^\dagger a_1^\dagger|0\rangle$
		0	$\frac{1}{\sqrt{3}}\left((a_2^\dagger)^2 + a_1^\dagger a_3^\dagger\right)|0\rangle$
		-1	$a_2^\dagger a_3^\dagger|0\rangle$
		-2	$\frac{1}{\sqrt{2}}(a_3^\dagger)^2|0\rangle$
2	0	0	$\frac{1}{\sqrt{6}}\left((a_2^\dagger)^2 - 2a_1^\dagger a_3^\dagger\right)|0\rangle$

It is clear that, given an angular momentum state in the irrep $(A, 0)$ of $\mathfrak{su}(3)$, we can unambiguously write it as a linear combination of occupational states, and vice versa. Thus, we may expand

$$\rho = \sum_{L_1 M_1 L_2 M_2} |L_1 M_1\rangle\langle L_2 M_2|\rho_{L_1 M_1, L_2 M_2}, \tag{64}$$

where L_1, L_2 run from A, $A - 2, \ldots, 1$ or 0 depending if A is even or odd.

As the evolution is necessarily an element of $\mathfrak{SO}(3)$, the tomogram takes the general form

$$\omega(\Omega) = \sum_{L_1 M_1 L_2 M_2} \langle A, -A|R(\Omega)|L_1 M_1\rangle\langle L_2 M_2|R^\dagger(\Omega)|A, -A\rangle\rho_{L_1 M_1, L_2 M_2},$$

$$= \sum_{M_1 M_2} \mathcal{D}^A_{-A, M_1}(\Omega)\mathcal{D}^{A*}_{-A, M_2}(\Omega)\rho_{A M_1, A M_2},$$

$$= \sum_{M_1 M_2 J} (-1)^{-A-M_2}\mathcal{D}^J_{0, M}(\Omega) C^{J0}_{A-A, AA} C^{JM}_{AM_1, AM_2}\rho_{AM_1, AM_2}, \tag{65}$$

with $C^{JM}_{L_1 M_1, L_2 M_2}$ a regular angular momentum Clebsch–Gordan coefficient.

In a manner similar to the previous cases, multiplication by $\mathcal{D}^{J'*}_{0, M}(\Omega)$, integration over $\mathfrak{SO}(3)$ and orthogonality of Clebsch–Gordan coefficients yields

$$(-1)^{A+M_2}\rho_{AM_1 AM_2} = \sum_J \frac{2J+1}{8\pi^2} C^{JM}_{AM_1, AM_2}\left(C^{J0}_{A-A, AA}\right)^{-1} \int \mathrm{d}\Omega\, \mathcal{D}^{J*}_{0, M}(\Omega)\omega(\Omega). \tag{66}$$

The result clearly shows that only those linear combinations of occupational state that transform by angular momentum $L = A$ can be reconstructed.

5.2. Examples: one- and two-atom cases

For a single atom, we see from table 2, that the tomogram is constructed from an $L = 1$ state. There is no other angular momentum multiplet and so the evolution, an element of $\mathfrak{SO}(3)$, will yield sufficiently many tomograms to guarantee complete reconstruction.

The matter is different for the two-atom case. In this case, the tomogram is constructed using an $L = 2$ state but the Hilbert space also contains an $L = 0$ subspace, which cannot

be reached from $L = 2$ with our evolution. Thus, if we are limited to measuring a total of $2A$ photons, it will only be possible to recover $\rho_{2M,2M'}$ and impossible to reconstruct $\rho_{00,2M}$, $\rho_{00,00}$, $\rho_{2M,00}$. This is because, in our scheme, it is not possible to extract photons from the $L = 0$ state, and the absence of photon does not pin down a particular state.

It may be possible to measure fewer than $2A$ photons, but this does not lead to more information. There is only one state with $M = A$ and one state with $M = A - 1$ (or $M = -A$ and $M = -(A - 1)$). It is possible to use the $L = A$, $M = A - 1$ state for the tomogram and measure $2A - 1$ or $2A - 2$ photons, but we will recover nothing more than if we had started with $L = A$, $M = A$.

