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To cite this article: M Enríquez and S Cruz y Cruz 2017 *J. Phys.: Conf. Ser.* **839** 012015

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Disentangling the Time-Evolution Operator of a Single Qubit

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Abstract. We show that the time-evolution equation for a two-level system can be turned into a system of non-linear differential equations when it is written in the disentangled form. The solutions are determined by solving a parametric-oscillator-like equation with a certain time-dependent frequency. The formalism is used to deal with the problem of a two-level atom interacting with a circularly polarized field. The possibility of generating exactly solvable Hamiltonians is briefly discussed.

1. Introduction

The search of exact solutions to the time-dependent Schrödinger equation represents a long-standing problem in quantum mechanics. Yet, the state of the system at any time $|\psi(t)\rangle$ fulfills the dynamical law

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \quad (1)$$

meaning that the evolution process is encoded in the family of unitary operators $U(t, t_0)$ defining the dynamics of the system from an initial moment t_0 to an arbitrary time t in the form $|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$. Then, the evolution operator satisfies the equation

$$i\frac{dU(t, t_0)}{dt} = H(t) \cdot U(t, t_0), \quad U(t_0, t_0) = \mathbb{I}, \quad (2)$$

where \mathbb{I} stands for the identity operator. The simplest case arises when the Hamiltonian H does not depend explicitly on time. In such a case the solution to equation (2) is readily written: $U(t, t_0) = \exp[-iH(t - t_0)]$. In general, if $H(t)$ does not commute with itself at different times one has to sum up the *continuous* Baker-Campbell-Hausdorff exponent [1], which is not a trivial problem. Therefore, it is essential the construction of different technics to solve the evolution equation (2).

The main goal of the present work is to develop a framework to approach the problem of the time-evolution of a two-level system. For this purpose it results convenient to write the Hamiltonian in terms of the Hubbard operators. Such set of operators is suitable to deal with the algebraic properties of the involved observables and represents an appropriate way to generalize our results to the case of multipartite systems [2]. The corresponding time-evolution operator



is then written in the so-called disentangled form and we show that the operator equation (2) is turned into a set of three non-linear differential equations. This way of approaching the problem is related to the well-known Wei-Norman theorem [3], which, in particular, has been applied to the case of the Lie groups $SU(2)$ [4] and $SU(1,1)$ [5]. In this sense, we discuss the equivalence of our results with those previously reported.

This contribution is organized as follows. In Section 2 some useful preliminaries are presented and the main results are given. This approach is applied to the case of one qubit interacting with a circularly polarized field in Section 3. Finally, in Section 4 we give some conclusions and discuss the possibility of obtaining exactly solvable time-dependent Hamiltonians for one qubit.

2. Two-level system driven by a time-dependent field

The Hubbard operators $X^{i,j}$ (also called X-operators) satisfy the following properties:

- (i) $X^{i,j} X^{k,m} = \delta_{jk} X^{i,m}$ (multiplication rule)
- (ii) $\sum_k X^{k,k} = \mathbb{I}$ (completeness)
- (iii) $(X^{i,j})^\dagger = X^{j,i}$ (non-hermiticity)

In the case of a qubit with eigenstates $|p\rangle$ and $|q\rangle$ and energies ϵ_p and ϵ_q , the Hubbard operator of order 2 is defined as

$$X_2^{k,\ell} := |k\rangle\langle\ell|, \quad k, \ell = p, q. \quad (3)$$

It is a simple matter to verify that the so-defined operators satisfy the properties (i)-(iii). Moreover, from the former definition it is straightforward to find the action of the X-operators on the basis vectors reads:

$$X_2^{k,\ell} |n\rangle = \delta_{\ell,n} |k\rangle, \quad k, \ell, n = p, q, \quad (4)$$

where $\delta_{i,j}$ stands for the Kronecker delta.

