Coarse-grained dynamics of ac-driven two-state systems

N. Macrì([1])([2]), L. Giannelli([1])([3]), J. Rajendran([1])([2]), E. Paladino([1])([2])([3])
and G. Falci([1])([2])([3])

([1]) *Dipartimento di Fisica e Astronomia "Ettore Majorana", Università di Catania*
Via S. Sofia 64, 95123, Catania, Italy
([2]) *Istituto Nazionale di Fisica Nucleare, Sezione di Catania - 95123, Catania, Italy*
([3]) *CNR-IMM, UoS Università - 95123 Catania, Italy*

Summary. — Magnus expansion is used to identify effective Hamiltonians describing the coarse-grained dynamics of more complex problems. Here, we apply this method to a two-level system driven by an AC field. We derive Stark and Bloch-Siegert shifts of both diagonal and off-diagonal entries of the Hamiltonian as a result of coarse graining only.

1. – Introduction: effective Hamiltonian by Magnus Expansion

The Magnus expansion is a mathematical tool allowing one to express the solution of a linear differential equation as an exponentiated series. In particular, the time-evolution operator $U(t, t_0) = -e^{-i F(t, t_0)}$ solving Schrödinger equation $\dot{U}(t, t_0) = -i H(t) U(t, t_0)$ with initial condition $U(t_0, t_0) = 1$ is expressed as a series $F(t, t_0) = \sum_i F_i(t, t_0)$ where (higher-order terms can be found in ref. [1])

$$(1) \qquad F_1 = \int_{t_0}^{t} ds\, H(s), \quad ; \quad F_2 = -\frac{i}{2} \int_{t_0}^{t} \int_{t_0}^{s_1} ds_1\, ds_2\, [H(s_1), H(s_2)].$$

The small expansion parameter is related to $[H(t), H(t')]$. The F_1 term yields the average Hamiltonian [2], while F_2 provides already an excellent approximation in many cases. Coarse graining over a time τ is obtained by approximating $U(t + \tau/2, t - \tau/2) \approx e^{-iH_{\text{eff}}(t)\tau}$, where the effective Hamiltonian is obtained by truncating the Magnus series, $H_{\text{eff}}(t) = \frac{1}{\tau} [F_1 + F_2 + \ldots]$. The coarse-grained dynamics is then expressed as $U_{eff}(t, t_0) = \text{T} \exp\left\{-i \int_{t_0}^{t} ds\, H_{\text{eff}}(s)\right\}$. If $[H(t'), H(t'')]$ is sufficiently small for $t'' \neq t' \in [t + \tau/2, t - \tau/2]$, the effective Hamiltonian involves few terms of the series and it is expected to be simpler than the original $H(t)$.

We validate the approximation via fidelity $\mathcal{F}(t) = \min_{|\psi_0\rangle} (|\langle\psi_0| \cdot U^\dagger(t) U_{\text{eff}}(t) |\psi_0\rangle|^2)$, which is a simple unitarily invariant figure of merit directly referring to the dynamics. Analytical expression $\mathcal{F} = \text{Tr}\left\{ U^\dagger U_{\text{eff}} \right\}$ holds for a two-state system.

2. – Results for ac driven 2-level atom

We consider a two-level system with Hamiltonian $H_0 = -\frac{\epsilon}{2}\hat{\sigma}_3$ driven by a monochromatic ac field $H_1 = H_{RW} + H_{CR}$ with corotating $H_{RW} = \mathscr{W} e^{i\omega t}\sigma^+ + \text{h.c.}$ and counterrotating $H_{CR} = \mathscr{W} e^{-i\omega t}\sigma^+ + \text{h.c.}$ terms. In the interaction picture, $\tilde{H}(t) = e^{iH_0 t} H_1 e^{-iH_0 t}$ the two lowest-order terms of the Magnus expansion are calculated

$$(2) \qquad \tilde{H}_{eff}^{(1)} = \frac{\mathscr{W}}{2}\left(e^{-i\,\delta t}\,\text{sinc}\frac{\delta\tau}{2} + e^{-i\,(\epsilon+\omega)t}\,\text{sinc}\frac{(\epsilon+\omega)\tau}{2} \right)\hat{\sigma}^- + \text{h.c.},$$

$$(3) \qquad \tilde{H}_{eff}^{(2)} = \left\{ -\frac{\mathscr{W}^2}{4}\left[\frac{1-\text{sinc}\,\delta\,\tau}{\delta} + \frac{1-\text{sinc}(\epsilon+\omega)\,\tau}{\omega+\epsilon} \right] - \frac{\mathscr{W}^2}{4} e^{2i\omega t}\left[\frac{\text{sinc}\,\omega\tau}{\delta(\omega+\epsilon)} \right.\right.$$
$$\left.\left. - \left(\frac{\text{sinc}(\delta\tau/2)}{\omega+\epsilon} e^{-i(\epsilon+\omega)\,\tau/2} + \frac{\text{sinc}[(\epsilon+\omega)\tau/2]}{\delta} e^{i\delta\,\tau/2} \right) \right] + \text{c.c.} \right\}\hat{\sigma}_3,$$