There are two states with $M = A - 2$; they belong different angular momentum multiplet. Thus, if we measure, say, a total of $2(A - 2)$ photons, it is not possible to know unambiguously if this is the result of a complete cascade within the $L = A - 1$ multiplet or a partial cascade within the $L = A$ multiplet. This kind of limitation becomes obviously more severe as the number of angular momentum multiplet containing a given M value increases.

6. Conclusions

We have proposed a physical realization applicable to the reconstruction of the quantum state of three-level atomic systems. The information about atomic states is extracted by measuring the total number of excitations after successive applications of electromagnetic field pulses.

We have shown that, in the non-degenerate case, the complete reconstruction of atomic states is possible. Although the number of independent parameters required for a complete reconstruction is less than needed for the complete parametrization of a generic element of $\mathfrak{SU}(3)$ group, a complete reconstruction is possible because, in addition to the usual evolution of the system, another tool is available in the reconstruction scheme: the projective measurement.

When degeneracies are present, the possibilities of reconstruction are limited. The origin of these limitations is essentially different for atoms in Λ and Ξ configuration. In both cases, the evolution operator operators belong to a subgroup of the whole $\mathfrak{SU}(3)$ group, and our work illuminates the subtle distinction between the global properties of $\mathfrak{SO}(3)$ and $\mathfrak{SU}(2)$ as subgroups of $\mathfrak{SU}(3)$.

In the Ξ case, the reconstruction is rooted in an $\mathfrak{SO}(3)$ symmetry of the physically available evolution operator; this symmetry provides information about a single subspace. In the one-atom case, the Hilbert space contains precisely a single $\mathfrak{SO}(3)$ subspace, so the density matrix can be completely reconstructed. In the multiple-atom case, only reconstruction in one pre-determined subspace is possible. In this case, our protocol would be to apply the sequence of pulses of equation (60) with a subsequent measurement of the number of $2A$ of photons in the irradiated field, giving us the tomogram appearing in the reconstruction formula of equation (66). For completeness, we note here that we did not consider the effective two-photon-like transition in the Ξ system due to extremely narrow width of such transitions ($\sim g^2/\Delta$), which leads to serious experimental difficulties in its detection.

In the case of Λ configuration, the evolution operator generates an $\mathfrak{SU}(2)$ transformation and, even in the one-atom case, there is always more than a single $\mathfrak{SU}(2)$ multiplet: a complete reconstruction is impossible because there always exists invariant $\mathfrak{SU}(2)$ 'dark' subspaces, which cannot be uniquely identified by measuring irradiated photons. We stress that the decomposition of the Hilbert space into invariant subspaces occurs as a result of the inability to access independent transitions separately; this to be contrasted with the approach of [9], wherein $\mathfrak{SU}(2)$ decomposability arises from considerations of perfectly general polarization

states. Note also that although the effective transitions between degenerate levels in the Λ case are not sensitive to the atom-field detunings, they still require long interaction times.

The tomographic protocol for Λ differs from the Ξ. After application of the sequence of pulses equation (24) to a Λ-type atom, we have to measure the probability of detecting zero irradiated photons, which leads to the tomogram used in equation (39).

Finally, we observe that the tomographic reconstruction process for a collection of non-degenerate three-level atoms is a simple generalization of the familiar process used for two-level quantum systems. In both instances, one uses the whole dynamic symmetry group to carry out the inversion process. In contrast to this, we are restricted to a specific subgroup in the degenerate cases, which essentially reduces our tools and actually limits the possibility of the complete tomographic reconstruction.

Acknowledgments

Appendix A. $\mathfrak{SU}(3)$ basis states and $\mathcal{D}$-functions

In this section, we review some notation useful mostly in section 3. Further details can be found in [18].

