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Magnus expansion applied to a dissipative driven two-level system

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ABSTRACT

One of the most powerful and potentially useful methods of time-dependent matrix differential equations is the Magnus expansion. In this work, we applied the Magnus expansion for Schrödinger and master equations of a dissipative two-level system interacting with a time-dependent π pulse. Two different models of dissipative two-level systems are considered, namely (i) the system decays from two considered levels into some other levels with given decay rates; (ii) the system decays from its excited level to its ground level. The obtained approximate solutions of a time dynamics by the first-order Magnus expansion are well consistent with the results of numerical calculations obtained by the fourth-order Runge-Kutta method.

Introduction

One of the simplest quantum systems that has ubiquitous applications in various fields of physics is the two-level system. The best examples of this system could be a half spin system in nuclear magnetic resonance, an atomic two-level system in quantum optics and a qubit (quantum bit) in quantum information theory. One of the potentially important applications of the two-level system is the qubit control in quantum computing [1–4]. In quantum computing, one needs to coherently control a qubit for fast processing and readout of quantum information. This can be done by perturbing a qubit (two-level system) by a time-dependent field or pulse. In that sense, a two-level system interacting with a time-dependent field is a potentially useful model for a qubit control design in quantum computing.

The two-level system is centennial problem as it has been extensively considered starting from 1930s just after the emerging of quantum mechanics. Only few exactly solvable models of two-level system have been discovered as yet, for example Landau-Zener model [5,6] and Rabi model [7]. However, a two-level system driven by a time-dependent field is not exactly solvable in general and a large number of approximately analytical solutions has been discovered until now [8–16]. Recent advances on the two-level system provide an impressive approximate solution that well describes a time dynamics of a two-level system interacting with far off-resonant time-dependent short pulse [17–19].

One alternative method for solving the problem of a two-level system interacting with time-dependent field is the Magnus expansion [20]. Magnus expansion is a powerful series method for solving an initial value problem given as

$$\frac{\mathrm{d}\mathbf{X}(t)}{\mathrm{d}t} = \mathbf{M}(t)\mathbf{X}(t), \quad \mathbf{X}(0) = \mathbf{I} \tag{1}$$

where $\mathbf{X}(t)$ and $\mathbf{M}(t)$ are operator (or matrix) functions of t, and $\mathbf{I}$ is the identity operator (or the unit matrix). In 1954, Wilhelm Magnus provided a solution of Eq. (1) in the following form [20]

$$\mathbf{X}(t) = \exp\left(\sum_{n=1}^{\infty} \mathbf{S}_n\right), \tag{2}$$

where $\mathbf{S}_n$ is the nth term of Magnus expansion or series[1]. The solution (2) looks compact and has wide applications in various areas of physics and chemistry for instance, nuclear magnetic resonance [21,22], quantum electrodynamics [23,24], numerical integrator [25–27] and so forth. Each term $\mathbf{S}_n$ of the Magnus series is expressed in terms of multiple integrals of nested commutators, and the first few of them are given by [28–30]

$$\mathbf{S}_1 = \frac{1}{1!}\int_0^t \mathrm{d}t_1 \mathbf{M}(t_1), \tag{3a}$$

$$\mathbf{S}_2 = \frac{1}{2!}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \left[\mathbf{M}(t_1), \mathbf{M}(t_2)\right], \tag{3b}$$

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[1] Terms of Magnus expansion are usually denoted by Ω_n. However, we denote it by $\mathbf{S}_n$ to avoid conflicting with driving term $\Omega(t)$ in the Hamiltonian (5).

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$$\mathbf{S}_3 = \frac{1}{3!}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 \left(\left[\mathbf{M}(t_1), \left[\mathbf{M}(t_2), \mathbf{M}(t_3) \right] \right] + \left[\mathbf{M}(t_3), \left[\mathbf{M}(t_2), \mathbf{M}(t_1) \right] \right] \right), \tag{3c}$$

$$\mathbf{S}_4 = \frac{1}{4!}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 \int_0^{t_3} \mathrm{d}t_4 \, ([[[\mathbf{M}(t_1), \mathbf{M}(t_2)], \mathbf{M}(t_3)], \mathbf{M}(t_4)] + [\mathbf{M}(t_1), [[\mathbf{M}(t_2), \mathbf{M}(t_3)], \mathbf{M}(t_4)]] + [\mathbf{M}(t_1), [\mathbf{M}(t_2), [\mathbf{M}(t_3), \mathbf{M}(t_4)]]] + [\mathbf{M}(t_2), [\mathbf{M}(t_3), [\mathbf{M}(t_4), \mathbf{M}(t_1)]]]). \tag{3d}$$

Expression of $\mathbf{S}_n$ becomes much complicated as the order increases. The Magnus expansion has been considered to be a useful tool to obtain analytic solution of a time dynamics of a two-level system, for details we refer Refs. [31–33].

