Trapped ions interacting with laser fields: a perturbative analysis without rotating wave approximation

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Abstract

The Hamiltonian describing a single ion placed in a potential trap in interaction with a laser beam is studied by means of a suitable perturbative approach. It is shown, in particular, that the rotating wave approximation does not provide the correct expression, already at the first perturbative order, of the evolution operator of the system.

1 Introduction

Trapped ions in interaction with laser beams are extremely useful tools for investigating fundamental aspects of quantum physics. For instance, they have been used for the generation of coherent, squeezed and Schrödinger-cat states, and for the preparation of entangled Bell and GHZ states. They have also had important experimental applications as, for instance, precision spectroscopy and laser cooling.

Recently, the interest for laser-driven ion traps has received a novel impulse in view of its applications in the fastly developing area of quantum computing. Indeed, in a quantum computer (QC), information is stored in a ‘quantum register’ composed of N two-level systems representing the quantum bits, or qubits. The storage of data and all the basic operations are implemented by inducing controlled dynamics on the quantum register. Since a QC is a quantum mechanical system, it can perform superpositions of computation...
operations with a remarkable gain of efficiency with respect to a classical computer; a typical example is the solution of the problem, fundamental for some cryptographic schemes, of factoring large numbers into primes [11]. In 1995 Cirac and Zoller [12] proposed a concrete model for a ion-trap computer consisting of $N$ atomic ions trapped in a parabolic potential well, each ion being regarded as a two-level system, hence as a realization of a qubit. The control of the quantum degrees of freedom is achieved by addressing the ions with time, frequency and intensity controlled laser beams (see also [13] [14]).

All the applications mentioned above are realized by ion traps with a linear geometry. In such traps a strong confinement is induced along the $y$ and $z$ axes, while a weak harmonic confinement is induced along the principal trap axis $x$. This confinement scheme is realized by the Paul linear trap [15]. $N$ ions in a linear trap will form a chain along the principal trap axis. This allows to reduce the initial $3N$-dimensional model to a $N$-dimensional one, which can be treated conveniently by the introduction of the normal coordinates of the ion chain [16].

As already mentioned, controlled dynamics can be induced on the ion trap by means of laser beams. The Hamiltonian describing the total system [16] [17] — which we will call simply the `ion trap Hamiltonian' (ITH) — in spite of its relative formal simplicity, gives rise to a Schrödinger equation whose exact solutions are not known and its study requires the adoption of suitable approximations. The standardly used method is the rotating wave approximation (RWA) [18] [19]. The RWA is a very popular technique in quantum optics and, in general, in the study of resonance phenomena since it leads to considerable simplifications in many calculation procedures. It consists essentially in passing to the interaction picture and then dropping those terms of the effective Hamiltonian which are rapidly oscillating (usually called 'counter rotating terms' or 'virtual terms'). Using this technique and the Lamb-Dicke approximation [20], the ITH can be reduced to an effective Hamiltonian formally identical to the Hamiltonian of the Jaynes-Cummings model (JCM) [21] [22] in the interaction picture, hence explicitly integrable.

Despite its great popularity, the general validity of the RWA is rather uncertain. In particular, the application of the RWA to the evaluation of the evolution operator is justified only by semiqualitative arguments and the ubiquity of this procedure is mainly due to the chance of performing explicit calculations partially supported by the prediction of some experimentally observable phenomena, for instance the typical ‘collapses and revivals’ in two-level systems [23] [24] [25]. Thus, some attempts of taking into account the impact of counter rotating terms have been made. Specifically, perturbative corrections to the energy spectrum [26], and corrections to the time evolution by means of path integral [27] and perturbative [28] [29] [30] techniques have been investigated. It should be also mentioned that an attempt of considering the counter rotating contributions is already present in the classical study of the magnetic resonance done by Bloch and Siegert [31] and in the later related work of Shirley [32]. Anyway, the validity of all these approaches, as well as of the RWA itself [33], rests on the smallness of the coupling constant, which in the case of a laser-driven ion trap is proportional to the intensity of the laser field. This is a severe drawback since
an intense laser field implies a fast coupling between the two internal energy levels of the trapped ions i.e., for instance, a fast QC.

In the present paper, we propose to study the ITH using a perturbative approach along new lines with respect to the existing literature. Since, by virtue of the normal coordinates of the ion chain, the $N$-ion case does not introduce any essential complication with respect to the single ion case (especially if the nonharmonic component of the ion-ion interaction can be neglected), we will restrict, for the sake of simplicity, to the latter case. Obviously, the $N$-ion case is of great interest for the applications and will deserve a particular attention in a forthcoming paper \[34\]. We proceed as follows. First, we notice that passing to a ‘rotating frame’, i.e. to a suitable interaction picture, the ITH transforms into a time-independent Hamiltonian which we will call the ‘rotating frame Hamiltonian’ (RFH). At this point, we use the fact that — as it has been shown by some of the authors \[35\] — the RFH is unitarily equivalent to a Hamiltonian formally similar to the RFH, except for the fact that the new coupling constant is not proportional any more to the field intensity but a simple bounded function of it (see section \[3\]). We will call this Hamiltonian the ‘balanced Hamiltonian’ (BH). The BH is an ideal starting point for a perturbative approach, since the results obtained by its study hold also in the strong field regime. Next, using the tools of perturbation theory for linear operators \[37\], \[38\], we develop a perturbative procedure which allows to give approximate expressions of the evolution operator associated with the BH (hence with the ITH) in terms of unitary operators.

Our basic idea is the following. The Jaynes-Cummings Hamiltonian is exactly solvable — i.e. its spectrum is discrete and its eigenvalues and eigenvectors are known — by virtue of the fact that it can be written as the sum of two commuting operators and one of the two is trivially solvable (see section \[2\]). Then, in general, we wonder if, given a perturbed Hamiltonian $H(\lambda) = H_0 + \lambda H\uparrow$, with $H_0$ exactly solvable, we can build a procedure which allows to compute, for each $n = 1, 2, \ldots$, hermitian operators $H_0^{(n)}(\lambda), C^{(n)}(\lambda)$ depending analytically on the parameter $\lambda$, such that

\begin{equation}
H(\lambda) = H_0^{(n)}(\lambda) + C^{(n)}(\lambda) + O(\lambda^{n+1}),
\end{equation}

\[ H_0^{(n)}(\lambda) \text{ is exactly solvable and } \]

\begin{equation}
\left[C^{(n)}(\lambda), H_0^{(n)}(\lambda)\right] = 0.
\end{equation}

Indeed, in this case the determination of an approximate expression, at each perturbative order, of the evolution operator associated with $H(\lambda)$ is greatly simplified. We will show in section \[4\] that this idea is correct and we will apply the method to the BH in section \[5\]. In sections \[6\] and \[7\] we compare the perturbative expressions obtained for the energy spectrum and the evolution operator with the results obtained applying the RWA to the BH. It will be shown that, while the RWA gives the right first order correction to the unperturbed eigenvalues, it does not give the right first order expression for the evolution operator since it neglects corrections to the eigenprojectors. Eventually, in section \[8\] conclusions are drawn.
2 The Jaynes-Cummings model

In this section we will give a very concise treatment of the classical JCM. This
will allow us to gain a better insight in our perturbative analysis of the ion trap
Hamiltonian.

The Hamiltonian of the JCM reads (\(\hbar = 1\)):

\[
H_{JC} = \nu \hat{n} + \frac{1}{2} \omega \sigma_z + \lambda \nu \left( a \sigma_+ + a^\dagger \sigma_- \right),
\]

(3)
where \(a, a^\dagger\), \(\hat{n}\) are the annihilation, creation and number operators and \(\sigma_z, \sigma_\pm\) the Pauli operators. In the following, we will denote by \(\{|n\}\}\) the Fock basis and by \(|g\rangle, |e\rangle\) the eigenvectors of \(\sigma_z\):

\[
\hat{n} |n\rangle = n |n\rangle, \quad \sigma_z |g\rangle = - |g\rangle, \quad \sigma_z |e\rangle = |e\rangle.
\]

The JCM is exactly solvable. This is due to the fact that its Hamiltonian can be
easily represented as the sum of two constants of the motion. Indeed, observe
that \(H_{JC}\) can be written as

\[
H_{JC} = N + S,
\]

where

\[
N := \nu \left( \hat{n} + \frac{1}{2} \sigma_z \right), \quad S := \frac{1}{2} (\omega - \nu) \sigma_z + \lambda \nu \left( a \sigma_+ + a^\dagger \sigma_- \right)
\]

(4)
and

\[
[N, S] = [N, H_{JC}] = [S, H_{JC}] = 0.
\]

(5)
It follows that the evolution operator of the JCM factorizes as

\[
e^{-iH_{JC}t} = e^{-iNt} e^{-iSt}.
\]

Moreover, \(N\) has a discrete spectrum and its eigenspaces, namely the one-
dimensional eigenspace \(H_0 = \text{Span}\{ |0\rangle \otimes |g\rangle \}\) and the two-dimensional eigenspaces

\[
H_n = \text{Span}\{ |n-1\rangle \otimes |e\rangle, \ |n\rangle \otimes |g\rangle \}, \quad n = 1, 2, \ldots,
\]

are invariant subspaces for \(S\), which can be diagonalized in each of these mutually orthogonal subspaces. This yields to a diagonalization of the whole Hamiltonian and to an explicit expression for the unitary operator \(e^{-iSt}\). If the resonance condition \(\nu = \omega\) is satisfied, then this operator assumes a particularly simple form and can also be computed by direct exponentiation. indeed, using the fact that

\[
(a \sigma_+ + a^\dagger \sigma_-)^2m = (a a^\dagger \sigma_+ \sigma_- + a^\dagger a \sigma_- \sigma_+)^m = \hat{n}^m |g\rangle \langle g| + (\hat{n} + 1)^m |e\rangle \langle e|,
\]

we find:

\[
\mathcal{J}(t) := \exp \left( -iSt \right)
\]

\[
= \cos \left( \lambda \nu \sqrt{\hat{n}} \ t \right) |g\rangle \langle g| + \cos \left( \lambda \nu \sqrt{\hat{n} + 1} \ t \right) |e\rangle \langle e|
\]

\[
- \ i \left( \frac{\sin \left( \lambda \nu \sqrt{\hat{n} + 1} \ t \right)}{\sqrt{\hat{n} + 1}} a \sigma_+ + \frac{\sin \left( \lambda \nu \sqrt{\hat{n}} \ t \right)}{\sqrt{\hat{n}}} a^\dagger \sigma_- \right).
\]

(6)
We will call \(J(t)\) the Jaynes-Cummings evolutor.