The correspondence between the occupational basis and states of the $(A, 0)$ is

$$|n_1 n_2 n_3\rangle \mapsto |(A, 0)nI\rangle. \tag{A.1}$$

In equation (A.1) and throughout this paper, n is a shorthand for $(n_1 n_2 n_3)$. Here, the $(A, 0)$ labels indicate that $|n_1 n_2 n_3\rangle$ can be reached, using the $\hat{S}_{ij}$ operators of equation (6), from the state $|A00\rangle$. This state is killed by the so-called $\mathfrak{su}(3)$ raising operators $\hat{S}_{12}$, $\hat{S}_{13}$ and $\hat{S}_{23}$. The eigenvalues of the $\mathfrak{su}(3)$ diagonal operators

$$\hat{\mathfrak{h}}_1 = \hat{S}_{11} - \hat{S}_{22}, \qquad \hat{\mathfrak{h}}_2 = \hat{S}_{22} - \hat{S}_{33}, \tag{A.2}$$

acting on $|A00\rangle$ are, respectively, $(A, 0)$.

The angular momentum label I is necessary to deal with the general case considered in [18], where states of more general families of the type (p, q) are constructed. A state $|(p, q)nI\rangle$ can be reached from the state $\left|(p, q)(p+q, q, 0)\frac{1}{2}p\right\rangle$, i.e. with $n_1 = p+q, n_2 = q, n_3 = 0$ and $I = \frac{1}{2}p$. $\left|(p, q)(p + q, q, 0)\frac{1}{2}p\right\rangle$ is killed by the $\mathfrak{su}(3)$ raising operators, and the eigenvalues of $(\hat{\mathfrak{h}}_1, \hat{\mathfrak{h}}_2)$ are (p, q). When p and q are both nonzero, it is possible to have distinct states in the same (p, q) family that have identical n, so the angular momentum label I is required to distinguish these distinct states.

Some calculations require the evaluation of the matrix elements

$$\langle n_1 n_2 n_3 | \bar{U}(\sigma) | n_1 n_2 n_3 \rangle^* = \langle (A, 0)nI | \bar{U}(\sigma) | (A, 0)\nu I' \rangle^*,$$
$$\equiv \mathcal{D}_{nI,\nu I'}^{(A,0)*}(\sigma). \tag{A.3}$$

This matrix element is related to the matrix element between basis states of the irrep $(0, A)$, which is conjugate to $(A, 0)$, by

$$\mathcal{D}_{nI,\nu I'}^{(A,0)*}(\tau) = (-1)^{n_2+\nu_2} \mathcal{D}_{n^*I,\nu^*I'}^{(0,A)}(\tau). \tag{A.4}$$

Here,

$$\mathcal{D}_{n^*I,\nu^*I'}^{(0,A)}(\tau) \equiv \langle (0, A)n^*I | \bar{U}(\sigma) | (0, A)\nu^*I' \rangle. \tag{A.5}$$

The relation between n and n^* is

$$n = (n_1, n_2, n_3) \mapsto n^* = (A - n_1, A - n_2, A - n_3). \tag{A.6}$$

Using this and the results from [18], one can verify equation (A.4).

   The dimension of $(0, A)$ is the same as the dimension of $(A, 0)$, but the construction of [18] for basis state of $|(0, A)n^*I\rangle$ requires twice as many quanta as the basis states of $|(A, 0)nI\rangle$.

   Using equation (A.4), one can also verify that the $\mathcal{D}$ functions are orthogonal, in the sense that

$$\frac{\dim(\lambda, \mu)}{1024\pi^5} \int d\Omega \, \mathcal{D}_{nI,vL}^{(\lambda,\mu)*}(\Omega) \mathcal{D}_{n'I',v'L'}^{(\lambda',\mu')}(\Omega) = \delta_{\lambda\lambda'}\delta_{\mu\mu'}\delta_{nn'}\delta_{II'}\delta_{vv'}\delta_{LL'}, \tag{A.7}$$

where

$$d\Omega = \sin\beta_1 \cos\tfrac{1}{2}\beta_2 \left(\sin\tfrac{1}{2}\beta_2\right)^3 \sin\beta_3 \, d\alpha_1 \, d\beta_1 \, d\gamma_1 \, d\alpha_2 \, d\beta_2 \, d\alpha_3 \, d\beta_3 \, d\gamma_3 \tag{A.8}$$

is the invariant measure, which can be found in the usual ways [21]. The normalization follows from the dimensionality formula

