Excitations in 2-state Systems

The Jaynes-Cummings Model

Paul Durham

Scientific Computing Department, STFC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK

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Abstract

These notes contain material on two-state systems (qubits) and their coupling with light. The key elements of this are

- 1. the Rabi Model (RM), in which a 2-level "atom" interacts with an electromagnetic field which is described classically;
- 2. the Jaynes-Cummings Model (JCM), in which the same system is described using a quantised photon field.

The Rabi Model is interesting as a simple spectroscopic problem which is exactly soluble to all orders in the field. Some illuminating comparisons can be made with first order perturbation theory, which gives Golden Rule-type results.

But the real focus is the Jaynes-Cummings Model. Here, the same 2-state excitation problem is solved exactly in full quantum electrodynamics. The idea of "dressed states" (products of electron and photon states) is useful in this. A further trick, potentially useful for any 2-state system, is to map the problem on to a spin ½ model. The appendices give some useful algebra for 2x2 matrices, using spin ½ language.

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1 Excitation by a periodic field: non-perturbative methods

The elementary theory of excitation by a periodic field is the standard time-dependent perturbation theory (see [1]) which, to first order, leads to expressions of the Golden Rule type. However, the simple system of 2 discrete electron levels coupled by a monochromatic periodic field of frequency ω is a surprising rich one, admitting exact analytic solutions correct to all orders in the field. The Rabi Model (RM) treats this problem semi-classically – quantised electrons, classical field – and solves it exactly, as we show in section 2. One illuminating aspect of this is the comparison with the results of the traditional first order time-dependent perturbation theory – \dot{a} la Dirac, Golden Rule etc.

Section 3 gives the fully quantised version of this problem – ie a two-level electronic system ("atom") plus a photon system. This is called the Jaynes-Cummings Model (JCM) [2]. It can be solved in many ways. Gerry and Knight [3] give a treatment involving the solution of the time-dependent Schrödinger equation, very similar to that of the RM in section 2. They also give alternative treatments, which are outlined here, involving first the so-called "dressed states" of the model (ie the full eigenfunctions of the coupled electron-photon system) and second the density matrix. Neither of these treatments would really be possible in the semi-classical description, so I'm using them here to emphasise the fully quantised character of the JCM. Since it is a full QED calculation, it contains quantum electrodynamical effects such as spontaneous emission. In addition, the density matrix treatment is convenient when looking at complex photon fields (mixed states, thermal states etc).

A couple of useful review articles ([4], [5]) give further details of these methods and of extensions of the JCM to, for example, 3-level atoms. The JCM can also be elaborated to describe multiple 2-state systems interacting with a periodic field; this is the so-called Tavis-Cummings Model [6], [7].

Finally, we note that 2-state systems are better known these days as qubits. Examples of qubits are too numerous to name; I evoke them just to emphasize that the techniques used here apply very widely to all qubit problems.

2 The Rabi Model

We first solve the time-dependent Schrödinger equation directly as an ordinary differential equation in time for this simple 2-discrete-level model:



Figure 1: the basic 2-level electron system considered in the RM and JCM

The Hamiltonian for this problem (see [1], working always in the Schrödinger picture) is:

$$\mathcal{H} = \mathcal{H}_{0} + \mathcal{V}(t) \tag{2.1}$$

where, guaranteeing that $\mathcal{V}(t)$ is Hermitian,

$$\mathcal{V}(t) = \frac{1}{2} \left(v e^{-i\omega t} + v^{\dagger} e^{i\omega t} \right)$$
(2.2)

Here v is the electron-photon interaction, but in this section the details don't matter; we only need to know that it is periodic and monochromatic, or single mode.

We start in the same way as the Dirac method described in [1], expanding in unperturbed states:

$$\begin{split} \left|\psi(t)\right\rangle = \sum_{n} c_{n}(t) \left|\varphi_{n}(t)\right\rangle = \sum_{n} c_{n}(t) e^{-i\varepsilon_{n}} \left|n\right\rangle \\ \left|\varphi_{n}(t)\right\rangle = e^{-i\varepsilon_{n}} \left|n\right\rangle \\ \mathcal{H}_{0}\left|n\right\rangle = \varepsilon_{n}\left|n\right\rangle \end{split}$$

and use this to write the time-dependent Schrödinger equation as follows

$$i\dot{c}_{m}(t) = \sum_{n} \langle \varphi_{m}(t) | \mathcal{V}(t) | \varphi_{n}(t) \rangle c_{n}(t)$$

Now assume that $\mathcal{V}^{s}(t)$ has no diagonal matrix elements in the unperturbed states – if it did you'd build them into the unperturbed Hamiltonian, wouldn't you? So we can write the time-dependent Schrödinger equation as

$$i\dot{c}_{m}(t) = \sum_{n \neq m} V_{mn}(t) e^{-i(\varepsilon_{n} - \varepsilon_{m})t} c_{n}(t)$$

where

$$V_{mn}(t) \equiv \langle m | \mathcal{V}(t) | n \rangle = \frac{1}{2} (v_{mn} e^{-i\omega t} + v_{nm}^* e^{i\omega t})$$
$$v_{mn} \equiv \langle m | v(t) | n \rangle$$

so that

$$\dot{c}_{m}(t) = -\frac{i}{2} \sum_{m \neq n} \left\{ v_{mn} e^{-i(\omega + \omega_{nm})t} + v_{nm}^{*} e^{i(\omega - \omega_{nm})t} \right\} c_{n}(t)$$
(2.3)

where $\omega_{nm} \equiv \varepsilon_n - \varepsilon_m = -\omega_{mn}$. Equation (2.3) is exact and pretty general for a single mode periodic perturbation; of course it is really a set of coupled equations, one for each state in the spectrum of the unperturbed system. We'll now go quite carefully through the application of the **rotating wave approximation (RWA)** [1] to the two-state model – it's not especially subtle but I want to write it out properly just once. It amounts to retaining only terms in the interaction that can lead to resonance, and is thus valid for detunings close to resonance.

Suppose that only the two states $|e\rangle$ and $|g\rangle$ need be considered and suppose that $|e\rangle$ lies at a higher energy than $|g\rangle$, as in the above diagram: $\omega_{eg} \equiv \omega_0 > 0$. Thus (2.3) reduces to the following two equations:

$$\dot{c}_{e}(t) = -\frac{i}{2} \left\{ v_{eg} e^{-i(\omega + \omega_{ge})t} + v_{ge}^{*} e^{i(\omega - \omega_{ge})t} \right\} c_{g}(t) = -\frac{i}{2} \left\{ v_{eg} e^{-i(\omega - \omega_{eg})t} + v_{ge}^{*} e^{i(\omega + \omega_{eg})t} \right\} c_{g}(t)$$
$$\dot{c}_{g}(t) = -\frac{i}{2} \left\{ v_{ge} e^{-i(\omega + \omega_{eg})t} + v_{eg}^{*} e^{i(\omega - \omega_{eg})t} \right\} c_{e}(t)$$

Now it's easy to identify the resonant terms and make the rotating wave approximation by dropping the others. In terms of the detuning parameter Δ defined by

$$\Delta = \omega_0 - \omega = \omega_{eg} - \omega = \varepsilon_e - \varepsilon_g - \omega$$

we obtain

$$\dot{c}_{e}(t) = -\frac{iv}{2} e^{i\Delta t} c_{g}(t)$$

$$\dot{c}_{g}(t) = -\frac{iv^{*}}{2} e^{-i\Delta t} c_{e}(t)$$
(2.4)

in which we've set $v = v_{eg}$ just to simplify the notation for a while. Note that the second equation of (2.4) contains the "negative frequency" component of the perturbation – it has to do with stimulated emission. So we just have to solve these equations subject to the initial conditions

$$c_e(t=0)=0$$

 $c_g(t=0)=1$
(2.5)

The usual way of proceeding (see [3] or [8]) is to differentiate one of these equations and substitute from the other to get an ordinary differential equation of 2^{nd} order for $c_e(t)$. This is solved using a simple ansatz and the two arbitrary constants are obtained from the initial conditions. But since this an initial value problem, let's solve it using Laplace transforms [9], just for fun and to vary a little from the standard path.

The Laplace transforms of a function f(t) and its derivative $\frac{df}{dt}$ are the following (see [10], for example) :

$$L\{f(t)\} \equiv \int_{0}^{\infty} dt f(t) e^{-pt} \equiv \overline{f}(p)$$

$$L\{\frac{df}{dt}\} = -f(t=0) + p\overline{f}(p)$$
(2.6)

The Laplace transforms of (2.4) are thus

$$-c_{e}(t=0) + p\overline{c}_{e}(p) = -\frac{i\nu}{2}\overline{c}_{g}(p-i\Delta)$$
$$-c_{g}(t=0) + p\overline{c}_{g}(p) = -\frac{i\nu^{*}}{2}\overline{c}_{e}(p+i\Delta)$$

where we have used the obvious extension $L\{fe^{iqt}\} = \overline{f}(p-iq)$. Using the initial conditions (2.5) we get

$$p\overline{c}_{e}(p) = -\frac{i\nu}{2}\overline{c}_{g}(p-i\Delta)$$

$$-1 + p\overline{c}_{g}(p) = -\frac{i\nu^{*}}{2}\overline{c}_{e}(p+i\Delta)$$
(2.7)

Replacing $p \rightarrow p - i\Delta$ in the second of these equations and substituting in the first, we get

$$\overline{c}_{e}(p) = \frac{-iv/2}{p(p-i\Delta) + |v|^{2}/4}$$
(2.8)

Now, en route to recognising the inverse transform, define the Rabi frequency Ω_R by

$$\Omega_{R} = \sqrt{\Delta^{2} + \left| \mathbf{v} \right|^{2}} \tag{2.9}$$

and use this in the last equation to get

$$\overline{c}_{e}(p) = -\frac{iv}{\Omega_{R}} \left[\frac{\Omega_{R}/2}{\left(p - i\Delta\right)^{2} + \left(\Omega_{R}/2\right)^{2}} \right]$$

Now we can use the result

$$L^{-1}\left\{\frac{b}{\left(p+a\right)^{2}+b^{2}}\right\}=e^{-at}\sin\left(bt\right)$$

to obtain

$$c_{e}(t) = -ive^{i\Delta t/2} \frac{\sin(\Omega_{R}t/2)}{\Omega_{R}}$$
(2.10)

Note that if $\Delta = 0$ then $\Omega_R = |v|$. Therefore exactly at resonance $c_e(t)$ oscillates between its extreme values of 0 and 1 regardless of the strength |v| of the coupling.