Now consider a qubit (*e.g.*, a two-level atom) in a time-dependent driving field. The corresponding Hamiltonian in the Hubbard representation has the form

$$H_2(t) = \epsilon_p X_2^{p,p} + \epsilon_q X_2^{q,q} + V(t) X_2^{p,q} + \bar{V}(t) X_2^{q,p}, \quad \epsilon_p, \epsilon_q \in \mathbb{R}, \quad (5)$$

where V is a complex-valued function and it will be referred to as the driving field. The over bar stands for complex conjugation. Since the energies ϵ_p, ϵ_q are real it is easy to verify that the Hamiltonian (5) is indeed Hermitian. Additionally, if the zero level energy is fixed at the middle of both levels, that is to say $\frac{1}{2}(\epsilon_p + \epsilon_q) = 0$, the Hamiltonian (5) can be written as

$$H_2(t) = \frac{\Delta}{2} (X_2^{p,p} - X_2^{q,q}) + V(t) X_2^{p,q} + \bar{V}(t) X_2^{q,p},$$

where $\Delta = \epsilon_p - \epsilon_q$ corresponds to the atomic transition frequency and the terms

$$H_0 = \frac{\Delta}{2} (X_2^{p,p} - X_2^{q,q}), \quad H_i = V(t) X_2^{p,q} + \bar{V}(t) X_2^{q,p}$$

are, respectively, the (free) atomic Hamiltonian and the interaction term. Remark that the operators

$$J_0 = \frac{1}{2} (X_2^{p,p} - X_2^{q,q}), \quad J_+ = X_2^{p,q} \quad \text{and} \quad J_- = X_2^{q,p} \quad (6)$$

constitute a representation of the $su(2)$ algebra generators [2].

The main problem of this work is to find the time-evolution operator $U(t) = U(t, 0)$ (we have fixed $t_0 = 0$ for the sake of simplicity) fulfilling the initial value problem (2). We assume that this operator can be written in the *disentangled* normal form

$$U(t) = \exp[\alpha(t)X_2^{p,q}] \exp[\Delta f(t)J_0] \exp[\beta(t)X_2^{q,p}], \quad (7)$$

where α , β and f are complex functions to be determined. Inserting (7) and (5) into (2) we get

$$\begin{aligned} \frac{dU}{dt} = & \alpha' X_2^{p,q} e^{\alpha X_2^{p,q}} e^{\Delta f J_0} e^{\beta X_2^{p,q}} \\ & + \Delta f' e^{\alpha X_2^{p,q}} J_0 e^{\Delta f J_0} e^{\beta X_2^{p,q}} + \beta' e^{\alpha X_2^{p,q}} e^{\Delta f J_0} X_2^{q,p} e^{\beta X_2^{p,q}} = -iH_2 U. \end{aligned} \quad (8)$$

Here the explicit time dependence of the functions α , f and β has been omitted for shortness and the prime stands for time derivation. The right multiplication of this expression by U^\dagger produces

$$-iH_2 = \alpha' X_2^{p,q} + \Delta f' e^{\alpha X_2^{p,q}} J_0 e^{-\alpha X_2^{p,q}} + \beta' e^{\alpha X_2^{p,q}} e^{\Delta f J_0} X_2^{q,p} e^{-\Delta f J_0} e^{-\alpha X_2^{p,q}}. \quad (9)$$

The similarity transformations in the right-hand side of (9) can be accomplished by using the well-known Baker-Campbell-Hausdorff formula [1]

$$e^{\lambda A} B e^{-\lambda A} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \{A^n, B\}, \quad (10)$$

where the bracket operation $\{ , \}$ is defined by

$$\{\mathbb{I}, B\} := B, \quad \{A^{n+1}, B\} = [A, \{A^n, B\}], \quad \{A^n, B\} := \underbrace{[A, [A, \dots [A, B \dots]]]}_{n\text{-times}},$$

leading to

$$\begin{aligned} -i\Delta J_0 - iV X_2^{p,q} - i\bar{V} X_2^{q,p} = & \alpha' X_2^{p,q} + \Delta f' (J_0 - \alpha X_2^{p,q}) \\ & + \beta' e^{-\Delta f} (X_2^{q,p} + 2\alpha J_0 - \alpha^2 X_2^{p,q}). \end{aligned}$$