$$\dim(\lambda, \mu) = \tfrac{1}{2}(\lambda + 1)(\mu + 1)(\lambda + \mu + 2) \tag{A.9}$$

for the irrep (λ, μ) and the use the parameter range

$$\begin{aligned}
0 \leqslant \alpha_1 \leqslant 4\pi, && 0 \leqslant \beta_1 \leqslant \pi, && 0 \leqslant \gamma_1 \leqslant 4\pi, \\
0 \leqslant \alpha_2 \leqslant 2\pi, && 0 \leqslant \beta_2 \leqslant \pi, && \\
0 \leqslant \alpha_3 \leqslant 4\pi, && 0 \leqslant \beta_3 \leqslant \pi, && 0 \leqslant \gamma_3 \leqslant 4\pi.
\end{aligned} \tag{A.10}$$

Appendix B. Reduced $\mathfrak{SU}(3)$ Clebsch–Gordan coefficients

B.1. Basis states

The construction of states in the irrep (p, q) of $\mathfrak{su}(3)$ is detailed in [18]. We can summarize this procedure by stating that one requires, at a minimum, a total of $p + 2q$ bosons. These bosons must be of at least two types when $q \neq 0$. Thus, if $a_{ij}^\dagger$ creates a boson of type j in mode i, we define, quite generally,

$$\hat{S}_{k\ell} = a_{k1}^\dagger a_{\ell 1} + a_{k2}^\dagger a_{\ell 2}. \tag{B.1}$$

   If $|0\rangle$ denotes state with no boson excitation, the state

$$\begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger \end{vmatrix}^q \left(a_{11}^\dagger\right)^p |0\rangle \sim \left|(p, q)(p + q, q, 0); \tfrac{1}{2}q\right\rangle, \tag{B.2}$$

containing $p + q$ bosons in mode 1, q boson in mode 2 and none in mode 3 , belongs to the (p, q) irrep. It is, in fact, killed by every $\hat{S}_{k\ell}$ with $\ell > k$ and is thus the highest weight state of (p, q). Here,

$$\begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger \end{vmatrix} = a_{11}^\dagger a_{22}^\dagger - a_{12}^\dagger a_{21}^\dagger \tag{B.3}$$

is the determinant of the matrix. Other states in (p, q) are obtained by laddering down from $\left|(p, q)(p + q, q, 0); \tfrac{1}{2}q\right\rangle$.

This is not the only possibility. One can verify that

$$\left|(p,q)(p+q+t, q+t, t); \tfrac{1}{2}q\right)$$

$$= \begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger & a_{13}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger & a_{23}^\dagger \\ a_{31}^\dagger & a_{32}^\dagger & a_{33}^\dagger \end{vmatrix}^t \begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger \end{vmatrix}^q (a_{11}^\dagger)^p |0\rangle,$$

$$\sim \begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger & a_{13}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger & a_{23}^\dagger \\ a_{31}^\dagger & a_{32}^\dagger & a_{33}^\dagger \end{vmatrix}^t \left|(p,q)(p+q, q, 0); \tfrac{1}{2}q\right\rangle, \tag{B.4}$$

visibly contains $p + 2q + 3t$ bosons but is equivalent to the state of equation (B.2) because the determinant

$$\begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger & a_{13}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger & a_{23}^\dagger \\ a_{31}^\dagger & a_{32}^\dagger & a_{33}^\dagger \end{vmatrix} \tag{B.5}$$

is an $\mathfrak{SU}(3)$ scalar.

More generally, if the usual ket $|(p,q)nI\rangle$ denotes a state in (p,q) containing $p + 2q$ bosons, then the (round) ket

$$|(p,q)nI) = \begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger & a_{13}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger & a_{23}^\dagger \\ a_{31}^\dagger & a_{32}^\dagger & a_{33}^\dagger \end{vmatrix}^t |(p,q)nI\rangle \tag{B.6}$$

differs from $|(p,q)nI\rangle$ by at most a normalization but contains $p + 2q + 3t$ bosons.