From (2.4) we immediately find

$$c_{g}(t) = \frac{e^{-i\Delta t/2}}{\Omega_{R}} \Big[\Omega_{R} \cos(\Omega_{R} t/2) + i\Delta \sin(\Omega_{R} t/2) \Big]$$

The transition probability is thus given by

$$P_{eg}(t) = |c_{e}(t)|^{2} = |v|^{2} \frac{\sin^{2}(\Omega_{R}t/2)}{\Omega_{R}^{2}}$$
(2.11)

This is the result for the transition probability as a function of time in the Rabi Model. Of course the solution for $c_g(t)$ can be found immediately, if required. Note that one recovers the result [1] of first order time-dependent perturbation theory, PT(1), immediately if $|\Delta| \gg |v|$, when $\Omega_R \rightarrow |\Delta|$. The exact result has the same form as the PT(1) result with the Rabi frequency acting as a *renormalised detuning* which removes the PT(1) divergence at resonance. To make a comparison between the two results for various times and frequencies, it's convenient to define scaled times and frequencies as follows:

$$\tilde{t} = |\mathbf{v}|t$$

$$\tilde{\Delta} = \Delta / |\mathbf{v}|$$

$$\tilde{\Omega}_{R} = \Omega_{R} / |\mathbf{v}| = \sqrt{\tilde{\Delta}^{2} + 1}$$
(2.12)

Now the PT(1) limit is $\tilde{\Delta} \gg 1$ and we get the following universal formulae (with the effect of the size of the matrix element removed):

$$P_{eg}(t) = \frac{\sin^{2}(\tilde{\Omega}_{R}\tilde{t})}{\tilde{\Omega}_{R}^{2}} \qquad Rabi Model$$

$$P_{eg}(t) = \frac{\sin^{2}(\tilde{\Delta}\tilde{t})}{\tilde{\Delta}^{2}} \qquad PT(1)$$
(2.13)

Exactly at resonance, $\Delta = 0$, the transition probability in the Rabi Model is still finite and oscillates with frequency $\Omega_R^0 = |v|$ between states $\{c_e(t)=0, c_g(t)=1\}$ and $\{c_e(t)=1, c_g(t)=0\}$. These are the famous Rabi oscillations:



Figure 2: Rabi oscillations

The system behaves somewhat like a pair of coupled classical oscillators in which the energy of motion moves back and forth between the oscillators with a frequency determined by the coupling strength. This is interesting in its own right, of course, and apparently useful in NMR, but it is dependent on a completely coherent, entirely monchromatic single mode perturbing field acting on two discrete electronic levels. These are quite special circumstances – perhaps they need microwave cavities etc. This sounds quite far from the standard set up for electronic spectroscopy in condensed matter.

The difference between the two results is illustrated for a small value of the scaled detuning parameter in the following diagram:



Figure 3: Exact result compared to 1st order perturbation theory

Clearly the PT(1) result continues to grow to large values comparable to 1 (in violation of the PT(1) assumption) as time increases, while the Rabi Model result is saturating.

3 The Jaynes-Cummings Model

The Jaynes-Cummings Model (JCM), described in detail by Gerry and Knight [3], looks at the same 2level electron system but treats the field in a fully quantised way; in quantum electrodynamics (QED), fields are observables and hence become operators. Note, as the algebra unfolds, that because the field is treated as a quantised dynamical variable in its own right, the JCM Hamiltonian does not depend on time, unlike that of the semi-classical RM. The time development of JCM states comes from the dynamical phase factors associated with energy eigenkets. Thus, the QED Rabi oscillations emerge in a somewhat different way from the RM, and have a richer behaviour.

3.1 Transforming to a pseudo-spin representation

The model is the same as that depicted above in Figure 1. The state space in the JCM is thus the product of the 2-level electron state space $\{|e\rangle, |g\rangle\}$ and the photon number state space $\{|n\rangle\}$. This section writes the Hamiltonian in terms of what are essentially annihilation and creation operators for the electron states and for the photon states, and then turns the electronic part of this into a pseudo-spin representation within the 2-level electronic state space. Underlying this, of course, is the fact that *any* 2x2 Hamiltonian matrix can be written (see Appendix A:) in terms of the Pauli matrices:

$$\boldsymbol{\sigma}_{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \boldsymbol{\sigma}_{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \boldsymbol{\sigma}_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ \text{plus} \ \boldsymbol{\sigma}_{0} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
(3.1)

Note that our convention for the ordering of the electron states in the 2x2 matrix representation is

 $|e\rangle$ then $|g\rangle$, thus $\begin{pmatrix} ee & eg\\ ge & gg \end{pmatrix}$.

The total Hamiltonian of the electron-photon system is

$$\mathcal{H} = \mathcal{H}_{A} + \mathcal{H}_{F} + \mathcal{H}_{int} \tag{3.2}$$

To get a symmetrical form for the Hamiltonian of the atom, we'll take the origin of electronic energies to be half way between the two levels:

$$\varepsilon_e = \frac{1}{2}\omega_0, \quad \varepsilon_g = -\frac{1}{2}\omega_0$$

so that

$$\mathbf{H}_{A} = \begin{pmatrix} \varepsilon_{e} & 0 \\ 0 & \varepsilon_{g} \end{pmatrix} = \frac{\omega_{0}}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\omega_{0}}{2} \boldsymbol{\sigma}_{3}$$
(3.3)

Thus the operator for the atom Hamiltonian is given by

$$\mathcal{H}_{A} = \frac{\omega_{0}}{2} \left(|e\rangle \langle e| - |g\rangle \langle g| \right)$$
(3.4)

Then the matrix elements of \mathcal{H}_{A} in the 2-level state space $\{|e\rangle, |g\rangle\}$ gives the matrices in (3.3).

The Hamiltonian of the field is given (omitting the zero-point energy – irrelevant to the dynamics here) in terms of the photon annihilation and creation operators:

$$\mathcal{H}_{r} = \omega a^{\dagger} a \tag{3.5}$$

Note that there's only one photon mode here, one frequency. We're considering a strictly singlemode field.

The interaction term is just

$$\mathcal{H}_{int} = -\boldsymbol{d} \cdot \boldsymbol{\mathcal{E}}$$

Where d is the electron dipole operator, and the electric field operator is given by

$$\mathcal{E} = \mathbf{e} \left(\frac{\hbar \omega}{\varepsilon_0 V} \right)^{1/2} \sin(kz) \left(\mathbf{a} + \mathbf{a}^{\dagger} \right)$$
(3.6)

This is a single-mode field of frequency ω propagating in the z-direction with polarisation along the unit vector **e** in the x,y-plane. Thus we can write

$$\mathcal{H}_{\rm int} = \mathcal{J}g\left(\mathbf{a} + \mathbf{a}^{\dagger}\right) \tag{3.7}$$

Where d = d.e and

$$g = -\left(\frac{\hbar\omega}{\varepsilon_0 V}\right)^{1/2} \sin(kz)$$

Now define the transition operators S_{\pm} and the inversion operator S_3 as follows:

$$s_{+} = |e\rangle\langle g| \qquad \mathbf{\sigma}_{+} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$s_{-} = |g\rangle\langle e| \qquad \mathbf{\sigma}_{+} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$s_{3} = (|e\rangle\langle e| - |g\rangle\langle g|) \qquad \mathbf{\sigma}_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(3.8)

The inversion operator is obviously represented in the 2-level state space $\{|e\rangle, |g\rangle\}$ by one of the Pauli matrices – hence the notation. In fact, the operators s_{\pm} are raising and lowering operators in a spin-1/2 algebra and s_3 is the z-component of the spin¹ (all easily checked by working out the commutators). To be explicit:

$$\boldsymbol{\sigma}_{\pm} = \frac{1}{2} \big(\boldsymbol{\sigma}_1 \pm i \boldsymbol{\sigma}_2 \big)$$

Now define the matrix element of the dipole operator:

$$\boldsymbol{d} = \langle \boldsymbol{e} | \boldsymbol{d} | \boldsymbol{g} \rangle \tag{3.9}$$

which we can take to be a real number. By parity, there can't be any diagonal matrix elements of the dipole operator in the 2-level state space, and so we can write the operator as follows:

$$d = d^* |e\rangle \langle g| + d|g\rangle \langle e| = d(s_+ + s_-)$$
(3.10)

Using this in (3.7) and defining $\lambda \equiv dg$, we obtain

$$\mathcal{H}_{\rm int} = \lambda \left(s_+ + s_- \right) \left(a + a^{\dagger} \right) \tag{3.11}$$

Now we make the rotating wave approximation which amounts to dropping the terms in s_+a^+ (corresponding to excitation of an electron from state g to e with *emission* of a photon) and s_-a^- (corresponding to de-excitation of an electron from state e to g with *absorption* of a photon). These terms contribute dynamical phase factors $e^{\pm i(\omega+\omega_0)t}$ which can't lead to resonance. The interaction term in the RWA is

$$\mathcal{H}_{\rm int} = \lambda \left(s_+ a + s_- a^{\dagger} \right) \tag{3.12}$$

and the full JCM Hamiltonian is thus

$$\mathcal{H} = \frac{\omega_0}{2} s_3 + \omega a^{\dagger} a + \lambda \left(s_+ a + s_- a^{\dagger} \right)$$
(3.13)

This Hamiltonian supports a couple of constants of the motion (ie operators that commute with \mathcal{H}):

• the "electron number" $\mathcal{P} \equiv |e\rangle \langle e| + |g\rangle \langle g|$, which is 1 in the 2-level state space;

¹ Actually *S* is twice the spin. This is the algebra of a spin $\frac{1}{2}$ system, but we are forgetting about the factor of $\frac{1}{2}$ that should relate the spin operators to the Pauli matrices – it's irrelevant here.