The solution (2) has a form of exponential function of series argument $\sum_{n=1}^{\infty}\mathbf{S}_n$. Therefore, one needs to answer two questions namely these are "does Magnus series converge?" and "if Magnus series was convergent, how fast does it converge?". The first question has drawn great attention since 1954 [28,34–36]. Commonly accepted i.e. "standard" condition of convergence of the Magnus series in the interval $[0, T]$ is given by [37,38]

$$\int_0^T \mathrm{d}t \left|\left|\mathbf{M}(t)\right|\right| < \pi \tag{4}$$

where $||\cdot||$ stands for the Frobenius norm [39]. This is sufficient but not necessary condition. That means Eq. (4) is not necessary to be satisfied for convergence of Magnus series but it guarantees convergence of the Magnus series. The second question about rate of convergence will be discussed in this paper.

In this work, we apply Magnus expansion method on a dissipative driven two-level system and compare it to standard perturbation method.

Probability amplitude method

The first model of interest is a two-level system whose levels $|1\rangle$ and $|2\rangle$ decay to third levels with decay rates Γ_1 and Γ_2, respectively (see Fig. 1a). When the system is interacting with a time-dependent field, Hamiltonian $\widehat{H}(t)$ of the system is given by

$$\widehat{H}(t) = \frac{\hbar\omega}{2}\widehat{\sigma}_z - \hbar\Omega(t)\widehat{\sigma}_x - i\frac{\hbar\Gamma_1}{2}|1\rangle\langle 1| - i\frac{\hbar\Gamma_2}{2}|2\rangle\langle 2| \tag{5}$$

where $\{\widehat{\sigma}_x, \widehat{\sigma}_z\}$ are the Pauli matrices, ω is transition frequency and $\Omega(t)$ is a time dependent driving term. This is the non-Hermitian Hamiltonian used to describe quantum open systems where the loss and dissipations are considered [40–42]. It is an alternative formalism to the master equation description of the system dynamics. The non-Hermitian Hamiltonian formalism has been applied to several fields, for example, to study the manifestation of resonance trapping in quantum dots [43,44], to explore the spectroscopic properties of highly excited states [45], to investigate the photosynthesis [46], to explain the unidirectional reflectionless light propagation [47], etc.

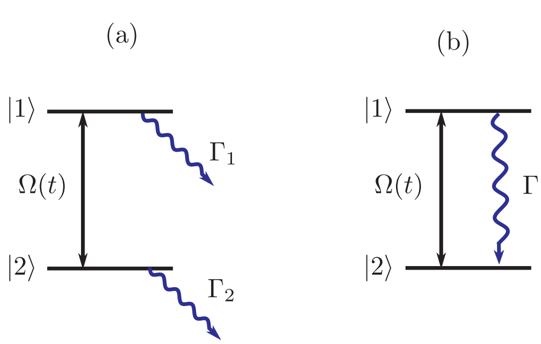

Fig. 1. Two considered models of driven two-level systems with dissipation are illustrated; (a) each level $|1\rangle$ or $|2\rangle$ decays to some levels other than $|1\rangle$ and $|2\rangle$, (b) excited level $|1\rangle$ decays to ground level $|2\rangle$. Driving field is depicted by the black vertical line with label $\Omega(t)$.