where $\delta = \epsilon - \omega$ is the detuning. Since $\omega, \epsilon > 0$ we can eliminate the fast dynamics by choosing $\tau \gg \frac{\pi}{\omega}, \frac{2\pi}{\omega+\varepsilon}$, meaning that the $\text{sinc}(x)$ terms are very small except possibly those containing δ. These latter can also be neglected if $\delta\tau \gg 2\pi$. In this case $\tilde{H}_{eff}^{(1)} \approx 0$ while $\tilde{H}_{eff}^{(2)} \approx -\frac{1}{2}[S_{RW} + S_{BS}]\sigma_3$, where Stark shift $S_{RW} = |\mathscr{W}|^2/(2\delta)$ and diagonal Bloch-Siegert shift $S_{BS} = |\mathscr{W}|^2/2\,(2\omega+\delta)$ [3] appear. This result is self-consistent if we can choose $\tau \ll 2\pi/S_{RW}$, such that the effect of the shifts on top of the bare dynamics is apparent. Thus the approximation holds only if $\delta/\mathscr{W} \gg 1$, *i.e.*, for large detuning.

The dynamics determined by H_{eff} conserves populations of the eigenstates of σ_3 accumulating a dynamical phase between them. We validate this result by the fidelity (see fig. 1(a)) with respect to the exact dynamics, evaluated up to relatively large times which amplify the effect of errors in the dynamical phase. Values of the parameters are chosen in order to test the limits of our approximation, as the quite large $\mathscr{W}/\omega = 0.5$ and not so large $\delta/\omega = 3$. It is seen that $\mathcal{F} \gtrsim 0.95$, the error being due to small changes in the populations. We also plot the fidelity for the rotating wave approximation (RWA) $H = H_{RW}$ showing that the diagonal S_{BS} cannot be neglected.

Notice that if we let $\delta \to 0$ in eq. (3) we would obtain $\tilde{H}_{eff}^{(1)} \to \tilde{H}_{RW}$ while in $\tilde{H}_{eff}^{(2)}$ terms containing δ vanish. Therefore, it is tempting to take $H_{eff} = -\frac{1}{2}S_{BS}\,\sigma_3 + H_{RW}$ as often done in the standard treatment of quantum optics [3]. However, this guess is not always accurate: in fact at resonance a new term appears which renormalizes $\mathscr{W}$. The calculation is carried in a rotating frame defined by transformation $U_x(t) = e^{-iH_0 t}e^{-i\tilde{H}_{RW}t}$. In this frame the Hamiltonian is $\bar{H}(t) = U_x^\dagger(t)\,\bar{H}_{CR}(t)\,U_x(t)$ and we use it to evaluate the first two terms of the Magnus expansion. Letting $\omega > \mathscr{W} > 0$ we choose $\frac{2\pi}{\mathscr{W}} \gg \tau \gg \frac{2\pi}{2\,\omega-\mathscr{W}}$. Thus, the first-order term averages out while at second order slowly varying terms are retained, obtaining

$$\bar{H}_{eff}^{(2)} = -\frac{S'_{BS}}{2}\,\sigma_1 - \frac{S_{BS}}{2}\,\frac{1-(\mathscr{W}/2\sqrt{2}\omega)^2}{1-(\mathscr{W}/2\omega)^2}\left[e^{-i\mathscr{W}t}\,|+\rangle\langle-| + \text{h.c.} \right],$$
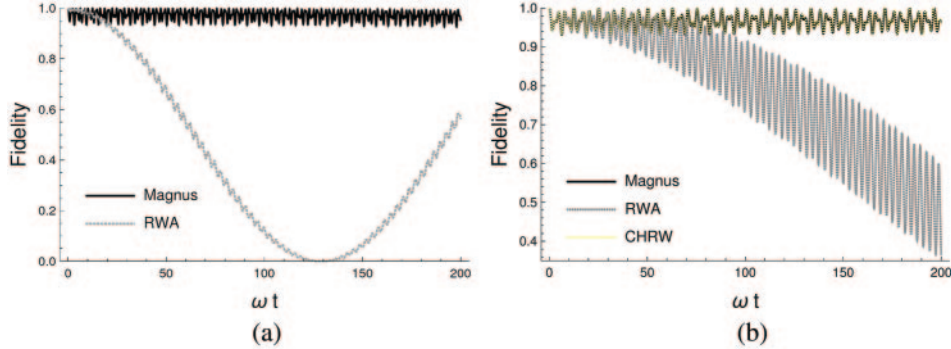
Fig. 1. – Fidelities for the Magnus effective Hamiltonian at second order for $\mathscr{W}/\omega = 0.5$. (a) For $\delta/\omega = 3$ and compared to the RWA. (b) At resonance, compared with the RWA plus diagonal S_{BS} and with the CHRW method [4,5].