• the "excitation number":

$$\mathcal{N} = \partial^{\dagger} \partial + |e\rangle \langle e| \tag{3.14}$$

It's obvious that $[\mathcal{P}, \mathcal{H}] = 0$. It's not so obvious that $[\mathcal{N}, \mathcal{H}] = 0$, but some algebra shows that it is so. Now it's easy to show that the full Hamiltonian (3.13) can also be written in terms of the detuning parameter $\Delta = \omega_0 - \omega$ as follows:

$$\mathcal{H} = \omega_0 \left(\mathcal{N} - \frac{1}{2} \right) - \Delta \mathfrak{z}^\dagger \mathfrak{z} + \lambda \left(s_+ \mathfrak{z} + s_- \mathfrak{z}^\dagger \right)$$
(3.15)

From this we can immediately see that exactly at resonance, when $\Delta = 0$, the free atom and field part of the Hamiltonian contains only a constant of the motion. The dynamics at resonance therefore depend only on the interaction term.

Note: Far from resonance in the JCM – dispersive interaction

When the detuning Δ becomes large, one can derive an effective Hamiltonian by expanding the evolution operator in powers of Δ^{-1} . In [I] this produces

$$\mathsf{T}\left[\exp\left(-\frac{i}{\hbar}\right)\int_{0}^{t}dt'\mathcal{H}(t')\right] \simeq 1 - \frac{it}{\hbar}\mathcal{H}_{eff}$$

where

$$\mathcal{H}_{eff} = \frac{\lambda^2}{\Delta} \left(S_+ S_- + a^{\dagger} a S_3 \right)$$

But $s_+s_- = |e\rangle\langle e|$. Thus \mathcal{H}_{eff} is diagonal in the product 2-level and photon state space. It doesn't cause any (real) transitions because they don't conserve energy. It amounts to a <u>dispersive</u> interaction. Gerry and Knight [3] show that it also evolves certain states, entangled in a Schrödinger's Cat sense, in an interesting way.

3.2 The product space of bare states

To summarize the previous section, the JCM Hamiltonian in the rotating wave approximation is

$$\mathcal{H} = \mathcal{H}_{A} + \mathcal{H}_{F} + \mathcal{H}_{int} = \frac{\omega_{0}}{2} s_{3} + \omega \overline{a}^{\dagger} \overline{a} + \lambda \left(s_{+} \overline{a} + s_{-} \overline{a} \right)$$
(3.16)

where

$$\lambda = -\left(\frac{\hbar\omega}{\varepsilon_0 V}\right)^{1/2} \sin(kz) \langle e | \mathbf{d} \cdot \mathbf{e} | \mathbf{g} \rangle$$
(3.17)

This Hamiltonian operates in a product space $S = |i\rangle \otimes |n\rangle$ spanned by the two electron states $|i\rangle = |e\rangle$ or $|g\rangle$ and field states of a definite photon number $|n\rangle$; in other words, in the state space of the JCM we can take as a basis the set of product states $|i\rangle \otimes |n\rangle$, where the first ket refers to the electron system - $|i\rangle = |e\rangle$ or $|g\rangle$ - and the second ket refers to the field – n is the number of photons.

These "bare" states are eigenstates of the non-interacting Hamiltonian $\mathcal{H}_A + \mathcal{H}_F$. Because the excitation number, whose operator is defined in (3.14), is a good quantum number, it can be used to classify the bare states thus:

Here I indicate explicitly that these are direct product states, and then omit the direct product symbol for notational simplicity.

The forms and energies, ie the eigenvalues of the non-interacting Hamiltonian are given in the following table:

Excitation number N	Bare state $\varphi_{_{\!N}}^{(\pm)}$	Energy $\varepsilon_{N}^{(\pm)} = \left\langle \varphi_{N}^{(\pm)} \middle \left(\frac{\omega_{0}}{2} s_{3} + \omega \beta^{\dagger} \beta \right) \middle \varphi_{N}^{(\pm)} \right\rangle$
1	$\left arphi_{1}^{(+)} ight angle \equiv \left e ight angle \left 0 ight angle$	$\varepsilon_1^{(+)} = \frac{\omega_0}{2} = \frac{1}{2}\omega + \frac{\Delta}{2}$
1	$\left arphi_{1}^{(-)} ight angle \equiv \left g ight angle \left 1 ight angle$	$\varepsilon_1^{(-)} = -\frac{\omega_0}{2} + \omega = \frac{1}{2}\omega - \frac{\Lambda}{2}$
2	$\left arphi_{2}^{(+)} ight angle \equiv \left oldsymbol{e} ight angle \left oldsymbol{1} ight angle$	$\varepsilon_2^{(+)} = \frac{\omega_0}{2} + \omega = \frac{3}{2}\omega + \frac{\Delta}{2}$
2	$\left arphi_{2}^{(-)} ight angle \equiv \left g ight angle \left 2 ight angle$	$\varepsilon_{2}^{(-)} = -\frac{\omega_{0}}{2} + 2\omega = \frac{3}{2}\omega - \frac{\Delta}{2}$
N	$\left \varphi_{N}^{(+)} \right\rangle \equiv \left e \right\rangle \left N - 1 \right\rangle$	$\varepsilon_{N}^{(+)} = \frac{\omega_{0}}{2} + (N-1)\omega = \left(N - \frac{1}{2}\right)\omega + \frac{\Delta}{2}$
N	$\left \left \varphi_{\scriptscriptstyle N}^{(-)} \right\rangle \equiv \left g \right\rangle \left N \right\rangle$	$\varepsilon_{N}^{(-)} = -\frac{\omega_{0}}{2} + N\omega = \left(N - \frac{1}{2}\right)\omega - \frac{\Delta}{2}$

where we used the detuning parameter defined in section 2:

$$\Delta = \omega - \omega_0 = \omega - \omega_{eq} = \omega - \varepsilon_e + \varepsilon_q \tag{3.19}$$

So the energy level diagram for these bare states looks like this:



Figure 4: Energies of the bare states in the JCM

At resonance, bare states $|\varphi_N^+\rangle$, $|\varphi_N^-\rangle$ are degenerate. Indeed, because the excitation number *N* is a good quantum number of the full Hamiltonian, only bare states with the same *N* can couple. Therefore the Hamiltonian matrix has a block-diagonal form

$$\mathbf{H} = \begin{pmatrix} \mathbf{h}^{(1)} & \cdots & 0 & \cdots \\ \vdots & \ddots & 0 & \cdots \\ 0 & 0 & \mathbf{h}^{(N)} & 0 \\ \vdots & \vdots & 0 & \ddots \end{pmatrix}$$
(3.20)

where the block corresponding to excitation number N has a 2x2 form which direct calculation now easily shows to be

$$\mathbf{h}^{(N)} = \begin{pmatrix} \varepsilon_N^{(+)} & \lambda N^{1/2} \\ \lambda N^{1/2} & \varepsilon_N^{(-)} \end{pmatrix} = \begin{pmatrix} (N-1/2)\omega + \Delta/2 & \lambda N^{1/2} \\ \lambda N^{1/2} & (N-1/2)\omega - \Delta/2 \end{pmatrix}$$
(3.21)

3.3 Dressed states

We can now find the exact eigenstates of the full Hamiltonian – the "dressed" states - by working only within the 2x2 subspace corresponding to a given excitation number. Consider only the subspace of states with excitation number N = n+1, that is the subspace spanned by bare states

Note that the photon number covers the interval $0 \le n \le \infty$, while the excitation number covers the interval $1 \le N \le \infty$. In this subspace we just have to diagonalise the 2x2 matrix given in (3.21) and we

can use the general results of Appendix A: to do this. We simply write (3.21) in the generic form given by (A.3).