B.2. $\mathfrak{SU}(3)$ Clebsch–Gordan coefficients

The $\mathfrak{SU}(3)$-coupling $(A, 0) \otimes (0, A)$ can be decomposed in the direct sum [19]

$$(A, 0) \otimes (0, A) = (A, A) \oplus (A - 1, A - 1) \oplus \cdots \oplus (0, 0),$$

$$= \bigoplus_{\lambda=0}^{A} (\lambda, \lambda).3 \tag{B.7}$$

The irrep (σ, σ) occurs at most once in the decomposition.

To compute $\mathfrak{SU}(3)$ Clebsch–Gordan coefficients for states in the series of equation (B.7), we must couple states of the form

$$|(A, 0)nI_1\rangle|(0, A)\nu^* I_2\rangle, \tag{B.8}$$

which contain a total of $3A$ bosons of three types. States in the irrep (σ, σ) of the series of equation (B.7) are of the form

$$|(\sigma, \sigma)NI_3\rangle = \begin{vmatrix} a_{11}^\dagger & a_{12}^\dagger & a_{13}^\dagger \\ a_{21}^\dagger & a_{22}^\dagger & a_{23}^\dagger \\ a_{31}^\dagger & a_{32}^\dagger & a_{33}^\dagger \end{vmatrix}^{A-\sigma} |(\sigma, \sigma)N^{(\sigma)}I_3\rangle, \tag{B.9}$$

where $|(\sigma, \sigma)N^{(\sigma)}I_3\rangle$ is the state with 3σ bosons described in [18].

Table B1. The one-atom case. Reduced $\mathfrak{SU}(3)$ Clesbsh–Gordan coefficients for $(1,0) \otimes (0,1) \to (0,0)$.

N_1	I_3	n_1	I_1	v_1^*	I_2	$\left\langle \begin{smallmatrix} (1,0) & (0,1) \\ n_1 I_1 & v_1^* I_2 \end{smallmatrix} \middle\| \begin{smallmatrix} (0,0) \\ N_1^{(\sigma)} I_3 \end{smallmatrix} \right\rangle$
0	0	0	$\frac{1}{2}$	1	$\frac{1}{2}$	$-\sqrt{\frac{2}{3}}$
		1	0	0	0	$+\sqrt{\frac{1}{3}}$

Table B2. The one-atom case. Reduced $\mathfrak{SU}(3)$ Clesbsh–Gordan coefficients for $(1,0) \otimes (0,1) \to (1,1)$.

N_1	I_3	n_1	I_1	v_1^*	I_2	$\left\langle \begin{smallmatrix} (1,0) & (0,1) \\ n_1 I_1 & v_1^* I_2 \end{smallmatrix} \middle\| \begin{smallmatrix} (1,1) \\ N_1^{(\sigma)} I_3 \end{smallmatrix} \right\rangle$
2	$\frac{1}{2}$	1	0	1	$\frac{1}{2}$	$+1$
1	1	0	$\frac{1}{2}$	1	$\frac{1}{2}$	$+1$
1	0	0	$\frac{1}{2}$	1	$\frac{1}{2}$	$+\sqrt{\frac{1}{3}}$
		1	0	0	0	$+\sqrt{\frac{2}{3}}$
0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	$+1$

Table B3. The two-atom case. Reduced $\mathfrak{SU}(3)$ Clesbsh–Gordan coefficients for $(2,0) \otimes (0,2) \to (0,0)$.

N_1	I_3	n_1	I_1	v_1^*	I_2	$\left\langle \begin{smallmatrix} (2,0) & (0,2) \\ n_1 I_1 & v_1^* I_2 \end{smallmatrix} \middle\| \begin{smallmatrix} (0,0) \\ N_1^{(\sigma)} I_3 \end{smallmatrix} \right\rangle$
0	0	0	1	2	1	$+\sqrt{\frac{1}{2}}$
		1	$\frac{1}{2}$	1	$\frac{1}{2}$	$-\sqrt{\frac{1}{3}}$
		2	0	0	0	$+\sqrt{\frac{1}{6}}$