We conclude this section observing that since
\[
e^{-i \frac{\pi}{2} \hat{n}} a e^{i \frac{\pi}{2} \hat{n}} = i a,
\]
where \(e^{i \frac{\pi}{2} \hat{n}}\) is nothing but the Fourier-Plancherel operator, the Hamiltonian \(H_{JC}\) is unitarily equivalent to the following one:
\[
\hat{H}_{JC} := e^{-i \frac{\pi}{2} \hat{n}} H_{JC} e^{i \frac{\pi}{2} \hat{n}} = \hat{N} + \hat{S},
\]
where
\[
\hat{S} := \frac{1}{2} (\omega - \nu) \sigma_z + i \lambda \nu \left( a \sigma_+ - a^\dagger \sigma_- \right).
\]

3 The ion trap Hamiltonian

A two-level ion of mass \(\mu\) in a potential trap, with strong confinement along the \(y\) and \(z\) axes, and weak harmonic binding of frequency \(\nu\) along the \(x\)-axis (the ‘trap axis’), can be described — neglecting the motion of the ions transverse to the trap axis — by a Hamiltonian of the following type (\(\hbar = 1\)):
\[
H_0 = \nu a^\dagger a + \frac{1}{2} \omega_{ge} \sigma_z,
\]
where \(a\) is the vibrational annihilation operator
\[
a = \left( \frac{\mu \nu}{2} \right)^{\frac{1}{2}} \left( \hat{x} + i \frac{\mu \nu}{\mu} \hat{p}_x \right)
\]
and \(\sigma_z\) the effective spin operator associated with the internal degrees of freedom of the ion. Let us suppose now that the ion is addressed by a laser beam of frequency \(\omega_L\) in a traveling wave configuration. Then, the Hamiltonian describing the physical system (ITH) becomes
\[
H(t) = H_0 + H_z(t),
\]
where
\[
H_z(t) := \Omega_R \left( e^{i \omega_L t} \sigma_- D(i \eta) \dagger + e^{-i \omega_L t} \sigma_+ D(i \eta) \right),
\]
with \(\Omega_R = \phi E\) the Rabi frequency and \(E\) the intensity of the laser field. Moreover, we have set:
\[
D(i \eta) := \exp \left( i \eta (a + a^\dagger) \right),
\]
where
\[
\eta := \frac{k_L \cos \phi}{\sqrt{2 \mu \nu}}
\]
— with \(k_L\) the wavevector and \(\phi\) the angle between the \(x\)-axis and \(k_L\) — is the Lamb-Dicke factor. Notice that \(D(\alpha)\), \(\alpha \in \mathbb{C}\), is a displacement operator, namely
\[
D(\alpha) := \exp \left( \alpha a^\dagger - \alpha^* a \right), \quad D(\alpha) a D(\alpha)^\dagger = a - \alpha.
\]
In order to work with operator matrices, the Hilbert space of the total system ('pointlike' ion + internal degrees of freedom of the ion), namely \( \mathcal{H} \otimes \mathbb{C}^2 \), \( \mathcal{H} \equiv L^2(\mathbb{R}) \), will be identified with the space \( \mathcal{H} \oplus \mathcal{H} \).

Now, the dynamical problem associated with the time-dependent Hamiltonian \( H(t) \) can be turned into a time-independent problem. Indeed, switching to the interaction picture with reference Hamiltonian \( \frac{1}{2} \omega_L t \sigma_z \) and setting

\[
R_t := \exp \left( \frac{i}{2} \omega_L t \sigma_z \right),
\]

one obtains the time-independent ‘rotating frame Hamiltonian’ (RFH)

\[
\tilde{H} = R_t \left( H(t) - \frac{1}{2} \omega_L \sigma_z \right) R_t^\dagger,
\]

\[
= \nu \hat{n} + \frac{1}{2} \delta \sigma_z + \Omega_R \left( \sigma_- D(i\eta) + \sigma_+ D(i\eta) \right),
\]

(15)

where \( \hat{n} = a^\dagger a \) is the number operator and \( \delta := \omega_{ge} - \omega_L \) is the ion-laser detuning.

At this point, in order to give an approximate expression of the evolution operator associated with the Hamiltonian \( \tilde{H} \), the rotating wave approximation (RWA) is usually applied. It consists in expanding the exponential \( D(i\eta) \), then passing to the interaction picture with reference Hamiltonian \( \tilde{H}_0 = \nu \hat{n} + \frac{1}{2} \delta \sigma_z \), so obtaining the interaction picture Hamiltonian

\[
\tilde{H}_{\text{int}}(t) = \Omega_R \left( 1 - i\eta \left( e^{i\nu t} a^\dagger + e^{-i\nu t} a + \ldots \right) e^{-i\delta t} + h.c. \right),
\]

and, finally, retaining only that terms in \( \tilde{H}_{\text{int}}(t) \) which are slowly rotating. Hence — assuming that \( \eta \ll 1 \) (Lamb-Dicke regime), so that one can keep only the terms which are at most linear in \( \eta \) — in correspondence to the three types of resonance

\[
\delta = \omega_{ge} - \omega_L \simeq 0, \quad \delta + \nu \simeq 0, \quad \delta - \nu \simeq 0,
\]

(16)

one obtains respectively the following three types of effective interaction picture Hamiltonian:

\[
\tilde{H}_{\text{eff}}^{(0)} = \Omega_R \left( \sigma_- + \sigma_+ \right),
\]

\[
\tilde{H}_{\text{eff}}^{(-)} = i\eta \Omega_R \left( a^\dagger \sigma_+ - a \sigma_- \right), \quad \tilde{H}_{\text{eff}}^{(+)} = i\eta \Omega_R \left( a \sigma_+ - a^\dagger \sigma_- \right).
\]

These effective Hamiltonians, in correspondence to the respective resonances, commute with the reference Hamiltonian \( \tilde{H}_0 \). This is due to the fact that the resonances (16) are associated with degeneracies of the reference Hamiltonian.

In fact, it turns out that the spectrum of \( \tilde{H}_0 \) is degenerate if and only if the condition \( m \nu = |\delta|, \ m = 0, 1, 2, \ldots \), holds. Notice that, in particular, \( \tilde{H}_{\text{eff}}^{(+)} \) is equal — up to a unitary transformation and setting \( \delta = \omega \) and \( \eta \Omega_R = \lambda \nu \) — to the constant of the motion \( S \) of the Jaynes-Cummings Hamiltonian in the resonant regime (see section 2).
It will be shown that the RWA is a rather poor approximation for the evaluation of the evolution operator. The argument usually adopted in order to support its validity is the following. Let us consider the Feynman-Dyson expansion of the evolution operator $U_{\text{int}}(t, t_0)$ associated with the interaction picture Hamiltonian $\tilde{H}_{\text{int}}(t)$. At the first order one has:

$$U_{\text{int}}(t, t_0) \simeq \text{Id} - i \int_{t_0}^{t} \tilde{H}_{\text{int}}(\tau) \, d\tau.$$ 

Then, it is argued that the fastly oscillating terms in $\tilde{H}_{\text{int}}$ give a smaller contribution to the integral in the r.h.s. of the previous formula with respect to the slowly rotating ones. As it will be seen later on, this argument turns out to be erroneous. The misunderstanding stems from the fact that one is using a perturbative expansion of the evolution operator whose terms (except the identity) are not unitary operators.