Here we give the results of putting the 2x2 sub-block $\mathbf{h}^{(N)}$ given by (3.21) into the canonical form (A.3). Straightforward algebra gives

$$h_{0}^{(N)} = (N - 1/2)\omega$$

$$h_{1}^{(N)} = \lambda N^{1/2}$$

$$h_{2}^{(N)} = 0$$

$$h_{3}^{(N)} = \Delta/2$$

$$h^{(N)} \equiv \left\{ \left(h_{1}^{(N)}\right)^{2} + \left(h_{2}^{(N)}\right)^{2} + \left(h_{3}^{(N)}\right)^{2} \right\} = \Omega_{N}/2$$
(3.23)

where the quantum electrodynamic Rabi frequency is defined by

$$\Omega_{N} = \sqrt{\Delta^{2} + 4\lambda^{2}N} = \sqrt{\Delta^{2} + 4\lambda^{2}(n+1)}$$
(3.24)

In terms of the angle parameters introduced in Appendix A:, we easily find the following results:

$$\phi_N = 0, \ \sin\theta_N = \frac{2\lambda N^{1/2}}{\Omega_N}, \ \cos\theta_N = \frac{\Delta}{\Omega_N}, \ \tan\theta_N = \frac{2\lambda N^{1/2}}{\Delta}$$
 (3.25)

Equivalently,

$$\sin\frac{\theta_{N}}{2} = \frac{\left(\Omega_{N} - \Delta\right)}{2\Omega_{N}}, \ \cos\frac{\theta_{N}}{2} = \frac{\left(\Omega_{N} + \Delta\right)}{2\Omega_{N}}$$
(3.26)

From (A.6), the exact eigenkets of the full electron-photon Hamiltonian, the "dressed" states, are given by

$$\left| \psi_{N}^{(+)} \right\rangle = \cos \frac{\theta_{N}}{2} \left| \varphi_{N}^{(+)} \right\rangle + \sin \frac{\theta_{N}}{2} \left| \varphi_{N}^{(-)} \right\rangle$$

$$\left| \psi_{N}^{(-)} \right\rangle = -\sin \frac{\theta_{N}}{2} \left| \varphi_{N}^{(+)} \right\rangle + \cos \frac{\theta_{N}}{2} \left| \varphi_{N}^{(-)} \right\rangle$$

$$(3.27)$$

Thus the eigenfunctions and eigenvalues of the dressed states corresponding to excitation number N or photon number n=N-1 can be written, using (3.26), as follows:

$$\left|\psi_{N}^{(+)}\right\rangle = \left(\frac{\Omega_{N}+\Delta}{2\Omega_{N}}\right)^{1/2} |e\rangle|n\rangle + \left(\frac{\Omega_{N}-\Delta}{2\Omega_{N}}\right)^{1/2} |g\rangle|n+1\rangle, \quad E_{N}^{(+)} = (N-1/2)\omega + \Omega_{N}/2$$

$$\left|\psi_{N}^{(-)}\right\rangle = \left(\frac{\Omega_{N}-\Delta}{2\Omega_{N}}\right)^{1/2} |e\rangle|n\rangle + \left(\frac{\Omega_{N}+\Delta}{2\Omega_{N}}\right)^{1/2} |g\rangle|n+1\rangle, \quad E_{N}^{(-)} = (N-1/2)\omega - \Omega_{N}/2$$
(3.28)

and the energy level diagram for the full interacting system with excitation number n+1 is as follows:



Figure 5: Energies of the dressed states in the JCM

Since we now have the exact eigenstates of the Hamiltonian, calculating the dynamics is easy:

- Specify the initial state $|\Psi(0)\rangle$ of the atom and field;
- Write $|\Psi(0)
 angle$ in terms of the dressed states $|\psi_{\scriptscriptstyle N}^{(\pm)}
 angle$;
- $|\Psi(t)
 angle$ is then obtained simply by including the dynamical phase factors $e^{-i\mathcal{E}_N^{(\pm)}t}$.

Applying this recipe to a specific case, let the atom be initially in $|e\rangle$ and the field in some pure state $\sum c_n |n\rangle$. Then

$$\Psi(\mathbf{0}) = \sum_{n=0}^{\infty} c_n |e\rangle |n\rangle = \sum_{N=1}^{\infty} c_{N-1} |\varphi_N^{(+)}\rangle$$
(3.29)

But from (3.27)

$$\left|\varphi_{N}^{(+)}\right\rangle = \cos\frac{\theta_{N}}{2}\left|\psi_{N}^{(+)}\right\rangle - \sin\frac{\theta_{N}}{2}\left|\psi_{N}^{(-)}\right\rangle$$
(3.30)

At later times, therefore, we simply have (omitting an irrelevant overall phase factor of $e^{-i(N-1/2)\omega t}$)

$$\left|\Psi(t)\right\rangle = \sum_{N=1}^{\infty} c_{N-1} \left(\cos\frac{\theta_N}{2} e^{-i\Omega_N t/2} \left|\psi_N^{(+)}\right\rangle - \sin\frac{\theta_N}{2} e^{i\Omega_N t/2} \left|\psi_N^{(-)}\right\rangle\right)$$
(3.31)

That's it! Let's use this to calculate the time-dependent inversion, the difference in the populations of states $|e\rangle$ and $|g\rangle$ given by the expectation value of the inversion operator s_3 (see (3.8))

$$W(t) \equiv \langle \Psi(t) | S_3 | \Psi(t) \rangle$$

We find (noting that S_3 can't connect states with different numbers of photons)

$$W(t) = \sum_{N=1}^{\infty} |c_{N-1}|^{2} \begin{cases} \cos^{2} \frac{\theta_{N}}{2} \langle \psi_{N}^{(+)} | s_{3} | \psi_{N}^{(+)} \rangle + \sin^{2} \frac{\theta_{N}}{2} \langle \psi_{N}^{(-)} | s_{3} | \psi_{N}^{(-)} \rangle \\ -\sin \frac{\theta_{N}}{2} \cos \frac{\theta_{N}}{2} \left(e^{i\Omega_{N}t} \langle \psi_{N}^{(+)} | s_{3} | \psi_{N}^{(-)} \rangle + e^{-i\Omega_{N}t} \langle \psi_{N}^{(-)} | s_{3} | \psi_{N}^{(+)} \rangle \right) \end{cases}$$

The matrix elements are easily found, using (3.27), to be

$$\left\langle \psi_{N}^{(+)} \middle| s_{3} \middle| \psi_{N}^{(+)} \right\rangle = \cos \theta_{N} = \left\langle \psi_{N}^{(-)} \middle| s_{3} \middle| \psi_{N}^{(-)} \right\rangle$$

$$\left\langle \psi_{N}^{(+)} \middle| s_{3} \middle| \psi_{N}^{(-)} \right\rangle = -\sin \theta_{N} = \left\langle \psi_{N}^{(-)} \middle| s_{3} \middle| \psi_{N}^{(+)} \right\rangle$$

$$(3.32)$$

Thus the inversion is given by

$$W(t) = \sum_{N=1}^{\infty} \left| c_{N-1} \right|^2 \left\{ \cos^2 \theta_N + \sin^2 \theta_N \cos(\Omega_N t) \right\}$$
(3.33)

From this equation we can see that when the field is in a particular number state $|m\rangle$, ie $c_n = \delta_{nm}$, we just get Rabi oscillations with the single frequency $\Omega_m = \sqrt{\Delta^2 + 4\lambda^2 (m+1)}$. This is pretty similar to the semi-classical Rabi Model itself (see, for example, equation (2.9) in section 2), except that now we can have oscillations even without any photons (ie if m = 0). This is a typical QED effect – vacuum Rabi oscillations in which the atom spontaneously emits and re-absorbs a photon.

At resonance
$$(\Delta = 0)$$
, $\sin \frac{\theta_N}{2} = \frac{1}{\sqrt{2}} = \cos \frac{\theta_N}{2}$ and thus $\theta_N = \pi / 2$. Hence $\cos \theta_N = 0$, $\sin \theta_N = 1$ and

$$W(t) = \sum_{N=1}^{\infty} |c_{N-1}|^2 \cos(\Omega_N (\Delta = 0)t) = \sum_{N=1}^{\infty} |c_{N-1}|^2 \cos(2\lambda t \sqrt{n+1})$$
(3.34)

Now suppose the field is initially in a *coherent state*. In this case the coefficients in (3.29) are given by [3]

$$c_n = e^{-|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}}$$
(3.35)

where the parameter α is related to the average photon number of the field by $|\alpha|^2 = \overline{n}$. Thus at resonance

$$W(t) = e^{-n} \sum_{n} \frac{\overline{n}^{n}}{n!} \cos\left(2\lambda t \sqrt{n+1}\right)$$
(3.36)

The behaviour of this formula is illustrated below for a coherent state with $\overline{n} = 5$.