Now we aim to solve Schrödinger equation with the Hamiltonian (5) and seek a solution in the following form

$$\left|\Psi(t)\right\rangle = C_1(t)\mathrm{e}^{-\frac{i\omega t}{2}-\frac{\Gamma_1 t}{2}}\left|1\right\rangle + C_2(t)\mathrm{e}^{\frac{i\omega t}{2}-\frac{\Gamma_2 t}{2}}\left|2\right\rangle, \tag{6}$$

where $C_1(t)$ and $C_2(t)$ are probability amplitudes of levels $|1\rangle$ and $|2\rangle$, respectively. Then equation for the probability amplitudes $\mathbf{C}(t) = (C_1(t) \;\; C_2(t))^T$ is given by

$$\dot{\mathbf{C}}(t) = \mathbf{M}(t)\mathbf{C}(t). \tag{7}$$

Here, the matrix $\mathbf{M}(t)$ has the following form

$$\mathbf{M}(t) = \begin{pmatrix} 0 & i\Omega(t)\mathrm{e}^{i\omega t-\gamma t} \\ i\Omega(t)\mathrm{e}^{-i\omega t+\gamma t} & 0 \end{pmatrix}, \tag{8}$$

where $\gamma = (\Gamma_2 - \Gamma_1)/2$. Solution of Eq. (7) with the use of Magnus expansion is obtained as

$$\mathbf{C}(t) = \mathbf{O}(t)\mathbf{C}(0), \tag{9}$$

where $\mathbf{O}(t) = \exp(\sum_{n=1}^{\infty}\mathbf{S}_n)$. As an approximation, infinite Magnus series in the exponent $\exp(\sum_{n=1}^{\infty}\mathbf{S}_n)$ is truncated at particular order and subsequently exponential function is analytically calculated without any approximations. Due to the simple form of the matrix $\mathbf{M}(t)$, the Magnus series is easily obtained as

$$\sum_{n=1}^{\infty}\mathbf{S}_n = \begin{pmatrix} \phi(t) & \theta_1(t) \\ \theta_2(t) & -\phi(t) \end{pmatrix}, \tag{10}$$

where

$$\begin{aligned} \phi(t) &= \phi^{(2)}(t) + \phi^{(4)}(t) + \ldots, \\ \theta_1(t) &= \theta_1^{(1)}(t) + \theta_1^{(3)}(t) + \ldots, \\ \theta_2(t) &= \theta_2^{(1)}(t) + \theta_2^{(3)}(t) + \ldots. \end{aligned} \tag{11}$$

The superscripts in above equation indicate the order of the Magnus terms. Therefore, only even (odd) Magnus terms contribute to function (s) $\phi(t)$ ($\theta_1(t)$ and $\theta_2(t)$). After exact calculation of exponential function we obtain the matrix $\mathbf{O}(t)$ in the following form

$$\mathbf{O}(t) = \begin{pmatrix} \cosh\eta(t) + \frac{\phi(t)\sinh\eta(t)}{\eta(t)} & \frac{\theta_1(t)\sinh\eta(t)}{\eta(t)} \\ \frac{\theta_2(t)\sinh\eta(t)}{\eta(t)} & \cosh\eta(t) - \frac{\phi(t)\sinh\eta(t)}{\eta(t)} \end{pmatrix}. \tag{12}$$

Here, the function $\eta(t)$ is expressed in terms of functions $\theta_1(t)$ and $\theta_2(t)$ in the following manner

$$\eta(t) = \sqrt{\phi^2(t) + \theta_1(t)\theta_2(t)}. \tag{13}$$

Furthermore, the functions in Eq. (11) can be expressed in terms of multiple integrals as follow

$$\theta_1^{(1)}(t) = i\int_0^t \mathrm{d}t_1 \Omega(t_1)\mathrm{e}^{i\omega t_1 - \gamma t_1}, \tag{14a}$$

$$\theta_2^{(1)}(t) = i\int_0^t \mathrm{d}t_1 \Omega(t_1)\mathrm{e}^{-i\omega t_1 + \gamma t_1}, \tag{14b}$$

$$\phi^{(2)}(t) = \frac{i^2}{2}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \Omega(t_1)\Omega(t_2)(\mathrm{e}^{-(i\omega-\gamma)(t_2-t_1)} - \mathrm{e}^{(i\omega-\gamma)(t_2-t_1)}), \tag{14c}$$

$$\theta_1^{(3)}(t) = \frac{i^3}{3}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 \Omega(t_1)\Omega(t_2)\Omega(t_3) \times (2\mathrm{e}^{(i\omega-\gamma)(t_1+t_3-t_2)} - \mathrm{e}^{(i\omega-\gamma)(t_1+t_2-t_3)} - \mathrm{e}^{(i\omega-\gamma)(t_2+t_3-t_1)}), \tag{14d}$$