Besides, any perturbative approach does not work in the strong field regime, since the Rabi frequency $\Omega_R$ which appears in the interaction component of the RFH is proportional to the intensity of the laser field. This problem can be bypassed by means of a suitable unitary transformation of the Hamiltonian $\tilde{H}$ (see [35]). This transformation allows to obtain a ‘balanced Hamiltonian’ (BH) $\hat{H}$ which is the sum of a large component having a simple ‘diagonal’ form — i.e. such that its matrix representation in the standard basis

$$\{|n \rangle \otimes |g\rangle, \, |n \rangle \otimes |e\rangle : \, n = 0, 1, 2, \ldots \}$$

is diagonal — and a small interaction component scarcely sensitive to the Rabi frequency $\Omega_R$. Indeed, introduced the dimensionless parameter $\Delta := \delta / \Omega_R$ (from this point onwards we will assume that $\Omega_R \neq 0$), there is a unitary operator $T_\Delta$ such that

$$\hat{H} := T_\Delta \tilde{H} T_\Delta^\dagger = \hat{H}_0 + \hat{H}_\uparrow,$$

where we have set:

$$\hat{H}_0 := \nu \hat{n} + \frac{1}{2} \delta \sigma_z + \lambda \bar{\eta} \nu,$$

with

$$\delta := \sqrt{4\Omega_R^2 + \delta^2}, \quad \bar{\eta} := \frac{\Delta}{\sqrt{4 + \Delta^2}} \eta, \quad \lambda := \frac{1}{\sqrt{4 + \Delta^2}} \eta = \frac{1}{\Delta} \bar{\eta},$$

and

$$\hat{H}_\uparrow := i \lambda \nu \left( (a - a^\dagger) \left( \sigma_+ D(i\bar{\eta}) + \sigma_- D(i\bar{\eta})^\dagger \right) - i\bar{\eta} \left( \sigma_+ D(i\bar{\eta}) - \sigma_- D(i\bar{\eta})^\dagger \right) \right) = i \lambda \nu \left( a - a^\dagger \right) \left( \sigma_+ + \sigma_- \right)$$

$$+ i \lambda \nu \sum_{m=1}^{\infty} \frac{(i\bar{\eta})^m}{m!} (a^2 - a^\dagger^2 + 1 - m) (a + a^\dagger)^{m-1} (\sigma_+ + (-1)^m \sigma_-).$$
Notice that the ‘balanced detuning’ $\tilde{\delta}$ is, unlike $\delta$, always positive so that the degeneracy condition for $\tilde{H}_0$ is now: $\nu = m \tilde{\delta}$, $m = 1, 2, \ldots$.

The unitary operator $T_\Delta$ has the following explicit form:

$$T_\Delta = \begin{bmatrix}
\kappa_\Delta^+ D(i \tilde{\eta} \eta) & \kappa_\Delta^- D(i \tilde{\eta} \eta) \\
-k_\Delta^- D(i \tilde{\eta} \eta)^\dagger & k_\Delta^+ D(i \tilde{\eta} \eta)^\dagger
\end{bmatrix} = \begin{bmatrix}
\kappa_\Delta^+ D(i(i \tilde{\eta} - \eta)/2) & \kappa_\Delta^- D(i(i \tilde{\eta} + \eta)/2) \\
-k_\Delta^- D(i(i \tilde{\eta} + \eta)/2)^\dagger & k_\Delta^+ D(i(i \tilde{\eta} - \eta)/2)^\dagger
\end{bmatrix},$$

(22)

with

$$k_\Delta^\pm = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 + \frac{1}{4 + \Delta^2}} \pm \text{sign}(\Delta) \sqrt{1 - \frac{1}{4 + \Delta^2}},$$

$$\epsilon_\Delta^\pm = \frac{\Delta}{2 \sqrt{4 + \Delta^2}} \pm \frac{1}{2}.$$  

(23)

(24)

The unitary operator $T_\Delta$ can be decomposed as the product of three unitary transformations:

$$T_\Delta = T_3 T_2 T_1.$$

The transformation $T_1$ has been introduced by Moya-Cessa et al. [36] and has the following form:

$$T_1 := \frac{1}{\sqrt{2}} \left( \frac{1}{2} (D + D^\dagger) - \frac{1}{2} (D - D^\dagger) \sigma_z + D \sigma_+ - D^\dagger \sigma_-, \right)$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix}
D & D^\dagger \\
-D^\dagger & D
\end{bmatrix}, \quad D \equiv D(i \eta/2).$$

The transformation $T_2$ is a spin rotation by the angle $\theta$ round the $y$-axis:

$$T_2 := \begin{bmatrix}
\cos \theta/2 & -\sin \theta/2 \\
\sin \theta/2 & \cos \theta/2
\end{bmatrix},$$

where the angle $\theta$, $-\pi/2 \leq \theta \leq \pi/2$, verifies the condition

$$\tan \theta = \frac{\Delta}{2} = \frac{\omega_{ge} - \omega_{L}}{2\Omega_R}.$$

The third transformation is given by

$$T_3 := \frac{1}{2} (D(i \tilde{\eta}/2) + D(i \tilde{\eta}/2)^\dagger) + \frac{1}{2} (D(i \tilde{\eta}/2) - D(i \tilde{\eta}/2)^\dagger) \sigma_z$$

$$= \begin{bmatrix}
D(i \tilde{\eta}/2) & 0 \\
0 & D(i \tilde{\eta}/2)^\dagger
\end{bmatrix}.$$
One can check that in the weak field limit $\Omega_R \to 0$ ($\Delta = \delta / \Omega_R \to \pm \infty$) and in the strong field limit $\Omega_R \to +\infty$ ($\Delta \to 0$) the transformation $T_\Delta$ has the following behaviour:

$$\lim_{\Delta \to +\infty} T_\Delta = \text{Id}, \quad \lim_{\Delta \to -\infty} T_\Delta = T_2(-\pi) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \text{(weak field limit);}$$

$$\lim_{\Delta \to 0} T_\Delta = T_1 \quad \text{(strong field limit).}$$

Thus, in the weak field limit, $T_\Delta$ goes to the identity if $\delta > 0$ and to a spin rotation which sends $\sigma_z$ into $-\sigma_z$ for $\delta < 0$ (so that, as already observed, $\delta$ is always positive); while, in the strong field limit, it goes to the transformation introduced by Moya-Cessa et alii.

The constant $\lambda$ which appears in the expression of the interaction component $\tilde{H}_\perp$ of the balanced Hamiltonian $\tilde{H}$ will play the role of perturbative parameter in our later analysis. Moreover, it will be seen that the constant $\tilde{\eta}$ rules the number of terms that have to be considered at each perturbative order. We remark that both $\lambda$ and $\tilde{\eta}$ are bounded functions of the Rabi frequency $\Omega_R$; indeed:

$$0 \leq |\lambda| = \frac{\Omega_R}{\sqrt{4\Omega_R^2 + \delta^2}} |\eta| \leq \frac{1}{2} |\eta|$$

and

$$0 \leq |\tilde{\eta}| = \frac{2}{\sqrt{4\Omega_R^2 + \delta^2}} |\eta| \leq |\eta|.$$ 

Thus, one can apply a perturbative approach also in the case of a large Rabi frequency (hence in presence of an intense laser field).

4 Perturbative analysis: outline of the method

Let $\mathfrak{H}_0$, $\mathfrak{H}_\perp$ be hermitian operators and assume that $\mathfrak{H}_0$ has a purely discrete spectrum (i.e. it has a pure point spectrum with finite-dimensional eigenspaces). Denote by

$$E_0 < E_1 < E_2 < \ldots$$

the (possibly degenerate) eigenvalues of $\mathfrak{H}_0$ and by $P_0, P_1, P_2, \ldots$ the associated eigenprojectors.

Now, consider the operator

$$\mathfrak{H}(\lambda) = \mathfrak{H}_0 + \lambda \mathfrak{H}_\perp \quad \lambda \in \mathbb{C},$$

which is hermitian if $\lambda$ is real. It is possible to show that, under certain conditions (see [37], [38]), there exist positive constants $r_0, r_1, r_2, \ldots$ and a simply connected neighbourhood $\mathcal{I}$ of zero in $\mathbb{C}$ such that the following contour integral on the complex plane

$$P_m(\lambda) = \frac{i}{2\pi} \oint_{|E - E_m| = r_m} dE \left( \mathfrak{H}(\lambda) - E \right)^{-1} \quad \lambda \in \mathcal{I},$$

(25)
defines a projection \((P_m(\lambda))^2 = P_m(\lambda))\), which is an orthogonal projection for real \(\lambda\), with \(P_m(0) = P_m\), and \(I \ni \lambda \mapsto P_m(\lambda)\) is an analytic operator-valued function. Moreover, the range of \(P_m(\lambda)\) is an invariant subspace for \(\H(\lambda)\), hence

\[
\mathcal{S}(\lambda) P_m(\lambda) = P_m(\lambda) \mathcal{S}(\lambda) P_m(\lambda),
\]

and there exists an analytic family \(U(\lambda)\) of invertible operators such that

\[
P_m = U(\lambda) P_m(\lambda) U(\lambda)^{-1}, \quad U(0) = \text{Id},
\]

and

\[
U(\lambda) = e^{iZ(\lambda)} \quad \lambda \in I,
\]

with \(Z(\lambda^*) = Z(\lambda)^\dagger\) (hence, for real \(\lambda\), \(Z(\lambda)\) is hermitian and \(U(\lambda)\) is unitary), where \(I \ni \lambda \mapsto Z(\lambda)\) is analytic. Let us observe explicitly that the following relation holds:

\[
U(\lambda^*) = e^{iZ(\lambda^*)} = e^{iZ(\lambda)^\dagger} = U(\lambda)^{-1},
\]

We remark that, as it is easily shown, the function \(\lambda \mapsto U(\lambda)\) is not defined uniquely by condition (27) even in the simplest case when \(\H_0\) has a nondegenerate spectrum.