Figure 6: The inversion with the field initially in a coherent state

Now, although coherent states are generally supposed to be the quantum field states that resemble most closely classical states, the inversion behaves in a quite complex way: the oscillations apparently collapse but revive at a later time. Gerry and Knight discuss this behaviour [3]

3.4 The evolution operator

The evolution operator is

$$\mathcal{U}(t) = e^{-i\mathcal{H}t} \tag{3.37}$$

where the Hamiltonian is given by (3.15). We want to find, essentially as an exercise, the matrix representation of the evolution operator in the bare state space classified by excitation number, ie the states $\left|\varphi_{N}^{(\pm)}\right\rangle$ defined by (3.18). From section 3.2 we know that the Hamiltonian matrix in this representation has the block-diagonal form (3.20) with the sub-blocks taking the 2x2 form given by (3.21) and repeated here:

$$\mathbf{h}^{(N)} = \begin{pmatrix} \varepsilon_N^{(+)} & \lambda N^{1/2} \\ \lambda N^{1/2} & \varepsilon_N^{(-)} \end{pmatrix} = \begin{pmatrix} (N-1/2)\omega + \Delta/2 & \lambda N^{1/2} \\ \lambda N^{1/2} & (N-1/2)\omega - \Delta/2 \end{pmatrix}$$

But from Appendix B: we know that we can write the corresponding evolution matrix in the same block-diagonal form:

$$\mathbf{U}(t) = \begin{pmatrix} \mathbf{u}^{(1)} & \cdots & \mathbf{0} & \cdots \\ \vdots & \ddots & \mathbf{0} & \cdots \\ \mathbf{0} & \mathbf{0} & \mathbf{u}^{(N)} & \mathbf{0} \\ \vdots & \vdots & \mathbf{0} & \ddots \end{pmatrix}$$
(3.38)

where the sub-blocks are given by

$$\mathbf{u}^{(N)}(t) = e^{-i\mathbf{h}^{(N)}t} \tag{3.39}$$

If, following Appendix A:, we introduce the diagonalising matrix $s^{(N)}$ such that

$$\mathbf{s}^{(N)^{+}} \cdot \mathbf{h}^{(N)} \cdot \mathbf{s}^{(N)} = \begin{pmatrix} E_{N}^{(+)} & 0\\ 0 & E_{N}^{(-)} \end{pmatrix} = \begin{pmatrix} (N-1/2)\omega + \Omega_{N}/2 & 0\\ 0 & (N-1/2)\omega - \Omega_{N}/2 \end{pmatrix}$$
(3.40)

then we can write

$$\mathbf{u}^{(N)}(t) = \mathbf{s}^{(N)} \cdot \begin{pmatrix} e^{-iE_{N}^{(+)}t} & 0\\ 0 & e^{-iE_{N}^{(-)}t} \end{pmatrix} \cdot \mathbf{s}^{(N)+}$$
(3.41)

More explicitly, using (A.21) we can write this in terms of the generic parameters given in (3.23):

$$\mathbf{u}^{(N)}(t) = e^{-ih_0^{(N)}t} \begin{pmatrix} \cos(h^{(N)}t) - i\sin(h^{(N)}t)\cos\theta_N & -i\sin(h^{(N)}t)\sin\theta_N e^{-i\phi_N} \\ -i\sin(h^{(N)}t)\sin\theta_N e^{i\phi_N} & \cos(h^{(N)}t) + i\sin(h^{(N)}t)\cos\theta_N \end{pmatrix}$$
(3.42)

Substituting from (3.25) we then obtain

$$\mathbf{u}^{(N)}(t) = e^{-i(N-1/2)\omega t} \begin{pmatrix} \cos\left(\frac{\Omega_N t}{2}\right) - i\frac{\Delta}{\Omega_N}\sin\left(\frac{\Omega_N t}{2}\right) & -\left(\frac{2i\lambda N^{1/2}}{\Omega_N}\right)\sin\left(\frac{\Omega_N t}{2}\right) \\ -\left(\frac{2i\lambda N^{1/2}}{\Omega_N}\right)\sin\left(\frac{\Omega_N t}{2}\right) & \cos\left(\frac{\Omega_N t}{2}\right) + i\frac{\Delta}{\Omega_N}\sin\left(\frac{\Omega_N t}{2}\right) \end{pmatrix}$$
(3.43)

Finally, we note that exactly at resonance, when $\Delta = 0$ and $\Omega_N = 2\lambda N^{1/2}$, we find

$$\mathbf{u}^{(N)}(t,\Delta=0) = e^{-i(N-1/2)\omega t} \begin{pmatrix} \cos(\lambda N^{1/2}t) & -i\sin(\lambda N^{1/2}t) \\ -i\sin(\lambda N^{1/2}t) & \cos(\lambda N^{1/2}t) \end{pmatrix}$$
(3.44)

There will be problems for which this bare state representation will be a convenient one in which to follow the dynamics. However, in the JCM problem we know the exact eigenstates of the Hamiltonian, the dressed states. Clearly, the evolution operator is diagonal in the dressed states:

$$\left\langle \psi_{N}^{(\alpha)} \left| \mathsf{U}(t) \right| \psi_{N'}^{(\alpha')} \right\rangle = e^{-E_{N}^{(\alpha)} t} \delta_{NN'} \delta_{\alpha\alpha'} \qquad \alpha, \alpha' = +, -$$
(3.45)

We'll use this is the next section.

3.5 The density matrix

The dressed state method of section 3.2 is a powerful approach to the dynamics when the field is in a pure state. It's not so easy to see how to deal with mixed states of the field – in other words an ensemble of systems about which we have only statistical information; hence the appeal of a density matrix description. The basic features of density matrices are revised in Appendix C:.

In particular, if one has the density operator ρ for a 2-component system (here it's the atom A + field F) one can capture the information available about the atom alone in the reduced, or partial, density operator for the atom:

$$\rho^{(A)} = Tr^{(F)} \left[\rho \right] \tag{3.46}$$

where the trace is carried out over the quantum numbers of the field (usually photon numbers in our problem). A similar partial density operator for the field can be defined:

$$\rho^{(F)} = Tr^{(A)} [\rho]$$

in which the trace covers the two atomic states \ket{e} and \ket{g} .

Regarding the dynamics, if one has a density operator $\rho(0)$ at t = 0, corresponding to an ensemble of systems prepared in some experiment, then at time t the density operator is given by

$$\rho(t) = \mathcal{U}(t)\rho(0)\mathcal{U}^{\dagger}(t) \tag{3.47}$$

where $\mathcal{U}(t) = e^{-i\mathcal{H}t}$ is the evolution operator (assuming the Hamiltonian is not time-dependent, as is the case in the JCM).

Our central problem is to calculate the inversion W(t) at time t, given an initial state described by a density operator $\rho(t)$ at t = 0. For this, we just trace the inversion operator s_3 , given in (3.8), with the density operator:

$$W(t) = Tr[s_3\rho(t)] \equiv Tr^{(A)}Tr^{(F)}[s_3\rho(t)]$$
(3.48)

Since s_3 operates in the atom state space only² we can write (see (3.46))

$$W(t) = Tr^{(A)} \left[s_3 Tr^{(F)} \left[\rho(t) \right] \right] = Tr^{(A)} \left[s_3 \rho^{(A)}(t) \right]$$
(3.49)

Thus we need to calculate

$$\rho^{(A)}(t) = Tr^{(F)} \left[\mathcal{U}(t)\rho(0)\mathcal{U}^{\dagger}(t) \right]$$
(3.50)

Of course, if one wanted to study the dynamics of the field $\rho^{(F)}(t)$ would be the central quantity.

3.5.1 General dynamics in the JCM

Now, to proceed to the actual calculation for the JCM, we'll take the $Tr^{(F)}$ operation to be a sum over photon number states $|n\rangle$ and for the coupled system we'll work in the dressed state representation so that we can exploit the diagonality of the evolution operator in this representation (see section 3.4, equation (3.45)). Using the completeness and orthogonality of the dressed states we can thus write (3.50) as follows:

$$\rho^{(A)}(t) = \sum_{n=0}^{\infty} \sum_{N,N'=1}^{\infty} \sum_{\alpha,\alpha'} \left\langle n \left| \psi_{N}^{(\alpha)} \right\rangle e^{-iE_{N}^{(\alpha)}t} \left\langle \psi_{N}^{(\alpha)} \right| \rho(0) \left| \psi_{N'}^{(\alpha')} \right\rangle e^{iE_{N}^{(\alpha')}t} \left\langle \psi_{N'}^{(\alpha')} \right| n \right\rangle$$
(3.51)

By (3.27) we can express the dressed states in terms of the bare states and easily find

² Strictly speaking, we should define an "extension" of the inversion operator into the full product space in the way described by Cohen-Tannoudji et al [11], but the result is the same as that found here.

$$\left\langle n \middle| \psi_{N}^{(+)} \right\rangle = \cos \frac{\theta_{N}}{2} \middle| e \right\rangle \delta_{n,N-1} + \sin \frac{\theta_{N}}{2} \middle| g \right\rangle \delta_{n,N}$$

$$\left\langle n \middle| \psi_{N}^{(-)} \right\rangle = -\sin \frac{\theta_{N}}{2} \middle| e \right\rangle \delta_{n,N-1} + \cos \frac{\theta_{N}}{2} \middle| g \right\rangle \delta_{n,N}$$

$$\left\langle \psi_{N}^{(+)} \middle| n \right\rangle = \cos \frac{\theta_{N}}{2} \left\langle e \middle| \delta_{n,N-1} + \sin \frac{\theta_{N}}{2} \left\langle g \middle| \delta_{n,N} \right\rangle$$

$$\left\langle \psi_{N}^{(-)} \middle| n \right\rangle = -\sin \frac{\theta_{N}}{2} \left\langle e \middle| \delta_{n,N-1} + \cos \frac{\theta_{N}}{2} \left\langle g \middle| \delta_{n,N} \right\rangle$$

$$(3.52)$$

Now it's a simple but lengthy piece of algebra to insert (3.52) into (3.51) and perform the sums over n and N' (which the Kronecker deltas in (3.52) allow us to do) and also over α , $\alpha' = \pm$. The result is

$$\rho^{(A)}(t) = \rho_{ee}(t)|e\rangle\langle e|+\rho_{eg}(t)|e\rangle\langle g|+\rho_{ge}(t)|g\rangle\langle e|+\rho_{gg}(t)|g\rangle\langle g|$$
(3.53)