where $|\pm\rangle$ are eigenstates of σ_1 and the off-diagonal Bloch-Siegert shift is defined as

$$S'_{BS} = \frac{\mathscr{W}^3}{16\,\omega^2[1 - (\mathscr{W}/2\omega)^2]}.$$

This result is self-consistent only if we can choose $\tau \ll 2\pi/S'_{RW}$ which implies that it must be $\mathscr{W}/\omega \gg (32)^{-1/3}$. Transforming back to the interaction picture we recover the more familiar structure

$$\tilde{H}_{eff} = -\frac{1}{2}\,S_{BS}\,\sigma_3 + \frac{1}{2}\,(\mathscr{W} - S'_{BS})\sigma_1.$$

Contrary to what previously guessed, this result shows that the field amplitude is renormalized by "off-diagonal" shift S'_{BS}. The fidelity for our H_{eff} and for RWA plus diagonal S_{BS} guess which neglects "off-diagonal" S'_{BS} is shown in fig. 1(b). We choose $\mathscr{W}/\omega = 0.5$ which is demanding for our approximation. It is clear that in this regime S'_{BS} cannot be neglected. This may be surprising at first sight since in regime $W/\omega < 1$ we consider $S_{BS} \sim \mathscr{W}^2/\omega$ larger than $S'_{BS} \sim \mathscr{W}^3/\omega^2$, but it can be understood by noticing that both shifts appear at the same order of $\mathscr{W}/\omega$ in the eigenvalues of $\tilde{H}_{eff}$.

3. – Conclusion

We studied the dynamics of a two-state system driven by a monochromatic ac classical field with both corotating and counterrotating components. This problem has been tackled in the past by several accurate and elaborated analytic methods. We show that a satisfactory and analytically solvable effective Hamiltonian can be found by deriving the coarse-grained dynamics, with no further basic assumption. Coarse graining was operated approximating the dynamics in short time intervals via the Magnus expansion. Our results agree with those obtained by more elaborated methods [4,5], as also shown in fig. 1 for the CHRW method of refs. [4,5] at first order in $\mathscr{W}/\omega$. The advantage of our approach is that it relies only on coarse-graining and it can be extended to more general instances, as slowly varying field amplitudes and frequency chirping [6], multitone drives and multilevel systems [7,8], operations in devices with realistic noise [9]. In view of

the accuracy we obtain for relatively large values of $\mathscr{W}$ we expect that extensions of our method to quantum fields may provide accurate effective Hamiltonians for atom-cavity systems in the ultrastrong coupling regime [10, 11], which are a subject of large interest in Condensed Matter physics and Quantum Technologies.

∗ ∗ ∗

REFERENCES

[1] Blanes S., Casas F., Oteo J. and Ros J., *Phys. Rep.*, **470** (2009) 151.
[2] Vandersypen L. M. K. and Chuang I. L., *Rev. Mod. Phys.*, **76** (2005) 1037.
[3] Allen L. and Eberly J. H., *Optical Resonance and Two-Level Atoms*, Vol. **28** (Courier Corporation) 1987.
[4] Lü Z. and Zheng H., *Phys. Rev. A*, **86** (2012) 023831.
[5] Ashhab S., Johansson J. R., Zagoskin A. M. and Nori F., *Phys. Rev. A*, **75** (2007) 063414.
[6] Falci G., Di Stefano P. G., Ridolfo A., D'Arrigo A., Paraoanu G. S. and Paladino E., *Fortschr. Phys.*, **65** (2017) 1600077.
[7] Di Stefano P. G., Paladino E., Pope T. J. and Falci G., *Phys. Rev. A*, **93** (2016) 051801.
[8] Di Stefano P. G., Paladino E., D'Arrigo A. and Falci G., *Phys. Rev. B*, **91** (2015) 224506.
[9] Paladino E., Galperin Y. M., Falci G. and Altshuler B. L., *Rev. Mod. Phys.*, **86** (2014) 361.
[10] Pellegrino M. D. F., Falci G. and Paladino E., *Commun. Phys.*, **3** (2020) 6.
[11] Falci G., Ridolfo A., Di Stefano P. G. and Paladino E., *Sci. Rep.*, **9** (2019) 9249.