Now, let us define the operator \(\H(\lambda)\) by

\[
\H(\lambda) := U(\lambda) \H(\lambda) U(\lambda)^{-1},
\]

which, for real \(\lambda\), is unitarily equivalent to \(\H(\lambda)\). Using relations (26) and (27), we find

\[
\mathcal{S}(\lambda) P_m = U(\lambda) \mathcal{S}(\lambda) P_m(\lambda) U(\lambda)^{-1} = U(\lambda) P_m(\lambda) \mathcal{S}(\lambda) P_m(\lambda) U(\lambda)^{-1}
\]

and hence:

\[
\mathcal{S}(\lambda) P_m = P_m \mathcal{S}(\lambda) P_m \quad m = 0, 1, \ldots
\]

It follows that

\[
[\H_0, \mathcal{S}(\lambda)] = 0
\]

and then we obtain the following important decomposition formula

\[
U(\lambda) \H(\lambda) U(\lambda)^{-1} = \H_0 + C(\lambda),
\]

where \([C(\lambda), \H_0] = 0\), i.e. \(C(\lambda)\) is a constant of the motion for the evolution generated by \(\H_0\). Notice that by virtue of relation (29) we have:

\[
C(\lambda^*) = U(\lambda^*) \H(\lambda^*) U(\lambda^*)^{-1} - \H_0
= U(\lambda)^{-1} \H(\lambda)^\dagger U(\lambda)^{\dagger} - \H_0
= C(\lambda)^\dagger.
\]

Thus, in particular, for real \(\lambda\), \(C(\lambda)\) is hermitian.
At this point, we are ready to build the perturbative decomposition of the operator $\mathcal{H}(\lambda)$ anticipated in section 1. Indeed, since the functions $\lambda \mapsto C(\lambda)$ and $\lambda \mapsto Z(\lambda)$ are analytic in $I$ and $C(0) = Z(0) = 0$, we can write:

$$C(\lambda) = \sum_{m=1}^{\infty} \lambda^m C_m, \quad Z(\lambda) = \sum_{m=1}^{\infty} \lambda^m Z_m, \quad \lambda \in I;$$  \hfill (34)

here we notice that — as $C(\lambda^*) = C(\lambda)^\dagger$ and $Z(\lambda^*) = Z(\lambda)^\dagger$ — for any $m$, $C_m = C_m^\dagger$ and $Z_m = Z_m^\dagger$. Then, if we set

$$\mathcal{H}(\lambda) := e^{-i(\lambda Z_1 + \cdots + \lambda^n Z_n)} H_0 e^{i(\lambda Z_1 + \cdots + \lambda^n Z_n)},$$  \hfill (35)

$$C(\lambda) := e^{-i(\lambda Z_1 + \cdots + \lambda^n Z_n)} (\lambda C_1 + \cdots + \lambda^n C_n) e^{i(\lambda Z_1 + \cdots + \lambda^n Z_n)},$$  \hfill (36)

by virtue of formula (33) we find that equation (1) is satisfied together with condition (2).

Now, in order to determine the operators $\{C_n(\lambda)\}$ and $\{Z_n(\lambda)\}$, let us substitute the exponential form $e^{iZ(\lambda)}$ of $U(\lambda)$ in formula (33); we obtain:

$$\mathcal{H}(\lambda) + \sum_{m=1}^{\infty} \frac{i^m}{m!} \text{ad}_{Z(\lambda)}^m \mathcal{H}(\lambda) = \mathcal{H}_0 + C(\lambda),$$  \hfill (37)

where we recall that $\text{ad}_K L = [K, L]$. Next, substituting the power expansions (34) in this equation, in correspondence to the various orders in the perturbative parameter $\lambda$, we get the following set of conditions:

$$C_1 - i[Z_1, \mathcal{H}_0] - \mathcal{H}_\uparrow = 0, \quad [C_1, \mathcal{H}_0] = 0$$  \hfill (38)

$$C_2 - i[Z_2, \mathcal{H}_0] + \frac{1}{2} [Z_1, [Z_1, \mathcal{H}_0]] - i[Z_1, \mathcal{H}_\uparrow] = 0, \quad [C_2, \mathcal{H}_0] = 0$$  \hfill (39)

$$\vdots$$

where we have taken into account also the additional constraint $[C(\lambda), \mathcal{H}_0] = 0$.

The generic term, after the first one, in this infinite sequence of equations is easily shown to be the following:

$$C_n = \sum_{m=1}^{n} \frac{i^m}{m!} \sum_{k_1 + \cdots + k_m = n} [Z_{k_1}, \ldots, [Z_{k_m}, \mathcal{H}_0], \ldots]$$

$$- \sum_{m=1}^{n-1} \frac{i^m}{m!} \sum_{k_1 + \cdots + k_m = n-1} [Z_{k_1}, \ldots, [Z_{k_m}, \mathcal{H}_\uparrow], \ldots] = 0,$$

$$[C_n, \mathcal{H}_0] = 0 \quad n = 2, 3, \ldots.$$  

The infinite set of equations can be solved recursively and the solution, as already anticipated, is not unique. The first equation, together with the first constraint, determines $Z_1$ up to an operator commuting with $\mathcal{H}_0$ and $C_1$ uniquely.
Indeed, since
\[ C_1 = \sum_{m=0}^{\infty} P_m C_1 P_m \quad \text{and} \quad [Z_1, \mathcal{H}_0] = \sum_{j \neq k} (E_k - E_j) P_j Z_1 P_k, \] (40)
we conclude that
\[ C_1 = \sum_{m=0}^{\infty} P_m \mathcal{H}_0 P_m \] (41)
and
\[ Z_1 = \sum_{m=0}^{\infty} P_m Z_1 P_m + i \sum_{j \neq k} (E_k - E_j)^{-1} P_j Z_1 P_k. \] (42)
This last equation admits a ‘minimal solution’ which is obtained by imposing a further condition, namely
\[ P_m Z_1 P_m = 0 \quad m = 0, 1, \ldots. \]
For \( n > 1 \), we will use an analogous reasoning. Indeed, let us define, for \( n \geq 2 \), the following operator function:
\[
G_n(Z_1, \ldots, Z_{n-1}) := \sum_{m=2}^{n} \frac{i^m}{m!} \sum_{k_1 + \cdots + k_m = n} [Z_{k_1}, \ldots, [Z_{k_m}, \mathcal{H}_0] \ldots] \\
+ \sum_{m=1}^{n-1} \frac{i^m}{m!} \sum_{k_1 + \cdots + k_m = n-1} [Z_{k_1}, \ldots, [Z_{k_m}, \mathcal{H}_0] \ldots].
\] (43)
Now, assume that the first \( n \) equations have been solved. Then, the operator \( G_{n+1}(Z_1, \ldots, Z_n) \) is known explicitly and hence
\[ C_{n+1} = \sum_{m=0}^{\infty} P_m G_{n+1}(Z_1, \ldots, Z_n) P_m, \] (44)
\[ [Z_{n+1}, \mathcal{H}_0] = i \sum_{j \neq k} P_j G_{n+1}(Z_1, \ldots, Z_n) P_k. \] (45)
Again, this last equation determines \( Z_{n+1} \) up to an operator commuting with \( \mathcal{H}_0 \). In general, the choice of a particular solution for \( Z_{n+1} \) will also influence the form of \( C_{n+2}, Z_{n+2}, \ldots \).
Thus, we conclude that the sequence of equations defined above admits infinite solutions (even in the case when \( \mathcal{H}_0 \) has a nondegenerate spectrum). This fact had to be expected as a consequence of the non-uniqueness of \( U(\lambda) \). Anyway, there is a unique ‘minimal solution’ \( \{C_1, Z_1, \ldots\} \) which fulfills the following additional condition:
\[ P_m Z_k P_m = 0 \quad m = 0, 1, \ldots, k = 1, 2, \ldots. \] (46)
The preceding scheme can be extended to the general case when the interaction component $H_\downarrow(\lambda)$ of $H(\lambda)$ does not depend linearly on $\lambda$:

$$H(\lambda) = H_0 + H_\uparrow(\lambda) = \sum_{m=0}^\infty \lambda^m H_m.$$  (47)

Indeed, given an operator $X$, let us set $F_0(X) \equiv X$ and

$$F_n(X; Z_1, \ldots, Z_n) := \sum_{m=1}^n \frac{i^m}{m!} \sum_{k_1 + \cdots + k_m = n} [Z_{k_1}, \ldots, [Z_{k_m}, X]],$$  (48)

for $n \geq 1$. Then we can define the operator function

$$G_n(H_0, \ldots, H_n; Z_1, \ldots, Z_{n-1}) := \sum_{m=0}^n F_{n-m}(H_m; Z_1, \ldots, Z_{n-1})$$

$$- i[Z_n, H_0], \quad n \geq 1,$$  (49)

which generalizes definition (43). At this point, one can show that this time the decomposition formula (33) leads to the following sequence of equations:

$$C_n - i[Z_n, H_0] = G_n(H_0, \ldots, H_n; Z_1, \ldots, Z_{n-1}),$$

$$[C_n, H_0] = 0 \quad n \in \mathbb{N}.$$  (50)

Again, the general solution of this set of equations can be obtained recursively by formulae (44) and (45). We want to show next that it is possible to give simple explicit expressions for the operators $C_n, Z_n$ which do not involve the eigenprojectors of $H_0$.