$$\theta_2^{(3)}(t) = \frac{i^3}{3}\int_0^t dt_1\int_0^{t_1}dt_2\int_0^{t_2}dt_3\,\Omega(t_1)\Omega(t_2)\Omega(t_3) \times\left(2e^{(i\omega-\gamma)(t_2-t_1-t_3)} - e^{(i\omega-\gamma)(t_3-t_2-t_1)} - e^{(i\omega-\gamma)(t_1-t_2-t_3)}\right), \quad (14e)$$

$$\phi^{(4)}(t) = \frac{i^4}{6}\int_0^t dt_1\int_0^{t_1}dt_2\int_0^{t_2}dt_3\int_0^{t_3}dt_4\,\Omega(t_1)\Omega(t_2)\Omega(t_3)\Omega(t_4) \times\left(e^{(i\omega-\gamma)(t_1+t_3-t_2-t_4)} + e^{(i\omega-\gamma)(t_3+t_4-t_1-t_2)} - e^{(i\omega-\gamma)(t_2+t_4-t_1-t_3)} - e^{(i\omega-\gamma)(t_1+t_2-t_3-t_4)}\right). \quad (14f)$$

Eq. (12) along with Eqs. (13), (1114) is an approximate analytical solution obtained by the Magnus expansion, and it can be applied for any time-dependent driving field. Restriction of the solution is only due to divergence of the Magnus expansion. Note that the solution reduces to the solution in Ref. [32] in the limit of $\gamma \to 0$.

In consideration of convergence, the integral in Eq. (4) is evaluated with Eq. (8) under the rotating wave approximation (RWA), and result is if

$$\int_0^\infty dt\left|\Omega'(t)\right|\sqrt{2\cosh(2\gamma t)} < \pi \quad (15)$$

then Magnus series Eq. (10) converges. Here, $\Omega'(t)$ is an envelope function of a pulse. Eq. (15) is the condition that must hold in order Magnus series to be convergent. However, in qubit control, it is common to use π pulse that is able to completely invert a qubit [48]. Therefore, we use π pulse in our calculations throughout this paper. Area of a pulse is defined as $A = \int_0^\infty dt\Omega'(t)$. As long as hyperbolic cosine function in Eq. (15) is always larger than 1 it is easy to see that $A < \pi$ to the Magnus series be convergent. Thus, for the π pulse Eq. (15) does not hold and as a consequence the Magnus series is not necessary to be convergent for π pulse. Nonetheless, results of the numerical calculation below demonstrate that for our specific model, Magnus expansion is convergent for π pulse.

Next, a time dynamics of a two-level system driven by Gaussian and hyperbolic secant π pulses is calculated.

Gaussian π pulse

Before we perform numerical analysis of the solution (13) we can obtain analytical solution in the case of Gaussian pulse of area π given by

$$\Omega(t) = \Omega_0 e^{-(t-t_0)^2/s^2}\cos(\nu(t-t_0)), \quad (16)$$

where ν is frequency of the pulse. Here, pulse parameters are Ω_0, t_0 and s. The functions $\theta_1^{(1)}(t)$ and $\theta_2^{(1)}(t)$ are calculated under RWA as follow

$$\theta_1^{(1)}(t) = -\frac{i\sqrt{\pi}s\Omega_0}{4}e^{\left(i\omega-\gamma\right)t_0+\frac{s^2(\gamma-i\Delta)^2}{4}}\left[\mathrm{erf}\left(\frac{s(\gamma-i\Delta)}{2}-\frac{t_0}{s}\right) - \mathrm{erf}\left(\frac{s(\gamma-i\Delta)}{2}+\frac{t-t_0}{s}\right)\right],$$
$$\theta_2^{(1)}(t) = \frac{i\sqrt{\pi}s\Omega_0}{4}e^{\left(-i\omega+\gamma\right)t_0+\frac{s^2(\gamma-i\Delta)^2}{4}}\left[\mathrm{erf}\left(\frac{s(\gamma-i\Delta)}{2}+\frac{t_0}{s}\right) - \mathrm{erf}\left(\frac{s(\gamma-i\Delta)}{2}-\frac{t-t_0}{s}\right)\right], \quad (17)$$

where $\Delta = \omega - \nu$ is detuning and erf() is the error function. With the help of the functions Eq. (17), and Eqs. (12) and (13), we analytically calculate excited- and ground-state probabilities as a function of time and compare it with numerically calculated results of fourth-order Runge-Kutta method. Not only the resonant interaction but also the non-resonant interaction which satisfies the adiabatic condition[2] is considered. Results of both cases are illustrated in Figs. 2(a-d). The graphs demonstrate that when $\nu = \omega$ the analytic solution based on first-order Magnus expansion well describes a time dynamics of a driven two-level system with dissipation. However, when $\Delta \neq 0$ and the adiabatic condition is satisfied, the first-order Magnus expansion is not sufficient to describe the dynamics of the system. Therefore, it is interesting to calculate higher order Magnus terms for the off-resonant adiabatic interaction.