Thus, the linear independence of the X-operators allows to reduce the problem to the following set of non-linear equations

$$\begin{aligned} \alpha' - \alpha \Delta f' - \alpha^2 \beta' e^{-\Delta f} &= -iV, \\ \Delta f' + 2\alpha \beta' e^{-\Delta f} &= -i\Delta, \\ \beta' e^{-\Delta f} &= -i\bar{V}, \end{aligned} \quad (11)$$

with the initial conditions $\alpha(0) = \beta(0) = f(0) = 0$ in order to fulfill the requirement that $U(0) = \mathbb{I}$. Substituting the second and third equations into the first one produces the following complex Ricatti equation for α

$$\alpha' + i\Delta \alpha - i\bar{V} \alpha^2 + iV = 0. \quad (12)$$

The introduction of the new variable η such that $\alpha = i(\ln \eta)' / \bar{V}$ turns (12) into the second-order differential equation

$$\eta'' - \left(-i\Delta + \frac{d}{dt} \ln \bar{V} \right) \eta' + |V|^2 \eta = 0. \quad (13)$$

In view of the forthcoming calculations, it is convenient to define the function $R(t) = e^{-i\Delta t}\bar{V}(t)$. Note that this function differs from the complex conjugate of V only in a phase factor, therefore, we will refer to both V and R , indistinctly, as the driving field. In these terms equation (13) becomes

$$\eta'' - \left(\frac{d}{dt} \ln R \right) \eta' + |R|^2 \eta = 0. \quad (14)$$

Finally, the change $\eta(t) = Q(t)\varphi(t)$, with $Q^2 = R$, turns this equation into the parametric oscillator equation

$$\varphi''(t) + \Omega^2(t)\varphi(t) = 0, \quad (15)$$

where the time-dependent frequency, given by

$$\Omega^2(t) = -\frac{1}{4} \left[\frac{d}{dt} \ln R(t) \right]^2 + \frac{1}{2} \frac{d^2}{dt^2} \ln R(t) + |R(t)|^2, \quad (16)$$

is, in general, a complex-valued function.

Now the solution to the equation (12) can be readily written by undoing the previous variable changes. Indeed, in terms of φ the function α has the form

$$\alpha(t) = i \frac{e^{-i\Delta t}}{R(t)} \left[\frac{\varphi'(t)}{\varphi(t)} + \frac{1}{2} \frac{R'(t)}{R(t)} \right]. \quad (17)$$

The functions f and β , in turn, are easily obtained from (11) by quadratures

$$\Delta f(t) = -2 \ln \left(\frac{\varphi(t)}{\varphi_0} \right) - \ln \left(\frac{R(t)}{R_0} \right) - i\Delta t, \quad \varphi_0 = \varphi(0), \quad R_0 = R(0), \quad (18)$$

and

$$\beta(t) = -iR_0\varphi_0^2 \int_0^t \frac{ds}{\varphi^2(s)}. \quad (19)$$

Remark that $f(t)$ and $\beta(t)$ were explicitly constructed to fulfill the initial conditions $f(0) = \beta(0) = 0$. Moreover, the condition $\alpha(0) = 0$ fixes the initial conditions of φ and its first derivative through

$$\lim_{t \rightarrow 0} \frac{1}{R(t)} \left[\frac{\varphi'(t)}{\varphi(t)} + \frac{1}{2} \frac{R'(t)}{R(t)} \right] = 0. \quad (20)$$