To this aim, let us denote by $\mathcal{H}_0, \mathcal{H}_1, \ldots$ the eigenspaces associated with the eigenvalues $E_0, E_1, \ldots$; namely, let us set:

$$\mathcal{H}_n \equiv \text{Ran}(P_n), \quad d_n \equiv \dim(\mathcal{H}_n) \quad n = 0, 1, \ldots, \quad d_{-1} \equiv 0.$$  

Now, let $\{|n\rangle : n = 0, 1, \ldots\}$ be an orthonormal basis formed by eigenvectors of $H_0$ such that

$$\mathcal{H}_n = \text{Span}(|c_n\rangle, \ldots, |c_n + d_n\rangle), \quad c_n \equiv \sum_{k=-1}^{n-1} d_n.$$  

We will denote by $A, A^\dagger, \hat{N}$ respectively the annihilation, creation and number operators relative to this basis:

$$A^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle, \quad \hat{N} |n\rangle = n |n\rangle.$$  

Then we can write

$$H_0 = E_N$$  (51)
and express the operators $G_1 \equiv \mathcal{H}_1$, $G_n \equiv G_n(\mathcal{H}_0, \ldots, \mathcal{H}_n; Z_1, \ldots, Z_{n-1})$, $n \geq 2$, in the following form:

$$G_n = g_n^{[0]}(\hat{N}) + \sum_{m=1}^{\infty} \left( g_n^{[m]}(\hat{N}) A^m + A^\dagger g_n^{[m]}(\hat{N}) \right).$$  (52)

At this point one can check that the operators

$$C_n = g_n^{[0]}(\hat{N}) + \sum_{m=1}^{d-1} \left( \chi(E_{\hat{N}+m} - E_{\hat{N}}) g_n^{[m]}(\hat{N}) A^m + h.c. \right),$$  (53)

$$Z_n = Z_n^{[0]} + i \sum_{m=1}^{\infty} \left( \gamma(E_{\hat{N}+m} - E_{\hat{N}}) g_n^{[m]}(\hat{N}) A^m - h.c. \right)$$  (54)

— where $d \equiv \sup \{ d_n : n = 0, 1, \ldots \}$, $Z_n^{[0]}$ is a hermitian operator such that $[Z_n^{[0]}, \mathcal{H}_0] = 0$ and the functions $\chi, \gamma$ are defined by

$$\chi(0) = 1, \quad \chi(x) = 0 \quad x \neq 0,$$

$$\gamma(0) = 0, \quad \gamma(x) = \frac{1}{x} \quad x \neq 0$$

— are solutions of eq. (50). This can be readily verified by direct substitution if one observes that

$$\chi(x) x = 0, \quad \gamma(x) x = 1 \chi(x).$$

We remark that if now $\{ |n \rangle : n = 0, 1, \ldots \}$ is any orthonormal basis of eigenvectors of $\mathcal{H}_0$, so that

$$\mathcal{H}_0 |n \rangle = E(n) |n \rangle,$$

where in general $E(n) \neq E_n$, and $A$, $A^\dagger$, $\hat{N}$ are respectively the annihilation, creation, and number operator associated with this basis, then formulae (53) and (54) still apply with the substitutions

$$E_{\hat{N}} \mapsto -E(\hat{N}), \quad d-1 \mapsto \infty.$$ 

We observe explicitly that with these modifications formulae (53) and (54) can be applied formally ignoring the possible degeneracies in the spectrum of $\mathcal{H}_0$.

5 Perturbative analysis: treatment of the BH

In this section, we want to apply the perturbative method outlined in the preceding one to the balanced Hamiltonian $\tilde{H}$. More precisely, for better illustrating the method, we will use, beside $\tilde{H}$, a Hamiltonian which is unitarily (hence
physically) equivalent to $\tilde{H}$. Indeed, let us consider the unitary operator

$$T := \exp \left( i \frac{\pi}{2} \hat{n} \sigma_x \right) \quad = \cos \left( \frac{\pi}{2} \hat{n} \right) + i \sin \left( \frac{\pi}{2} \hat{n} \right) \sigma_x. \quad (55)$$

One checks easily that the following transformation formulae hold:

$$T a T^\dagger = -i a \sigma_x, \quad (56)$$

$$T \sigma_z T^\dagger = e^{i\pi \hat{n}} \sigma_z, \quad (57)$$

$$T \sigma_\pm T^\dagger = \cos^2 \left( \frac{\pi}{2} \hat{n} \right) \sigma_\pm + \sin^2 \left( \frac{\pi}{2} \hat{n} \right) \sigma_\mp. \quad (58)$$

With the aid of this formulae, we find that

$$\check{H} := T \tilde{H} T^\dagger = \check{H}_0 + \check{H}_\uparrow, \quad (59)$$

where:

$$\check{H}_0 := \nu \hat{n} + \frac{1}{2} \delta e^{i\pi \hat{n}} \sigma_z + \lambda \eta \nu \quad (60)$$

and

$$\check{H}_\uparrow := \lambda \nu (a + a^\dagger) \quad (61)$$

$$+ \lambda \nu \sum_{m=1}^{\infty} \frac{\eta^m}{m!} (a^\dagger - a^2 + 1 - m) (a^\dagger - a)^{m-1} e^{im\pi \hat{n}} (\sigma_+ + (-1)^m \sigma_-).$$

Now, if we assume that $\eta \ll 1$, we can drastically reduce the number of terms that need to be considered in the interaction components of the Hamiltonians $\check{H}$ and $\check{H}_\uparrow$; namely, we can set:

$$\check{H}_\uparrow \simeq i \lambda \nu (a^\dagger - a^2) (\sigma_+ + \sigma_-) + \lambda \eta \nu \left( a^\dagger - a \right)^2 (\sigma_+ - \sigma_-) \quad (62)$$

$$\check{H}_\uparrow \simeq \lambda \nu (a + a^\dagger) + \lambda \eta \nu \left( a^\dagger - a \right)^2 e^{i\pi \hat{n}} (\sigma_- - \sigma_+). \quad (63)$$

Moreover, in order to treat $H_\uparrow$ and $\check{H}_\uparrow$ as perturbations, with perturbative parameter $\lambda$, we will also assume that $\lambda \ll 1$. For simplicity, we will set

$$\check{H} = e^{-i (\check{Z}_1 + \check{Z}_2 + \cdots)} \left( \check{H}_0 + \check{C}_1 + \check{C}_2 + \cdots \right) e^{i (\check{Z}_1 + \check{Z}_2 + \cdots)}, \quad (64)$$

$$\check{H} = e^{-i (\check{Z}_1 + \check{Z}_2 + \cdots)} \left( \check{H}_0 + \check{C}_1 + \check{C}_2 + \cdots \right) e^{i (\check{Z}_1 + \check{Z}_2 + \cdots)}. \quad (65)$$

Thus, differently from section 4, the perturbative parameter $\lambda$ will be included in the operators $\check{C}_n$, $\check{C}_n$, $\check{Z}_n$, $\check{Z}_n$.

Our purpose is to perform the perturbative analysis up to the second order; precisely, since we want to compute the first and second order corrections to the energy spectrum and the first order expression of the evolution operator, we need to compute the operators $\check{C}_1$, $\check{Z}_1$, and $\check{C}_2$. 

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At this point, it is convenient to distinguish three cases: when \( \bar{\eta} \) is much smaller than \( \lambda \), when \( \bar{\eta} \) is of the same order of magnitude of \( \lambda \), when \( \bar{\eta} \) is much larger than \( \lambda \).

Let us consider the case when \( \bar{\eta} \ll \lambda \).

In this case, the second term which appears respectively in the r.h.s. of eq. (52) and eq. (53), due to the presence of the factor \( \lambda \bar{\eta} \ll \lambda^2 \), can be skipped in a second order treatment; hence we can set

\[
\hat{H}_t \simeq i \lambda \nu \left( a - a^\dagger \right) \left( \sigma_+ + \sigma_- \right), \quad \hat{H}_z \simeq \lambda \nu \left( a + a^\dagger \right).
\]

Let us use the Hamiltonian \( \hat{H} \) first. Observe that, within the given approximation, the subspaces \( \mathcal{H}_g, \mathcal{H}_e \) of the total Hilbert space \( \mathcal{H} \), \( \mathcal{H}_g \oplus \mathcal{H}_e = \mathcal{H} \), are invariant subspaces for \( \hat{H} \). Thus, it will be convenient to split the perturbative problem by restricting to each invariant subspace. In order to do this, let us denote by \( a_g, \hat{n}_g, \hat{H}_g, \hat{H}^g_0, \hat{H}^g_t \) (resp. \( a_e, \hat{n}_e \)) the restriction of the operators \( a, \hat{n}, \hat{H}, \hat{H}_0, \hat{H}_t \) to \( \mathcal{H}_g \) (resp. to \( \mathcal{H}_e \)). Then, we have:

\[
\hat{H}_g = \hat{H}^g_0 + \hat{H}^g_t = \nu \hat{n}_g - \frac{1}{2} \delta e^{i \pi \hat{n}_g} + \lambda \nu \left( a_g + a_g^\dagger \right).
\]

At this point, identify the basis \( \left\{ |n\rangle \otimes |g\rangle : n = 0, 1, \ldots \right\} \) in \( \mathcal{H}_g \) with the basis \( \left\{ ||n|| : n = 0, 1, \ldots \right\} \) of section 4 and the operators \( a_g, \hat{n}_g \) with \( A, \hat{N} \). Then, applying formula (54), we find:

\[
\hat{C}^g_1 = \lambda \nu \chi(\nu + \delta e^{i \pi \hat{n}_g}) a_g + h.c. .
\]