One interesting point here to briefly discuss is about what would be happen if the pulse duration is longer than the period considered in the simulation (1 ns)? Clearly the dynamics of the system would change much if we have longer pulse keeping the same intensity i.e. the peak value of the Rabi frequency Ω_0. Nevertheless, the Magnus expansion limits pulse area A to the values less than or equal to π, and it requires to keep the pulse area rather than the intensity. Therefore, if we have longer pulse with the same area as $A = \pi$ then the dynamics would be the same, and Figs. 2 would not change except scaling of the horizontal time axis. This is also true for all graphs in this paper.

Hyperbolic secant π pulse

Another pulse shape function that we consider here is $\mathrm{sech}(x) = 1/\cosh(x)$ function. In this case, Rabi frequency of a pulse has a following shape

$$\Omega(t) = \Omega_0\mathrm{sech}((t-t_0)/s)\cos(\nu(t-t_0)), \quad (18)$$

where s and t_0 are real-valued parameters. We calculate the functions $\theta_1^{(1)}(t)$ and $\theta_2^{(1)}(t)$ under RWA as follow

$$\theta_1^{(1)}(t) = \frac{is\Omega_0 e^{\left(\frac{1}{s}+i\nu\right)t_0}}{1+s(\gamma-i\Delta)}\left[{}_2F_1\left(1, \frac{1+s(\gamma-i\Delta)}{2}, \frac{3+s(\gamma-i\Delta)}{2}, -e^{\frac{2t_0}{s}}\right) - e^{-t\left(\frac{1}{s}+(\gamma-i\Delta)\right)}{}_2F_1\left(1, \frac{1+s(\gamma-i\Delta)}{2}, \frac{3+s(\gamma-i\Delta)}{2}, -e^{-\frac{2(t-t_0)}{s}}\right)\right],$$
$$\theta_2^{(1)}(t) = \frac{is\Omega_0 e^{\left(\frac{1}{s}-i\nu\right)t_0}}{1-s(\gamma-i\Delta)}\left[{}_2F_1\left(1, \frac{1-s(\gamma-i\Delta)}{2}, \frac{3-s(\gamma-i\Delta)}{2}, -e^{\frac{2t_0}{s}}\right) - e^{-t\left(\frac{1}{s}-(\gamma-i\Delta)\right)}{}_2F_1\left(1, \frac{1-s(\gamma-i\Delta)}{2}, \frac{3-s(\gamma-i\Delta)}{2}, -e^{-\frac{2(t-t_0)}{s}}\right)\right], \quad (19)$$

where ${}_2F_1()$ is the hypergeometric function. Time evolutions of the excited-state probability $|C_1(t)|^2$ and the ground-state probability $|C_2(t)|^2$ are shown in Figs. 2(e-h) for the resonant and non-resonant interactions as well. For the resonant driving field $\nu = \omega$, the Figs. 2(e-f) show that first-order Magnus expansion governed by Eq. (19) provides a solution well consistent with the result of numerical simulation implemented by a standard fourth-order Runge-Kutta method. Nonetheless, Figs. 2(g-h) exhibits inconsistencies between the first-order Magnus expansion and the fourth-order Runge-Kutta method. This is the reason why we compute higher order Magnus terms in the following.