If we define the following notation for matrix elements of the density operator:

$$\rho_{N,N'}^{\alpha\alpha'} \equiv \left\langle \psi_{N}^{(\alpha)} \middle| \rho(0) \middle| \psi_{N'}^{(\alpha')} \right\rangle$$
(3.54)

then the matrix elements of $ho^{\scriptscriptstyle (A)}(t)$ in (3.53) are given by

$$\rho_{ee}(t) = \sum_{N=1}^{\infty} \left[\rho_{N,N}^{++} \cos^2 \frac{\theta_N}{2} - \rho_{N,N}^{+-} \sin \frac{\theta_N}{2} \cos \frac{\theta_N}{2} e^{-i(\mathcal{E}_N^{(+)} - \mathcal{E}_N^{(-)})t} - \rho_{N,N}^{-+} \sin \frac{\theta_N}{2} \cos \frac{\theta_N}{2} e^{-i(\mathcal{E}_N^{(-)} - \mathcal{E}_N^{(+)})t} + \rho_{N,N}^{--} \sin^2 \frac{\theta_N}{2} \right]$$
(3.55)

$$\rho_{eg}(t) = \sum_{N=1}^{\infty} \left[\rho_{N,N-1}^{++} \cos\frac{\theta_N}{2} \sin\frac{\theta_{N-1}}{2} e^{-i(E_N^{(+)} - E_{N-1}^{(+)})t} + \rho_{N,N-1}^{+-} \cos\frac{\theta_N}{2} \cos\frac{\theta_{N-1}}{2} e^{-i(E_N^{(+)} - E_{N-1}^{(-)})t} - \rho_{N,N-1}^{-+} \sin\frac{\theta_N}{2} \cos\frac{\theta_{N-1}}{2} e^{-i(E_N^{(-)} - E_{N-1}^{(-)})t} \right]$$
(3.56)

$$\rho_{ge}(t) = \sum_{N=1}^{\infty} \left[\rho_{N,N+1}^{++} \sin\frac{\theta_{N}}{2} \cos\frac{\theta_{N+1}}{2} e^{-i\left(\varepsilon_{N}^{(+)} - \varepsilon_{N+1}^{(+)}\right)t} - \rho_{N,N+1}^{+-} \sin\frac{\theta_{N}}{2} \sin\frac{\theta_{N+1}}{2} e^{-i\left(\varepsilon_{N}^{(+)} - \varepsilon_{N+1}^{(-)}\right)t} + \rho_{N,N+1}^{-+} \cos\frac{\theta_{N}}{2} \cos\frac{\theta_{N+1}}{2} e^{-i\left(\varepsilon_{N}^{(-)} - \varepsilon_{N+1}^{(+)}\right)t} - \rho_{N,N+1}^{--} \cos\frac{\theta_{N}}{2} \sin\frac{\theta_{N+1}}{2} e^{-i\left(\varepsilon_{N}^{(-)} - \varepsilon_{N+1}^{(-)}\right)t} \right]$$
(3.57)

$$\rho_{gg}(t) = \sum_{N=1}^{\infty} \left[\rho_{N,N}^{++} \sin^2 \frac{\theta_N}{2} + \rho_{N,N}^{+-} \sin \frac{\theta_N}{2} \cos \frac{\theta_N}{2} e^{-i(E_N^{(+)} - E_N^{(-)})t} + \rho_{N,N}^{-+} \sin \frac{\theta_N}{2} \cos \frac{\theta_N}{2} e^{-i(E_N^{(-)} - E_N^{(+)})t} + \rho_{N,N}^{--} \cos^2 \frac{\theta_N}{2} \right]$$
(3.58)

These formulae, (3.53) to (3.58), express the general dynamics of the JCM in the atom subspace. To determine the actual dynamics in a given case one must specify the initial density operator $\rho(0)$. Before considering a couple of specific cases, note that, from (3.55) and (3.58),

$$Tr^{(A)} \left[\rho^{(A)}(t) \right] = \rho_{ee}(t) + \rho_{gg}(t) = \sum_{N=1}^{\infty} \left(\rho_{NN}^{++} + \rho_{NN}^{--} \right) = Tr \left[\rho(0) \right] = 1$$

So $\rho^{(A)}(t)$, as we've just calculated it, remains correctly normalised at all times. It's also clear from (3.49) and (3.53) that the inversion is given by

$$W(t) = \rho_{ee}(t) + \rho_{qg}(t)$$
(3.59)

Then, using (3.55) and (3.58) again, and noting that $E_N^{(+)} - E_N^{(-)} = \Omega_N$ (see (3.28)) we easily obtain

$$W(t) = \sum_{N=1}^{\infty} \left[\left(\rho_{N,N}^{++} - \rho_{N,N}^{++} \right) \cos \theta_{N} - \left(\rho_{N,N}^{+-} e^{-i\Omega_{N}t} + \rho_{N,N}^{-+} e^{i\Omega_{N}t} \right) \sin \theta_{N} \right]$$
(3.60)

3.5.2 Pure Initial States

Suppose that initially the atom is in state $|e\rangle$ and the field is in some pure state expressed as a superposition of number states $|n\rangle$. The system as a whole, then, is in the pure state

$$\left|\Psi(0)\right\rangle = \left|e\right\rangle \sum_{n=0}^{\infty} c_{n}\left|n\right\rangle = \sum_{N=1}^{\infty} b_{N}\left|\varphi_{N}^{(+)}\right\rangle$$
(3.61)

where $b_N = c_{N-1}$. It will be useful to express this in terms of the dressed states. Using (3.30) we have

$$\left|\Psi(0)\right\rangle = \sum_{N=1}^{\infty} b_{N}\left(\cos\frac{\theta_{N}}{2}\left|\psi_{N}^{(+)}\right\rangle - \sin\frac{\theta_{N}}{2}\left|\psi_{N}^{(-)}\right\rangle\right)$$
(3.62)

By definition, the density operator for this initial state is

$$ho(0) = |\Psi(0)\rangle\langle\Psi(0)|$$
 (3.63)

and now it's straightforward to evaluate the matrix elements defined in (3.54); the results are

$$\rho_{N,N'}^{++} = b_N b_{N'}^* \cos \frac{\theta_N}{2} \cos \frac{\theta_{N'}}{2} \qquad \qquad \rho_{N,N'}^{+-} = -b_N b_{N'}^* \cos \frac{\theta_N}{2} \sin \frac{\theta_{N'}}{2} \rho_{N,N'}^{-+} = -b_N b_{N'}^* \sin \frac{\theta_N}{2} \cos \frac{\theta_{N'}}{2} \qquad \qquad \rho_{N,N'}^{--} = b_N b_{N'}^* \sin \frac{\theta_N}{2} \sin \frac{\theta_{N'}}{2}$$
(3.64)

Using these results in (3.60) we immediately find

$$W(t) = \sum_{N=1}^{\infty} \left| \boldsymbol{b}_{N} \right|^{2} \left(\cos^{2} \theta_{N} + \sin^{2} \theta_{N} \cos \Omega_{N} t \right)$$
(3.65)

This is identical to the result we found in section 3.3 – see equation (3.33).

3.5.3 Mixed initial states

Now we'll consider an initial state that has to be described as an ensemble of systems in all of which the atom is in state $|e\rangle$ but the field by itself is described by a density operator

$$\rho_{F} = \sum_{n=0}^{\infty} p_{n} \left| n \right\rangle \left\langle n \right| \tag{3.66}$$

where p_n is the probability of the field being in a state of *n* photons (of course $\sum_{n=0}^{\infty} p_n = 1$). This is

different in principle from the partial density operator for the field. Then we can write the full initial density operator as

$$\rho(0) = |e\rangle \langle e| \otimes \rho_{F} = \sum_{n=0}^{\infty} \rho_{n} |e\rangle \langle e| \otimes |n\rangle \langle n|$$
(3.67)

It's almost obvious that the partial density operators implied by (3.67) are just

$$\rho^{(A)}(0) = |e\rangle\langle e|$$

$$\rho^{(F)}(0) = \sum_{n=1}^{\infty} p_n |n\rangle\langle n| = \rho_F$$

Following our well-trodden path of expressing this density operator in terms of the dressed states, we can easily find, using (3.27) and (3.67), that the matrix elements (3.54) we need to calculate the inversion via (3.60) are given by

$$\rho_{N,N}^{++} = \rho_{N-1} \cos^2 \frac{\theta_N}{2}$$

$$\rho_{N,N}^{+-} = -\frac{1}{2} \rho_{N-1} \sin \theta_N = \rho_{N,N}^{-+}$$

$$\rho_{N,N}^{--} = \rho_{N-1} \sin^2 \frac{\theta_N}{2}$$
(3.68)

The inversion dynamics for this general mixed state of the field is thus given by inserting (3.68) into (3.60) to obtain

$$W(t) = \sum_{N=1}^{\infty} p_{N-1} \left(\cos^2 \theta_N + \sin^2 \theta_N \cos \Omega_N t \right)$$
(3.69)

Gerry and Knight [3] follow a somewhat different route through the density matrix theory and treat only the case of exact resonance ($\Delta = 0$) when

$$\cos \theta_{N} = 0$$
, $\sin \theta_{N} = 1$, $\Omega_{N} = 2\lambda N^{1/2}$

Then (3.69) becomes

$$W(t) = \sum_{N=1}^{\infty} p_{N-1} \cos(2\lambda t N^{1/2}) = \sum_{n=0}^{\infty} p_n \cos(2\lambda t (n+1)^{1/2})$$
(3.70)

which is Gerry and Knight's result.