Hence, \( \hat{C}^g_1 = 0 \) unless the resonance condition \( \nu = \delta \) is satisfied; in this case, we have:

\[
\hat{C}^g_1 = \frac{1}{2} \lambda \nu \left( a_g + a_g^\dagger \right) + \frac{1}{2} \lambda \nu \left( a_g - a_g^\dagger \right) e^{i \pi \hat{n}_g}.
\]

In the subspace \( \mathcal{H}_e \), arguing as above, we find that \( \hat{C}^e_1 \) is zero unless \( \nu = \delta \), in which case:

\[
\hat{C}^e_1 = \frac{1}{2} \lambda \nu \left( a_e + a_e^\dagger \right) - \frac{1}{2} \lambda \nu \left( a_e - a_e^\dagger \right) e^{i \pi \hat{n}_e}.
\]

Hence, considering the total Hilbert space \( \mathcal{H} \), at the first perturbative order in \( \lambda \) we find that

\[
\hat{C}_1 = \begin{cases} 0 & \text{for } \nu \neq \delta, \\ \frac{1}{2} \lambda \nu \left( a + a^\dagger \right) - \frac{1}{2} \lambda \nu \left( a - a^\dagger \right) e^{i \pi \hat{n}_z} & \text{for } \nu = \delta. \end{cases} \tag{66}
\]

Moreover, one can check that the minimal solution for \( \hat{Z}_1 \) is given by:

\[
\hat{Z}_1 = \frac{i}{2} \lambda \nu (\nu - \delta) \left( (a - a^\dagger) - (a + a^\dagger) e^{i \pi \hat{n}_z} \right) + \frac{i}{2} \lambda \frac{\nu}{\nu + \delta} \left( (a - a^\dagger) + (a + a^\dagger) e^{i \pi \hat{n}_z} \right). \tag{68}
\]
The operator \( \tilde{Z}_1 \) allows us to compute the second order constant of the motion \( \tilde{C}_2 \). The result is found to be:

\[
\tilde{C}_2 = \lambda^2 \nu^2 \left( \left( \hat{n} + \frac{1}{2} \right) e^{i\pi \hat{n} \sigma_z} - \frac{1}{2} \right) - \lambda^2 \nu^2 \gamma (\nu - \bar{\delta}) \left( \left( \hat{n} + \frac{1}{2} \right) e^{i\pi \hat{n} \sigma_z} + \frac{1}{2} \right). \tag{69}
\]

On the other hand, in the ‘reference frame’ associated with \( \tilde{H} \), at the first order we have:

\[
\tilde{C}_1 = T^\dagger \tilde{C}_1 T = 0 \quad \text{for} \quad \nu \neq \bar{\delta}, \tag{70}
\]

\[
\tilde{C}_1 = i \lambda \nu (a \sigma_+ - a^\dagger \sigma_-) \quad \text{for} \quad \nu = \bar{\delta}. \tag{71}
\]

Notice that, in correspondence to the resonance condition \( \nu = \bar{\delta} \), \( \tilde{C}_1 \) coincides with the constant of the motion \( \tilde{S} \), with \( \omega = \bar{\delta} \), of the Hamiltonian \( \tilde{H}_{JC} \) which is unitarily equivalent to the Jaynes-Cummings Hamiltonian (see section 2) and hence with the prescription of the RWA (see section 3). We could have obtained this result using directly the Hamiltonian \( \tilde{H} \), observing that \( m \nu = \bar{\delta}, \ m = 1, 2, \ldots \), is the degeneracy condition for \( \tilde{H}_0 \) and then applying formula (41).

Thus, it could seem that, in the resonant regime \( \nu = \bar{\delta} \), the first order approximation of \( \tilde{H} \) coincides with the RWA Hamiltonian \( \tilde{H}_0 + \tilde{C}_1 \). Actually, it would be so if \( \tilde{Z}_1 \) was identically zero (recall formula (64)), but we have:

\[
\tilde{Z}_1 = T^\dagger \tilde{Z}_1 T
= -\lambda \nu \gamma (\nu - \bar{\delta}) (a \sigma_+ + a^\dagger \sigma_-) - \lambda \frac{\nu}{\nu + \delta} (a \sigma_- + a^\dagger \sigma_+). \tag{72}
\]

We will see the effects of this fact in section 7.

At the second order, we find:

\[
\tilde{C}_2 = T^\dagger \tilde{C}_2 T
= \lambda^2 \nu^2 \left( \left( \hat{n} + \frac{1}{2} \right) \sigma_z - \frac{1}{2} \right) - \lambda^2 \nu^2 \gamma (\nu - \bar{\delta}) \left( \left( \hat{n} + \frac{1}{2} \right) \sigma_z + \frac{1}{2} \right). \tag{73}
\]

Let us now consider the case when \( \bar{\eta} \sim \lambda \).

In this case, since \( \lambda \bar{\eta} \sim \lambda^2 \), we have to consider the second term in the r.h.s. respectively of eq. (62) and eq. (63) at the second perturbative order. In this case, one can work directly with the Hamiltonian \( \tilde{H} \). Then, the result is the following. At the first order, the constant of the motion \( \tilde{C}_1 \) is still given by formulae \( 60 \) and \( 61 \). \( \tilde{Z}_1 \) by formula \( 62 \). At the second order, one finds:

\[
\tilde{C}_2 = \lambda^2 \nu^2 \left( \left( \hat{n} + \frac{1}{2} \right) \sigma_z - \frac{1}{2} \right) - \lambda^2 \nu^2 \gamma (\nu - \bar{\delta}) \left( \left( \hat{n} + \frac{1}{2} \right) \sigma_z + \frac{1}{2} \right)
- \lambda \bar{\eta} \nu \chi (2\nu - \bar{\delta}) (a^2 \sigma_+ + a^{1^2} \sigma_-). \tag{74}
\]
Hence an extra term, with respect to formula (73), appears in the expression of \( \tilde{C}_2 \). This term is related to the resonance \( 2\nu = \tilde{\delta} \).

Eventually, let us consider the case when \( \tilde{\eta} \gg \lambda \).

In this case, we have:

\[ \lambda^2 \ll \lambda \tilde{\eta} \ll \lambda \ll \tilde{\eta} \ll 1. \]

Hence, the term proportional to \( \lambda \tilde{\eta} \) can now be regarded as the leading term at the second perturbative order. Then, the operators \( \tilde{C}_1, \tilde{Z}_1 \) and \( \tilde{C}_2 \) are given again by formulae (70), (71), (72) and (74).

A special attention is deserved by the nearly resonant regime. Indeed, if the condition \( |\nu - \tilde{\delta}| \ll \nu \) is satisfied, it is convenient to set \( \tilde{H} = \tilde{H}_0' + \tilde{H}_0'' \), where:

\[ \tilde{H}_0' = \nu \left( \hat{n} + \frac{1}{2} \sigma_z \right) + \lambda \tilde{\eta} \nu, \]

\[ \tilde{H}_0'' = \frac{1}{2} \left( \tilde{\delta} - \nu \right) \sigma_z + \lambda \tilde{\eta} \nu \left( a \sigma_+ - a^\dagger \sigma_- \right). \]

Thus, the zeroth order Hamiltonian \( \tilde{H}_0' \) has degeneracies in its spectrum as in the resonant case and an extra term appears in the perturbation. This strategy, which is analogous to carefully choosing the origin of the power expansion of an analytic function, allows to obtain larger convergence radii for our perturbative expansions. In the nearly resonant case, one finds that the expressions of the operators \( \tilde{C}_1, \tilde{Z}_1 \) and \( \tilde{C}_2 \) are the following:

\[ \tilde{C}_1 = \frac{1}{2} \left( \tilde{\delta} - \nu \right) \sigma_z + i \lambda \nu \left( a \sigma_+ - a^\dagger \sigma_- \right), \]

\[ \tilde{Z}_1 = -\frac{1}{2} \lambda \left( a \sigma_- + a^\dagger \sigma_+ \right), \]

\[ \tilde{C}_2 = \frac{1}{2} \lambda^2 \nu \left( \hat{n} + \frac{1}{2} \sigma_z - \frac{1}{2} \right). \]

Notice that, as in the exactly resonant regime, the operator \( \tilde{H}_0'' + \tilde{C}_1 \) coincides with the RWA Hamiltonian (now obtained using as reference Hamiltonian \( \tilde{H}_0' \)), but again, since \( \tilde{Z}_1 \neq 0 \), it is not the correct first order approximation of \( \tilde{H} \).

### 6 Corrections to eigenvalues: the RWA and the Bloch-Siegert shift

By means of the perturbative method discussed in the previous sections one can obtain approximate expressions, at each perturbative order, of the eigenvalues, the eigenprojectors and of the evolution operator associated with the BH.