Note that, because the state $|(\sigma,\sigma)N^{(\sigma)}I_3\rangle$ does not contain $3A$ bosons, we do not have $n_i + v_i^* = N_i^{(\sigma)}$ etc but rather

$$n_i + v_i^* = N_i^{(\sigma)} + (A - \sigma). \tag{B.10}$$

Thus we have

$$|(\sigma,\sigma)N^{(\sigma)}I_3\rangle = \sum_{n v I_1 I_2} |(A,0)n I_1\rangle |(0,A)v^* I_2\rangle \left\langle \begin{matrix} (A,0) & (0,A) \\ n I_1 & v^* I_2 \end{matrix} \middle| \begin{matrix} (\sigma,\sigma) \\ N^{(\sigma)} I_3 \end{matrix} \right\rangle, \tag{B.11}$$

where $M_1 = \frac{1}{2}(n_2 - n_3)$, $M_2 = \frac{1}{2}(v_3 - v_2)$. The phases of the states $|(A,0)n I_1\rangle$, $|(0,A)v^* I_2\rangle$ and $|(\sigma,\sigma)N^{(\sigma)}I_3\rangle$ are those of [18]. The phase of the Clebsch–Gordan coefficient is determined by forcing

$$\text{sign}\left(\left\langle \begin{matrix} (A,0) & (0,A) \\ (A00)\frac{1}{2}A & v^* I_2 \end{matrix} \middle| \begin{matrix} (\sigma,\sigma) \\ (2\sigma,\sigma,0)\frac{1}{2}\sigma \end{matrix} \right\rangle\right) = +. \tag{B.12}$$

As always, it is convenient to rewrite equation (B.11) as

$$|(\sigma,\sigma)N^{(\sigma)}I_3\rangle = \sum_{n v} |(A,0)n I_1\rangle |(0,A)v^* I_2\rangle \left\langle \begin{matrix} (A,0) & (0,A) \\ n_1 I_1 & v_1^* I_2 \end{matrix} \middle\| \begin{matrix} (\sigma,\sigma) \\ N_1^{(\sigma)} I_3 \end{matrix} \right\rangle C_{I_1 M_1, I_2 M_2}^{I_3 M_3} \tag{B.13}$$

Table B4. The two-atom case. Reduced $\mathfrak{SU}(3)$ Clesbsh–Gordan coefficients for $(2,0) \otimes (0,2) \rightarrow (1,1)$.

N_1	I_3	n_1	I_1	v_1^*	I_2	$\left\langle \begin{smallmatrix} (2,0) & (0,2) \\ n_1 I_1 & v_1^* I_2 \end{smallmatrix} \middle\| \begin{smallmatrix} (1,1) \\ N_1^{(\sigma)} I_3 \end{smallmatrix} \right\rangle$
2	$\frac{1}{2}$	1	$\frac{1}{2}$	2	1	$-\sqrt{\frac{3}{5}}$
		2	0	1	$\frac{1}{2}$	$+\sqrt{\frac{2}{5}}$
1	0	0	1	2	1	$-\sqrt{\frac{2}{5}}$
		1	$\frac{1}{2}$	1	$\frac{1}{2}$	$-\sqrt{\frac{1}{15}}$
		2	0	0	0	$\sqrt{\frac{8}{15}}$
1	1	0	1	2	1	$-\sqrt{\frac{4}{5}}$
		1	$\frac{1}{2}$	1	$\frac{1}{2}$	$+\sqrt{\frac{1}{5}}$
0	$\frac{1}{2}$	0	1	1	$\frac{1}{2}$	$-\sqrt{\frac{3}{5}}$
		1	$\frac{1}{2}$	0	0	$+\sqrt{\frac{2}{5}}$

Table B5. The two-atom case. Reduced $\mathfrak{SU}(3)$ Clesbsh–Gordan coefficients for $(2,0) \otimes (0,2) \rightarrow (2,2)$.