If, to take a specific case, the field is initially in a thermal distribution, the probabilities are given by [3]

$$p_n^{th} = \frac{\overline{n}^n}{\left(1 + \overline{n}\right)^{n+1}} \tag{3.71}$$

Here the average photon number \overline{n} at temperature T is determined by

$$\frac{\overline{n}}{1+\overline{n}} = e^{-\frac{\omega}{k_B T}}$$
(3.72)

so that

$$p_{n}^{th} = \frac{e^{-n\frac{\omega}{k_{B}T}}}{e^{-\frac{\omega}{k_{B}T}} - 1}$$
(3.73)

Here's what (3.70) looks like for a thermal field with $\overline{n} = 5$:



Figure 7: The inversion dynamics for a thermal photon field

4 Coda

If I were writing a review of the JCM, I would now go on to describe the experimental situation: have the theoretical predictions been observed; what is the significance of the model for cavity QED and for quantum optics in general; what are its applications? Actually, though, I'm not writing a review but rather expounding the model itself and the mechanics of is solution, essentially as a technical exercise. So these notes will stop here, recalling that full reviews are available [4], [5].

References

- [1] <u>Elementary Quantum Dynamics</u>, PJD (DL 2020)
- [2] E Jaynes and F Cummings, Proc. IEEE 51, 89 (1963)
- [3] "Introductory Quantum Optics", Chris Gerry and Peter Knight (CUP, 2004)
- [4] H-I Yoo and J H Eberle, Physics Reports 118, 239 (1985)
- [5] B W Shore and P L Knight, J Modern Optics 40, 1195 (1993)
- [6] R H Dicke, Phys. Rev. 93, 99 (1954)
- [7] M Tavis and F W Cummings, Phys. Rev. 170, 379 (1968)
- [8] "Quantum Mechanics (2nd edition)", L D Landau and E M Lifshitz (Pergamon, 1965)
- [9] "Methods in Theoretical Quantum Optics" by S M Barnett and P M Radmore (OUP 1997)
- [10] "Fourier and Laplace Transforms", P D Robinson (Routledge and Keegan Paul 1971)
- [11] "Quantum Mechanics Vol I", C Cohen-Tannoudji, Diss and Laloë (Wiley 2005)
- [12] Coordinate Rotations, Spherical Harmonics and Rotation Matrices, PJD (DL 2013)
- [13] Density matrix, PJD (DL 2019)

Appendix A: Basic results for 2x2 Hamiltonian matrices

The canonical 2x2 Hamiltonian matrix

Any 2x2 matrix can be written [11]

$$\mathbf{M} = \boldsymbol{a}_0 \boldsymbol{i} + \boldsymbol{a} \cdot \boldsymbol{\sigma} \tag{A.1}$$

where $\mathbf{a} = (a_1, a_2, a_3)$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a vector of Pauli matrices

$$\boldsymbol{\sigma}_{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \boldsymbol{\sigma}_{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \boldsymbol{\sigma}_{1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ \text{plus} \ \boldsymbol{\sigma}_{0} = \boldsymbol{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
(A.2)

In general, the parameters a_0 , a are complex numbers. In particular, the Hamiltonian matrix of a 2-level system with state space $(|\alpha\rangle, |\beta\rangle)$ can be written in terms of the following canonical form:

$$\mathbf{H} = h_0 \mathbf{1} + \mathbf{h} \cdot \boldsymbol{\sigma} \tag{A.3}$$

in which the parameters h_0 , h are real to ensure that H is Hermitian. If we write

$$h_1 = h\sin\theta\cos\phi, \ h_2 = h\sin\theta\sin\phi, \ h_3 = h\cos\theta$$

$$h = |\mathbf{h}| = \sqrt{h_1^2 + h_2^2 + h_3^2}$$
(A.4)

then the Hamiltonian matrix takes the following form

$$\mathbf{H} = \begin{pmatrix} h_0 + h\cos\theta & h\sin\theta e^{-i\phi} \\ h\sin\theta e^{i\phi} & h_0 - h\cos\theta \end{pmatrix}$$
(A.5)

which is explicitly Hermitian.

Eigenvectors and eigenvalues:

The orthonormal eigenkets and eigenvalues of **H** are as follows:

$$|\psi_{+}\rangle = \cos(\theta/2)e^{-i\phi/2}|\alpha\rangle + \sin(\theta/2)e^{i\phi/2}|\beta\rangle, \qquad e_{+} = h_{0} + h$$

$$|\psi_{-}\rangle = -\sin(\theta/2)e^{-i\phi/2}|\alpha\rangle + \cos(\theta/2)e^{i\phi/2}|\beta\rangle, \qquad e_{-} = h_{0} - h$$
(A.6)

These kets correspond to the following eigenvectors:

$$\psi_{+} = \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} \end{pmatrix}, \qquad e_{+} = h_{0} + h$$

$$\psi_{-} = \begin{pmatrix} -\sin(\theta/2)e^{-i\phi/2} \\ \cos(\theta/2)e^{i\phi/2} \end{pmatrix}, \qquad e_{-} = h_{0} - h$$
(A.7)

Note that in this notation $|\psi_{\pm}\rangle$ is represented by one of the above column vectors $|\psi_{\pm}\rangle$ while $\langle\psi_{\pm}|$ is represented by one of the row vectors:

$$\left(\tilde{\psi}_{+} \right)^{*} = \left(\cos(\theta/2) e^{i\phi/2} \quad \sin(\theta/2) e^{-i\phi/2} \right)$$

$$\left(\tilde{\psi}_{-} \right)^{*} = \left(-\sin(\theta/2) e^{i\phi/2} \quad \cos(\theta/2) e^{-i\phi/2} \right)$$
(A.8)

In this vector/matrix notation, orthonormality means

Diagonalisation:

The unitary matrix **S** that diagonalises the canonical Hamiltonian matrix:

$$\mathbf{S}^{\dagger} \cdot \mathbf{H} \cdot \mathbf{S} = \begin{pmatrix} e_{+} & 0 \\ 0 & e_{-} \end{pmatrix} = \begin{pmatrix} h_{0} + h & 0 \\ 0 & h_{0} - h \end{pmatrix}$$
(A.10)

is that matrix whose columns are the orthonormal eigenvectors:

$$\mathbf{S} = \begin{pmatrix} \cos(\theta/2)e^{-i\phi/2} & -\sin(\theta/2)e^{-i\phi/2} \\ \sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{i\phi/2} \end{pmatrix}$$

$$\mathbf{S}^{\dagger} = \begin{pmatrix} \cos(\theta/2)e^{i\phi/2} & \sin(\theta/2)e^{-i\phi/2} \\ -\sin(\theta/2)e^{i\phi/2} & \cos(\theta/2)e^{-i\phi/2} \end{pmatrix}$$
(A.11)

From these equations it is easy to verify that (A.10) holds and that

$$\begin{pmatrix} \tilde{\psi}_{+} \end{pmatrix}^{*} \cdot \mathbf{S} = \begin{pmatrix} 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} \tilde{\psi}_{-} \end{pmatrix}^{*} \cdot \mathbf{S} = \begin{pmatrix} 0 & 1 \end{pmatrix}$$

$$\mathbf{S}^{\dagger} \cdot \psi_{+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \mathbf{S}^{\dagger} \cdot \psi_{-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
(A.12)

Rotations of a Spin ½ System

The canonical Hamiltonian (A.3) describes a system characterised by a \mathbb{R}^3 vector **h** pointing in a direction specified by polar angles θ, ϕ referred to a Cartesian coordinate system (x, y, z). The effect of diagonalisation is (must be) to produce a Hamiltonian matrix of the form

$$h_0 \mathbf{1} + h \boldsymbol{\sigma}_3 = h_0 \boldsymbol{\sigma}_0 + h \mathbf{z} \cdot \boldsymbol{\sigma}$$

which represents the same system but with the vector **h** now pointing along the z-axis. Thus the effect of diagonalisation is to **rotate** the physical system so that **h** points along the z-axis, or, equivalently, to rotate the coordinate system so that the z-axis points along **h**. This argument shows that the unitary matrix **S** given by (A.11) is actually the spin ½ rotation matrix $\mathfrak{D}^{1/2}(\alpha, \beta, \gamma)$ which angular momentum theory gives as

$$\mathfrak{D}^{1/2}(\alpha,\beta,\gamma) = \begin{pmatrix} e^{-i\alpha/2} & 0\\ 0 & e^{i\alpha/2} \end{pmatrix} \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2)\\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix} \begin{pmatrix} e^{-i\gamma/2} & 0\\ 0 & e^{i\gamma/2} \end{pmatrix}$$

General rotation matrices are functions of the 3 Euler angles (α, β, γ) . In this case the system under rotation has axial symmetry and so only 2 angles are required. In fact, geometry shows³ that we should identify α with ϕ , β with θ and set $\gamma = 0$. It's easy to see from (A.11) that

$$\mathbf{S} = \mathfrak{D}^{1/2} \left(\alpha = \phi, \beta = \theta, \gamma = 0 \right)$$

Moreover (A.12) shows that

$$\mathbf{S} \cdot \begin{pmatrix} \mathbf{1} \\ \mathbf{0} \end{pmatrix} = \boldsymbol{\psi}_{+} \qquad \mathbf{S} \cdot \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix} = \boldsymbol{\psi}_{-}$$

This means that a method of finding the eigenvectors of $\mathbf{n} \cdot \boldsymbol{\sigma}$ is to take the vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and rotate them through the polar angles corresponding to unit vector \mathbf{n} .