For instance, recalling formulae (74) and (77), one finds that approximate expressions, at the second perturbative order, of the energy levels of the BH in
the nearly resonant regime, i.e. for $|\nu - \tilde{\delta}| \ll \nu$, are given by the eigenvalues of the hermitian operator

$$
\mathfrak{h}^{(2)} = \nu \left( \hat{n} + \frac{1}{2} \sigma_z \right) + \frac{1}{2} \left( \tilde{\delta} - \nu \right) \sigma_z \\
+ i \lambda \nu \left( a \sigma_+ - a^\dagger \sigma_- \right) + \frac{1}{2} \lambda^2 \nu \left( \left( \hat{n} + \frac{1}{2} \right) \sigma_z - \frac{1}{2} \right).
$$

Observe that the eigenspaces of the operator $\mathfrak{h}^{(2)}$ are the one-dimensional subspace $\mathcal{H}_0 = \text{Span}\{ |0 \rangle \otimes |g \rangle \}$ and the two-dimensional subspaces

$$
\mathcal{H}_n = \text{Span}\{ |n-1 \rangle \otimes |e \rangle, \; |n \rangle \otimes |g \rangle \}, \; n = 1, 2, \ldots .
$$

Hence, all one has to do is to diagonalize the matrix representation of $\mathfrak{h}^{(2)}$ in each of these two-dimensional subspaces; namely, one has to diagonalize the $2 \times 2$ matrices

$$
\begin{bmatrix}
\mathfrak{A}_n + \mathfrak{B}_n & i \lambda \nu \sqrt{n} \\
- i \lambda \nu \sqrt{n} & \mathfrak{A}_n - \mathfrak{B}_n
\end{bmatrix}, \; n = 1, 2, \ldots ,
$$

(80)

where:

$$
\mathfrak{A}_n = \nu \left( n - \frac{1}{2} \right) + \lambda \tilde{\eta} \nu - \frac{1}{2} \lambda^2 \nu, \\
\mathfrak{B}_n = \frac{1}{2} \left( \tilde{\delta} - \nu \right) + \frac{1}{2} \lambda^2 \nu n.
$$

(81)

(82)

Thus, the energy levels of the BH $\hat{H}$, in the nearly resonant regime, are given by

$$
E_0 \simeq -\frac{1}{2} \nu + \lambda \tilde{\eta} \nu - \frac{1}{2} \lambda^2 \nu,
$$

$$
E_{n, \pm} \simeq \nu \left( n - \frac{1}{2} \right) + \lambda \tilde{\eta} \nu \pm \frac{1}{4} \left( \lambda^2 \nu n \right)^2 + \lambda^2 \nu^2 n - \frac{1}{2} \lambda^2 \nu.
$$

(83)

with $n = 1, 2, \ldots$. The previous expressions coincide, skipping the second order corrections, with the ones obtained applying the RWA. This is due to the fact that, as already observed in section 5, the operator $\hat{H}_0 + i \lambda \nu \left( a \sigma_+ + a^\dagger \sigma_- \right)$ coincides with the result of the application of the RWA to the Hamiltonian $\hat{H}$, in the nearly resonant regime $|\nu - \tilde{\delta}| \ll \nu$. Hence, on the one hand, the RWA gives the correct first order expressions for the eigenvalues. In the next section we will show that, on the other hand, the RWA does not give the correct first order approximation of the evolution operator associated with the BH (hence, with the ITH).

There is also a second order effect that cannot be predicted if one simply applies the RWA. This effect may be compared with the so called ‘Bloch-Siegert shift’. In order to clarify this point, let us consider the matrix representation of a hermitian operator $\mathfrak{h}$ (which can be thought as a perturbative approximation of

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the Hamiltonian of a physical system) in a two-dimensional invariant subspace, with respect to an orthonormal basis \(|1\rangle, |2\rangle\) in this space:

\[
M = \begin{bmatrix}
  h_{11} & h_{12} \\
  h_{21} & h_{22}
\end{bmatrix}, \quad h_{11} = h_{11}^*, \quad h_{22} = h_{22}^*, \quad h_{12} = h_{21}^*.
\]

Now, if one sets

\[
A = \frac{h_{11} + h_{22}}{2}, \quad b = \frac{h_{11} - h_{22}}{2}, \quad c = h_{12} = h_{21}^*,
\]

the matrix \(M\) can be rewritten as

\[
M = \begin{bmatrix}
  A + b & c \\
  c^* & A - b
\end{bmatrix}.
\]

and the eigenvalues of the hermitian matrix \(M\) are given by the following simple formula:

\[
E_\pm(b) = A \pm \sqrt{b^2 + |c|^2}.
\]

Let us assume that \(c \neq 0\). Then the vectors \(|1\rangle, |2\rangle\) are not eigenvectors of \(h\) and the graphics of the functions \(b \mapsto E_\pm(b)\) are the two branches of a hyperbola whose asymptotes intersect at the point of coordinates \((0, \hat{A})\). Thus the difference between the two eigenvalues \(E_+(b) - E_-(b)\) attains its minimum ('level anticrossing') at \(b = 0\). This is also the condition for which the transition probability \(P_{1\rightarrow 2}(t)\) assumes periodically the value 1 (otherwise \(P_{1\rightarrow 2}(t) < 1\)). Indeed, according to a well known formula, we have:

\[
P_{1\rightarrow 2}(t) := |\langle 2 | \exp(-i h t) | 1 \rangle|^2 = \frac{|c|^2}{b^2 + |c|^2} \sin^2 \left( \sqrt{b^2 + |c|^2} t \right).
\]

At this point, suppose that — due, for instance, to (higher order) perturbative corrections — the matrix \(M\) undergoes a modification of the type

\[
M \rightarrow M + \begin{bmatrix}
  \epsilon & 0 \\
  0 & -\epsilon
\end{bmatrix}.
\]

Then the level anticrossing condition undergoes a shift: \(b + \epsilon = 0\). In our case, we can do the following identifications:

\[
\hat{A} \equiv \hat{A}_n, \quad b \equiv \frac{1}{2} \left( \delta - \nu \right), \quad \epsilon \equiv \epsilon_n \equiv \frac{1}{2} \lambda^2 \nu n, \quad n = 1, 2, \ldots.
\]

Thus, the second order level anticrossing shift for the subspace \(\mathcal{H}_n\) is given by

\[
\frac{1}{2} \lambda^2 \nu n = \frac{1}{2} \sqrt{\Omega R + \delta^2} \eta^2 \nu n, \quad n = 1, 2, \ldots.
\]

A similar phenomenon appears in the classical work of Bloch and Siegert on the magnetic resonance, whose Hamiltonian can be replaced, using Floquet’s theorem, by a time-independent effective Hamiltonian containing virtual terms, as shown later by Shirley. The presence of these virtual terms gives rise, at the second perturbative order, to a level anticrossing shift, which translates into a shift of the magnetic resonance condition, the Bloch-Siegert shift.
7 The evolution operator

From this point onwards, for the sake of conciseness, we will use the following notation. Given a couple of functions \( f \) and \( h \) of the perturbative parameter \( \lambda \), if \( f(\lambda) = h(\lambda) + O(\lambda^2) \), we will write simply

\[
 f(\lambda) \overset{\lambda^2}{=} h(\lambda).
\]

Then, let \( \mathcal{U}(t, t_0) \) be the evolution operator associated with the ion trap Hamiltonian \( H(t) \):

\[
 \left( \frac{i}{\hbar} \frac{d}{dt} \mathcal{U} \right)(t, t_0) = H(t) \mathcal{U}(t, t_0), \quad \mathcal{U}(t_0, t_0) = \text{Id}. \tag{84}
\]

As we have seen, \( \mathcal{U}(t, t_0) \) can be decomposed as

\[
 \mathcal{U}(t, t_0) = R^\dagger T^\dagger e^{-i\tilde{H}(t-t_0)} T_{\Delta}. \tag{85}
\]

Moreover, the evolution operator associated with \( \tilde{H} \), namely \( \mathcal{E}(t) = e^{-i\tilde{H}t} \), admits a perturbative decomposition. At the first order, we have:

\[
 \mathcal{E}(t) \overset{\lambda^2}{=} \exp \left( -i e^{-i\tilde{Z}_1} \left( \tilde{H}_0 + \tilde{C}_1 \right) e^{i\tilde{Z}_1} t \right)
 = e^{-i\tilde{Z}_1} e^{-i(\tilde{H}_0+\tilde{C}_1)t} e^{i\tilde{Z}_1}
 = e^{-i\tilde{Z}_1} e^{-i\tilde{H}_0 t} e^{-i\tilde{C}_1 t} e^{i\tilde{Z}_1} =: \mathcal{E}_1(t), \tag{86}
\]

where for obtaining the third line we have used the fact that \( [\tilde{C}_1, \tilde{H}_0] = 0 \). In order to deal with simpler formulae, let us consider the case when the resonance condition \( \nu = \delta \) is exactly satisfied. In this case, we have that \( \tilde{H}_0 = \nu (\hat{n} + \frac{1}{2} \sigma_z) \) and \( \tilde{C}_1 = i \lambda \nu (a \sigma_+ - a^\dagger \sigma_-) \). Thus, \( \tilde{C}_1 \) is, up to a unitary transformation, the infinitesimal generator of the Jaynes-Cummings evaporator \( \mathcal{J}(t) \); hence:

\[
 \tilde{\mathcal{J}}(t) := \exp \left( -i \tilde{C}_1 t \right)
 = e^{-i\tilde{\mathcal{J}}^\dagger} \mathcal{E}(t) e^{i\tilde{\mathcal{J}}^\dagger}
 = \begin{bmatrix}
 \cos(\lambda \nu \sqrt{\hat{n} + 1} t) & \sin(\lambda \nu \sqrt{\hat{n} + 1} t) \frac{a}{\sqrt{\hat{n} + 1}} \\
 -\sin(\lambda \nu \sqrt{\hat{n}} t) \frac{a^\dagger}{\sqrt{\hat{n}}} & \cos(\lambda \nu \sqrt{\hat{n}} t)
\end{bmatrix}. \tag{87}
\]