N_1	I_3	n_1	I_1	v_1^*	I_2	$\left\langle \begin{smallmatrix} (2,0) & (0,2) \\ n_1 I_1 & v_1^* I_2 \end{smallmatrix} \middle\| \begin{smallmatrix} (2,2) \\ N_1^{(\sigma)} I_3 \end{smallmatrix} \right\rangle$
0	1	0	1	0	0	$+1$
1	$\frac{1}{2}$	0	1	1	$\frac{1}{2}$	$+\sqrt{\frac{2}{5}}$
		1	$\frac{1}{2}$	0	0	$+\sqrt{\frac{3}{5}}$
1	$\frac{3}{2}$	0	1	1	$\frac{1}{2}$	$+1$
2	2	0	1	2	1	$+1$
2	1	0	1	2	1	$+\sqrt{\frac{1}{5}}$
		1	$\frac{1}{2}$	1	$\frac{1}{2}$	$+\sqrt{\frac{4}{5}}$
2	0	0	1	2	1	$+\sqrt{\frac{1}{10}}$
		1	$\frac{1}{2}$	1	$\frac{1}{2}$	$+\sqrt{\frac{3}{5}}$
		2	0	0	0	$+\sqrt{\frac{3}{10}}$
3	$\frac{1}{2}$	1	$\frac{1}{2}$	2	1	$+\sqrt{\frac{2}{5}}$
		2	0	1	$\frac{1}{2}$	$+\sqrt{\frac{3}{5}}$
3	$\frac{3}{2}$	1	$\frac{1}{2}$	2	1	$+1$
4	1	2	0	2	1	$+1$

where $C^{I_3 M_3}_{I_1 M_1, I_2 M_2}$ is the usual $\mathfrak{su}(2)$ coupling coefficient and the reduced Clebsch–Gordan $\left\langle \begin{smallmatrix} (A,0) & (0,A) \\ n_1 I_1 & v_2^* I_2 \end{smallmatrix} \middle\| \begin{smallmatrix} (\sigma,\sigma) \\ N_1^{(\sigma)} I_3 \end{smallmatrix} \right\rangle$ does not depend on M_i. Tables B1 to B5 are provided for calculations involving $A = 2$ and $A = 1$.

Appendix C. Final form of the density matrix for the non-degenerate case

In this section, we present the technical steps to obtain equation (39) from equation (38).

First, multiply both sides of equation (38) by $\mathcal{D}^{(\mu,\mu)*}_{(\mu\mu\mu)0,N^{(\mu)}J'}(\tau)$ for fixed $N^{(\mu)}$ and fixed J', integrate over the $\mathfrak{SU}(3)$-invariant measure of equation (A.8) and rearrange. This produces

$$
\frac{(\mu+1)^3}{1024\pi^5}
\left\langle \begin{matrix} (A,0) & (0,A) \\ (A00)0 & (0AA)0 \end{matrix} \middle| \begin{matrix} (\mu,\mu) \\ (\mu\mu\mu)0 \end{matrix} \right\rangle^{-1}
\int \mathrm{d}\tau\, \mathcal{D}^{(\mu,\mu)*}_{(\mu\mu\mu)0,N^{(\mu)}J'}(\tau)\omega(\tau)
$$

$$
= \sum_{n\nu}(-1)^{\nu_2}\rho_{n,\nu}
\left\langle \begin{matrix} (A,0) & (0,A) \\ nI & \nu^*I' \end{matrix} \middle| \begin{matrix} (\mu,\mu) \\ N^{(\mu)}J' \end{matrix} \right\rangle . \tag{C.1}
$$

In this last expression, the sums over n and ν are not independent but linked by equation (36).

To complete the inversion, we use orthogonality of $\mathfrak{SU}(3)$ CGs:

$$
\sum_{\mu J'}
\left\langle \begin{matrix} (A,0) & (0,A) \\ nI & \nu^*I' \end{matrix} \middle| \begin{matrix} (\mu,\mu) \\ N^{(\mu)}J' \end{matrix} \right\rangle
\left\langle \begin{matrix} (A,0) & (0,A) \\ \bar{n}\bar{I} & \bar{\nu}^*\bar{I}' \end{matrix} \middle| \begin{matrix} (\mu,\mu) \\ N^{(\mu)}J' \end{matrix} \right\rangle
= \delta_{\bar{n}n}\delta_{\bar{I}I}\delta_{\bar{\nu}\nu}\delta_{\bar{I}'I'}, \tag{C.2}
$$

and rearrange the notation to finally yield equation (39).

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