On the other hand, from the Hubbard operators properties one can see that $(X_2^{p,q})^2 = (X_2^{q,p})^2 = 0$, $(X_2^{p,p})^2 = X_2^{p,p}$ and $(X_2^{q,q})^2 = X_2^{q,q}$. Then, using the completeness property (iii), we may write

$$\begin{aligned} \exp[\alpha(t)X_2^{p,q}] &= 1 + \alpha(t)X_2^{p,q}, \quad \exp[\beta(t)X_2^{q,p}] = 1 + \beta(t)X_2^{q,p} \\ \exp \left[\frac{\Delta f(t)}{2} X_2^{p,p} \right] &= X_2^{q,q} + e^{\Delta f(t)/2} X_2^{p,p}, \quad \exp \left[\frac{-\Delta f(t)}{2} X_2^{q,q} \right] = X_2^{p,p} + e^{-\Delta f(t)/2} X_2^{q,q} \\ \exp [\Delta f(t)J_0] &= e^{\Delta f(t)/2} X_2^{p,p} + e^{-\Delta f(t)/2} X_2^{q,q}. \end{aligned} \quad (21)$$

The time-evolution operator of the system follows immediatly:

$$\begin{aligned} U(t) &= [e^{\Delta f(t)/2} + e^{-\Delta f(t)/2} \alpha(t)\beta(t)] X_2^{p,p} + e^{-\Delta f(t)/2} X_2^{q,q} \\ &\quad + e^{-\Delta f(t)/2} [\alpha(t)X_2^{p,q} + \beta(t)X_2^{q,p}]. \end{aligned} \quad (22)$$

Summarizing, we have reduced the problem of constructing the evolution operator for a driven two-level system, to the problem of finding out the solutions of the parametric oscillator (15) with the appropriate initial conditions. Equivalent results can be found, *e.g.*, in the works by Dattoli *et al.* [4, 5] for a different ordering in the factorization of the time-evolution operator. It is important to point out that the introduction of Hubbard operators [2] in our approach allows the possibility of extending the method to the case of multipartite systems [6].

3. A simple example

In this section we deal with a physical example to illustrate the convenience of our approach. To begin with, observe that a simple inspection to equation (16) allows us to conclude that the driving field of the form $R(t) = \bar{g}e^{i\delta t}$, with g and δ constants and $\delta \in \mathbb{R}$, produce $\Omega = \text{constant}$. In this case $V(t) = ge^{-i\omega t}$, with $\omega = \delta + \Delta$. The corresponding interaction Hamiltonian

$$H_i = ge^{-i\omega t} X_2^{p,q} + \bar{g}e^{i\omega t} X_2^{q,p}, \quad (23)$$

can be identified as the interaction term of a two-level atom driven by a classical circularly polarized electromagnetic field, of frequency ω , in the dipole approximation: $H_i = -\mathbf{p} \cdot \mathbf{E}(t)$ with $\mathbf{p} = e\mathbf{r}$ the electric dipole operator and $\mathbf{E}(t) = (\mathcal{E}_0 \cos \omega t, \mathcal{E}_0 \sin \omega t, 0)$ the electric field amplitude, provided that the coupling constant g takes the value (see, *e.g.*, Klimov and Chumakov [7], pp. 26)

$$g = -\frac{e\mathcal{E}_0}{2} \langle p|x + iy|q \rangle.$$

We now follow the formalism of the previous section to construct the time-evolution operator in the form (7). The functions α , f and β are expressed in terms of the solution of the parametric oscillator equation (15) with the frequency given by

$$\Omega^2(t) = -\frac{1}{4} \left[\frac{d}{dt} \ln R(t) \right]^2 + \frac{1}{2} \frac{d^2}{dt^2} \ln R(t) + |R(t)|^2 = \frac{\delta^2}{4} + |g|^2 \equiv \Omega_0^2, \quad (24)$$

where we have used the fact that

$$R(0) = R_0 = \bar{g}, \quad \frac{d}{dt} \ln R(t) = i\delta = i(\omega - \Delta). \quad (25)$$