Then it turns out that the expression of the evolution operator \( \mathcal{R}(t) \) obtained applying the RWA to \( \tilde{H} \), namely

\[
 \mathcal{R}(t) = \exp(-i\tilde{H}_0 t) \tilde{\mathcal{J}}(t), \tag{88}
\]

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would be correct at the first perturbative order only if the operator $\hat{Z}_1$ was identically zero. But this is not the case since, for $\nu = \delta$, it turns out that $\hat{Z}_1 = -\frac{i}{2} \lambda (a \sigma_- + a^\dagger \sigma_+)$ and we have:

$$\exp \left( i \hat{Z}_1 \right) = \begin{bmatrix} \cos \left( \frac{1}{2} \lambda \sqrt{n} \right) & -i \frac{\sin \left( \frac{1}{2} \lambda \sqrt{n} \right)}{\sqrt{n}} a^\dagger \\ -i \frac{\sin \left( \frac{1}{2} \lambda \sqrt{n + 1} \right)}{\sqrt{n + 1}} a & \cos \left( \frac{1}{2} \lambda \sqrt{n + 1} \right) \end{bmatrix}.$$  \hspace{1cm} (89)

This result can be also expressed saying that the RWA neglects the first order correction to the unperturbed eigenprojectors.

In order to get a more explicit comparison of the correct first order approximate evolution operator $\mathcal{E}_1(t)$ with the RWA evolution operator $\mathcal{R}(t)$, we proceed as follows. First, we observe that

$$\mathcal{E}_1(t) = e^{-i\hat{Z}_1} e^{-i\hat{H}_{0t}} \mathcal{L}(t) e^{i\hat{Z}_1} \approx \frac{\lambda^2}{2} e^{-i\hat{Z}_1} e^{-i\hat{H}_{0t}} e^{i\hat{Z}_1} \mathcal{L}(t).$$

Then, using formula (89), we find that the operator $e^{-i\hat{Z}_1} e^{-i\hat{H}_{0t}} e^{i\hat{Z}_1}$ has the following expression:

$$\begin{bmatrix} (\alpha_\lambda (\hat{n}) + \beta_\lambda (\hat{n}) e^{i2\nu t}) e^{-i\nu (\hat{n} + \frac{1}{2}) t} & \kappa_\lambda (\hat{n}) (1 - e^{i2\nu t}) e^{-i\nu (\hat{n} + \frac{1}{2}) t} a^\dagger \\
\kappa_\lambda (\hat{n} + 1) (1 - e^{-i2\nu t}) e^{-i\nu (\hat{n} - \frac{1}{2}) t} a & (\alpha_\lambda (\hat{n} + 1) + \beta_\lambda (\hat{n} + 1) e^{-i2\nu t}) e^{-i\nu (\hat{n} - \frac{1}{2}) t} \end{bmatrix};$$

where we have set

$$\alpha_\lambda (\hat{n}) := \cos^2 \left( \frac{1}{2} \lambda \sqrt{n} \right), \quad \beta_\lambda (\hat{n}) := \sin^2 \left( \frac{1}{2} \lambda \sqrt{n} \right),$$

$$\kappa_\lambda (\hat{n}) := -i \frac{\cos \left( \frac{1}{2} \lambda \sqrt{n} \right) \sin \left( \frac{1}{2} \lambda \sqrt{n} \right)}{\sqrt{n}}.$$

Thus, due to the fact that $\kappa_\lambda (\hat{n}) \approx -\frac{i}{2} \lambda \text{Id}$, we have:

$$e^{-i\hat{Z}_1} e^{-i\hat{H}_{0t}} e^{i\hat{Z}_1} \lambda^2 \approx e^{-i\hat{H}_{0t}}, \quad \text{for } t \neq 0.$$

It follows that, for $t \neq 0$,

$$\mathcal{E}(t) \lambda^2 \approx \mathcal{E}_1(t) \lambda^2 \approx e^{-i\hat{Z}_1} e^{-i\hat{H}_{0t}} e^{i\hat{Z}_1} \mathcal{L}(t) \lambda^2 \approx e^{-i\hat{H}_{0t}} \mathcal{L}(t) = \mathcal{R}(t).$$

This proves that the RWA does not provide, already at the first perturbative order, the correct approximate expression of the evolution operator associated
with the BH (hence with the ITH).

Now, in order to obtain a direct comparison of \( E(t) \) with \( R(t) \), observe that

\[
E(t) \simeq e^{-i\tilde{Z}_1(t)} e^{-i\tilde{H}_0 t} e^{i\tilde{Z}_1} \tilde{L}(t)
\]

\[
= e^{-i\tilde{Z}_1} (e^{-i\tilde{H}_0 t} e^{i\tilde{Z}_1} e^{i\tilde{H}_0 t}) e^{-i\tilde{H}_0 t} \tilde{L}(t)
\]

\[
= e^{-i\tilde{Z}_1(0)} e^{i\tilde{Z}_1(-t)} e^{-i\tilde{H}_0 t} \tilde{L}(t)
\]

\[
\simeq e^{-i(\tilde{Z}_1(0)-\tilde{Z}_1(-t))} e^{-i\tilde{H}_0 t} \tilde{L}(t),
\]

where \( t \mapsto \tilde{Z}_1(t) \) is solution of the Heisenberg equation

\[
\left( \frac{d}{dt} \tilde{Z}_1 \right)(t) = -i[\tilde{Z}_1(t), \tilde{H}_0], \quad \tilde{Z}_1(0) = \tilde{Z}_1.
\]

Then, since

\[
-i[\tilde{Z}_1(-t), \tilde{H}_0] = i \lambda \nu (a \sigma_- e^{i2\nu t} + a^\dagger \sigma_+ e^{-i2\nu t}) =: \tilde{Y}_1(t),
\]

we find the following formula:

\[
E(t) \simeq \exp \left( -i \int_0^t \tilde{Y}_1(\tau) \, d\tau \right) \mathcal{R}(t). \tag{90}
\]

This expression provides a direct relation between \( E(t) \) and \( \mathcal{R}(t) \). Notice that it contains the integral of an oscillating function. Anyway, since this integral appears as the argument of an exponential, we are not led to the erroneous conclusion that its contribution can be neglected, as it is often incorrectly argued using a Feynman-Dyson expansion of the interaction picture evolution operator (see section 3).

### 8 Discussion

In writing the present paper, the authors had in mind two main aims:

- to show that the Hamiltonian of a trapped ion interacting with a laser field can be studied even if the condition \( \Omega_R \ll \nu \) is not satisfied, since this condition is incompatible with applications that physicists consider to be relevant nowadays, for instance fast ion trap quantum computers;

- to show that a rigorous perturbative approach can improve the results obtained by simply applying the RWA, still preserving the chance of performing explicit and manageable calculations.

With regard to the first point, it has been shown that the study of the ion trap Hamiltonian can be reduced to the study of a time-independent effective Hamiltonian (the BH) in which the coupling constant is scarcely sensitive to the
Rabi frequency $\Omega_R$, hence perfectly fit for our aims. The resonance condition for the BH has a very simple form:

$$m \nu = \delta = \sqrt{4\Omega_R^2 + \delta^2}, \quad m = 1, 2, \ldots ,$$

where we recall that $\delta$ denotes the ion-laser detuning.

With regard to the second point, we have shown that a suitable perturbative approach allows to write a very powerful perturbative expansion of the evolution operator of the system. Indeed, using the notation of section 4 we have:

$$e^{-i S(\lambda) t} = \exp\left(-i \left( e^{-i (\lambda Z_1 + \lambda^2 Z_2 + \cdots)} (H_0 + \lambda C_1 + \cdots) e^{i (\lambda Z_1 + \lambda^2 Z_2 + \cdots)} \right) t \right)$$

$$= e^{-i (\lambda Z_1 + \lambda^2 Z_2 + \cdots)} e^{-i (H_0 + \lambda C_1 + \cdots)} e^{i (\lambda Z_1 + \lambda^2 Z_2 + \cdots)}, \quad (91)$$

where the operators $C_1, Z_1, C_2, Z_2, \ldots$ can obtained by a recursive algebraic procedure. Notice that any truncation of this perturbative expansion is a unitary operator, a very valuable feature for an approximate expression of the evolution operator. Our approach, whose general validity goes beyond the argument of this paper, can be applied successfully to the BH pointing out two main facts. First, the RWA terms and the counter rotating terms play different roles (but with the same dignity) in the perturbative expansion $91$. The former appear in the time-dependent component of the expansion (the one associated with the operators $C_1, C_2, \ldots$), while the latter appear in the time-independent component (associated with the operators $Z_1, Z_2, \ldots$). Second, already at the first perturbative order the counter rotating terms, completely neglected by the RWA, give rise to a correction that can be regarded as a perturbative correction to the unperturbed eigenprojectors (while, as we have seen, the first order correction to the eigenvalues coincides with the prescription of the RWA). In conclusion, we believe that our approach can provide more accurate expressions of the evolution operator of the ion trap Hamiltonian for a wide range of intensities of the driving laser field.

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