Functions of the Hamiltonian:

Consider a function f(x) with a well-behaved expansion in powers of x:

$$f(x) = \sum_{n=0}^{\infty} f_n x^n \tag{A.13}$$

Then the same function of any Hamiltonian matrix, ie

$$f(\mathbf{H}) = \sum_{n=0}^{\infty} f_n \mathbf{H}^n \tag{A.14}$$

is itself a 2x2 matrix. If H has the diagonal form H_{p} , where

$$\mathbf{H}_{D} = \begin{pmatrix} \varepsilon_{+} & 0 \\ 0 & \varepsilon_{-} \end{pmatrix}$$
(A.15)

then clearly

$$\left(\mathbf{H}_{D}\right)^{n} = \begin{pmatrix} \left(\mathcal{E}_{+}\right)^{n} & \mathbf{0} \\ \mathbf{0} & \left(\mathcal{E}_{-}\right)^{n} \end{pmatrix}$$

and

$$f(\mathbf{H}_{D}) = \begin{pmatrix} f(\varepsilon_{+}) & 0\\ 0 & f(\varepsilon_{-}) \end{pmatrix}$$
(A.16)

To evaluate $f(\mathbf{H})$ when **H** isn't diagonal, we use the diagonalising matrix **S** given by (A.11). Since

³ The definitions of Euler angles are all over the place. For my definitions, see my notes on rotation matrices [12].

$$\mathbf{S}^{\dagger} \cdot \mathbf{H} \cdot \mathbf{S} = \mathbf{H}_{D} = \begin{pmatrix} e_{+} & 0 \\ 0 & e_{-} \end{pmatrix}$$

then

$$\mathbf{S}^{\dagger} \cdot \mathbf{H}^{2} \cdot \mathbf{S} = \mathbf{S}^{\dagger} \cdot \mathbf{H}\mathbf{S}\mathbf{S}^{\dagger}\mathbf{H} \cdot \mathbf{S} = (\mathbf{H}_{D})^{2} = \begin{pmatrix} (e_{+})^{2} & 0\\ 0 & (e_{-})^{2} \end{pmatrix}$$

Thus

$$\mathbf{S}^{\dagger} \cdot f(\mathbf{H}) \cdot \mathbf{S} = \sum_{n=0}^{\infty} f_n \begin{pmatrix} (e_+)^n & 0\\ 0 & (e_-)^n \end{pmatrix} = \begin{pmatrix} f(e_+) & 0\\ 0 & f(e_-) \end{pmatrix}$$
(A.17)

So the result we seek is

$$f(\mathbf{H}) = \mathbf{S} \cdot \begin{pmatrix} f(e_{+}) & 0 \\ 0 & f(e_{-}) \end{pmatrix} \cdot \mathbf{S}^{\dagger}$$
(A.18)

In Appendix B: these results are generalised to block diagonal matrices of arbitrary dimension.

Evolution operator in matrix form:

We can immediately apply the results of the preceding subsection to find the 2x2 matrix representation of the evolution operator $U(t) = e^{-i\mathcal{H}t}$. Considering the canonical Hamiltonian (A.3) we get

$$\mathbf{U}(t) = e^{iHt} \tag{A.19}$$

and so, by inspection of (A.18),

$$\mathbf{U}(t) = \mathbf{S} \cdot \begin{pmatrix} u_{+} & 0 \\ 0 & u_{-} \end{pmatrix} \cdot \mathbf{S}^{\dagger}, \qquad u_{\pm} = e^{-ie_{\pm}t}$$
(A.20)

To get an explicit form for this, use (A.7), (A.11) and (A.12) in (A.20):

$$\mathbf{U}(t) = e^{-ih_0 t} \begin{pmatrix} \cos(ht) - i\sin(ht)\cos\theta & -i\sin(ht)\sin\theta e^{-i\phi} \\ -i\sin(ht)\sin\theta e^{i\phi} & \cos(ht) + i\sin(ht)\cos\theta \end{pmatrix}$$
(A.21)

Clearly (A.21) satisfies $\mathbf{U}^{\dagger}(t) = \mathbf{U}(-t)$ and it is a European flight's worth of algebra to demonstrate that it is also unitary, ie that $\mathbf{U}^{\dagger}(t) \cdot \mathbf{U}(t) = \mathbf{1}$ identically for all values of t, h, θ, ϕ .

Appendix B: Functions of block-diagonal matrices

Here we generalise the section on functions of matrices in the previous appendix to apply to matrices of the following block-diagonal form:

$$\mathbf{H} = \begin{pmatrix} \mathbf{h}^{(1)} & 0 & 0 & \cdots \\ 0 & \ddots & 0 & \cdots \\ 0 & 0 & \mathbf{h}^{(n)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$
(B.1)

in which the diagonal blocks $\mathbf{h}^{(n)}$ are square matrices of arbitrary dimension.

Consider again a function f(x) with the well-behaved power series expansion given in (A.13). We want to evaluate the same function of the matrix **H** in (B.1). To do this, we note that it is obvious that

$$(\mathbf{H})^{m} = \begin{pmatrix} (\mathbf{h}^{(1)})^{m} & 0 & 0 & \cdots \\ 0 & \ddots & 0 & \cdots \\ 0 & 0 & (\mathbf{h}^{(n)})^{m} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$
(B.2)

From this it follows immediately that

$$f(\mathbf{H}) = \sum_{m} f_{m} \mathbf{H}^{m} = \begin{pmatrix} f(\mathbf{h}^{(1)}) & 0 & 0 & \cdots \\ 0 & \ddots & 0 & \cdots \\ 0 & 0 & f(\mathbf{h}^{(n)}) & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$
(B.3)

Thus a function of a block-diagonal matrix has the same block-diagonal form in which the blocks are given by the same function of the individual block matrices.

In particular, if a Hamiltonian \mathcal{H} has a block-diagonal matrix representation, then the corresponding evolution operator $\mathcal{U}(t) = e^{-i\mathcal{H}t}$ has a matrix representation of this block-diagonal form. If the individual blocks are 2x2 matrices, as they are in the JCM, then the results of the previous appendix can be used.

Appendix C: The density matrix revised

This appendix simply gives some results expounded fully in [13].

In terms of some basis set $\{|\varphi_n\rangle\}$, a pure state can be written

$$\left|\psi^{(i)}\right\rangle = \sum_{n} c_{n}^{(i)} \left|\varphi_{n}\right\rangle \tag{C.1}$$

while a mixed state must be described by a density operator in [S]

$$\rho(t) = \sum_{i} |\psi^{(i)}(t)\rangle \rho^{(i)} \langle \psi^{(i)}(t)|$$
(C.2)

in which $p^{(i)}$ is the probability of being in state $|\psi^{(i)}\rangle$; of course $0 \le p^{(i)} \le 1$. The density operator above is manifestly Hermitian. The density matrix *per se* is just the matrix representation of the density operator in some basis (usually $\{|\varphi_n\rangle\}$.

Normalisation:

$$Tr[\rho] = \sum_{i} \rho^{(i)} = 1 \tag{C.3}$$

Magnitude:

If the system is in a pure state $|\psi^{(i)}\rangle$, ie $\rho^{(i)} = \delta_{ij}$, then $\rho^2 = \rho$: this is idempotency. For such a pure state $Tr[\rho^2]$ takes its maximum size. For a mixed state the density matrix is smaller in magnitude in the following sense:

- Pure state: $Tr[\rho^2]=1$
- Mixed state: $Tr[\rho^2] < 1$

Dynamics:

In general the time-dependence of the density operator is given in terms of the evolution operator $\mathcal{U}(t,t_{_0})$ by [1]

$$\rho(t) = \mathcal{U}(t,0)\rho(0)\mathcal{U}^{\dagger}(t,0) \tag{C.4}$$

If the Hamiltonian is independent of time, then (in [S])

$$i\frac{\partial\rho(t)}{\partial t} = \left[\mathcal{H}, \rho(t)\right] \tag{C.5}$$

Observables:

For any observable $\mathcal O$, the expectation value is

$$\langle \mathcal{O} \rangle = Tr[\rho \mathcal{O}]$$
 (C.6)

Reduced Density Matrix:

If the full Hilbert space of the system is the product of those of two subsystems A and B (eg atom and photon field) and ρ is the density operator of the system, then the reduced density operator of subsystem A is

$$\rho^{(A)} = Tr_{B}[\rho] \tag{C.7}$$

where Tr_{B} means the trace over the states in the Hilbert space of subsystem B.

Entanglement:

An entangled state of two subsystems A and B is one whose wave-function can't be factorised, in any basis, into a direct product of the states of A and B. Here's an example:

$$\left|entangled\right\rangle = \frac{1}{\sqrt{2}} \left(\left|\psi_{1}^{(A)}\right\rangle \otimes \left|\psi_{2}^{(B)}\right\rangle + \left|\psi_{2}^{(A)}\right\rangle \otimes \left|\psi_{1}^{(B)}\right\rangle\right) \neq \left|\psi_{any}^{(A)}\right\rangle \otimes \left|\psi_{any}^{(B)}\right\rangle \right) \tag{C.8}$$

In such a state, $Tr[(\rho^{(A)})^2] < 1$, ie it looks like subsystem A is in a mixed state, even though the whole system is in a pure state: $\rho = |entangled\rangle\langle entangled|$.