Here $\delta = \omega - \Delta$ is the *detuning* given by the difference between the atomic and the driving field frequencies. In the same sense, the quantity Ω_0 is nothing but the *Rabi frequency* of the atomic driven system. Accordingly, the parametric oscillator equation becomes

$$\varphi''(t) + \Omega_0^2 \varphi(t) = 0, \quad (26)$$

whose general solution is given by $\varphi(t) = c_1 \cos(\Omega_0 t) + c_2 \sin(\Omega_0 t)$, with c_1 and c_2 two complex constants related to each other through (20) as $c_2 = -i\delta c_1 / 2\Omega_0$. By setting, without loss of generality $\varphi(0) = c_1 = 1$ we get

$$\varphi(t) = \cos(\Omega_0 t) - \frac{i\delta}{2\Omega_0} \sin(\Omega_0 t), \quad (27)$$

and the solutions of the non-linear system are then computed from (17-19)

$$\begin{aligned} \alpha(t) &= \frac{-2ige^{-i\omega t} \sin(\Omega_0 t)}{2\Omega_0 \cos(\Omega_0 t) - i\delta \sin(\Omega_0 t)}, \\ \Delta f(t) &= -2 \ln \left[\cos(\Omega_0 t) - \frac{i\delta}{2\Omega_0} \sin(\Omega_0 t) \right] - i\omega t, \\ \beta(t) &= \frac{-2i\bar{g} \sin(\Omega_0 t)}{2\Omega_0 \cos(\Omega_0 t) - i\delta \sin(\Omega_0 t)}. \end{aligned} \quad (28)$$

A similar approach has been done by Klimov and Chumakov [7] for a system consistent on A qubits interacting with a circularly polarized field. Our results are equivalent to theirs for the lowest representation, or, equivalently, for $A = 1$, as the dynamical group in both cases is $SU(2)$. Since in that work the authors focus in the case of exact resonance, their results are retrieved by setting $\delta = 0$ in our expressions (28).

Let us assume that the system is, initially, in the upper-level energy state, *i.e.*, $|\psi(0)\rangle = |p\rangle$. The state of the system at any time reads

$$|\psi(t)\rangle = U(t)|p\rangle = [e^{\Delta f(t)/2} + e^{-\Delta f(t)/2}\alpha(t)\beta(t)]|p\rangle + e^{-\Delta f(t)/2}\beta(t)|q\rangle. \quad (29)$$

After some algebra we retrieve the known expressions for the time-evolution

$$|\psi(t)\rangle = e^{-i\omega t/2} \left[\cos(\Omega_0 t) + \frac{i\delta}{2\Omega_0} \sin(\Omega_0 t) \right] |p\rangle - \frac{i\bar{g}}{\Omega_0} e^{i\omega t/2} \sin(\Omega_0 t) |q\rangle. \quad (30)$$

The atomic population inversion \mathcal{P} is also computed to give

$$\mathcal{P}(t) = |c_p|^2 - |c_q|^2 = \frac{|g|^2}{\Omega_0^2} \cos(2\Omega_0 t) + \frac{\delta^2}{4\Omega_0^2}. \quad (31)$$

We stress that this problem is exactly solvable since the general solution to the parametric oscillator equation (26) is well-known. However, in general, the problem is not so simple to deal with and there are a limited number of cases for which exact solutions to (15) can be explicitly constructed (see for instance [4, 5]).

4. Conclusions and perspectives

The evolution operator of one qubit interacting with a time-dependent driving field has been constructed, in the disentangled form, by using the Hubbard representation. First, the evolution equation is reduced to a set of three coupled nonlinear equations whose solution can be expressed in terms of the solution of a single complex Riccati-type one. Next, with some appropriate changes of variable, this equation is transformed into a classical parametric oscillator equation with a time-dependent frequency defined by the form of the driving field. As a particular case, we have determined the time-evolution operator for a two-level atom interacting with a circularly polarized field. The well-known expressions for the time evolution of the state of the system and the population inversion were also obtained. Yet, it is widely recognized that there is only a limited number cases for which the solution of the general problem can be explicitly constructed. In this sense, an alternative to generate exactly solvable time-dependent Hamiltonians is constituted by the inverse technic: assuming that the solutions of the equation (15) for a given $\Omega(t)$ are known, the problem then is to find the driving field $R(t)$ which yields such time-dependent frequency. The results on this matter will be reported elsewhere [8].

Acknowledgments

The financial support of CONACyT through ME's postdoctoral scholarship (233036) and from the Instituto Politécnico Nacional through project SIP20170233 is acknowledged.

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