Numerical analysis

In addition to the analytical solutions in the case of Gaussian and hyperbolic secant pulses presented in previous subsection, we perform numerical calculation based on Eqs. (12), (1314) up to fourth-order Magnus expansion. Here, the numerical calculation means that the multiple integrals (14), which are analytically not solvable in general, are numerically integrated by 5-point Gaussian quadrature method. Results of the calculation are plotted in Fig. 3 for resonant driving and in Fig. 4 for non-resonant driving, and compared with the results of standard perturbation method of the same order. As shown in Fig. 3, the

[2] Adiabatic condition means that the inverse of the detuning is much smaller than the full width at half maximum values of duration i.e. $1/\Delta \ll FWHM$

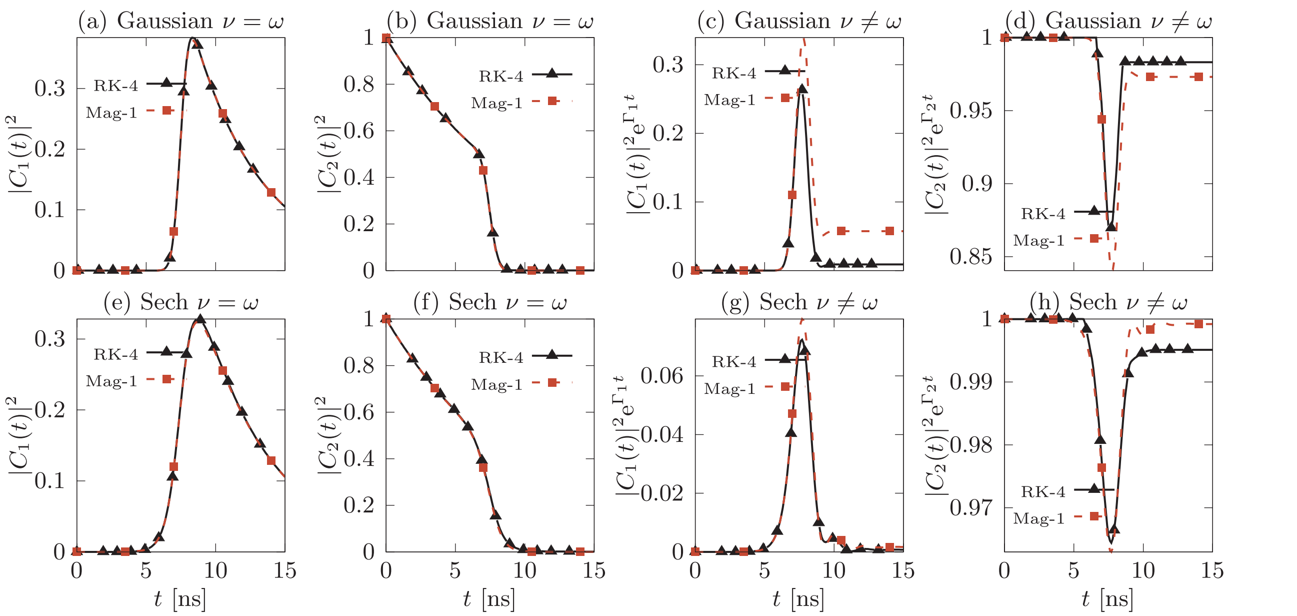

Fig. 2. Analytical results of the first-order Magnus approximation (red dashed line with rectangular nodes) are compared with the results of numerical calculations (black solid line with triangular nodes) obtained by the fourth-order Runge-Kutta method. Excited- and ground-state probabilities $|C_1(t)|^2$ and $|C_2(t)|^2$ of two-level systems driven by resonant Gaussian pulse are plotted in (a-b), and by resonant hyperbolic secant pulse are plotted in (e-f). For the non-resonant adiabatic interaction, the same quantities without decay factors $e^{-\Gamma_1 t}$ and $e^{-\Gamma_2 t}$ are plotted in (c-d) for the Gaussian pulse and in (g-h) for the hyperbolic secant pulse. Frequency of the driving field is $\nu = 0.999997\omega$ for plots (c-d) and (g-h). Eq. (17) is used in the case of the Gaussian pulse whereas Eq. (19) is used for the case of the hyperbolic secant pulse. Initial state of the system is ground state. Numerical values of parameters used in the calculations are following $\omega = 10^{15}$ 1/s, $\Omega_0 = 1.77 \times 10^9$ 1/s for Gaussian pulse, $\Omega_0 = 10^9$ 1/s for hyperbolic secant pulse, $\Gamma_1 = 2 \times 10^8$ 1/s, $\Gamma_2 = 10^8$ 1/s, $s = 1$ ns and $A = \pi$. The corresponding full width at half maximum is $FWHM = 1.18$ ns for the Gaussian pulse and $FWHM = 1.76$ ns for the hyperbolic secant pulse.

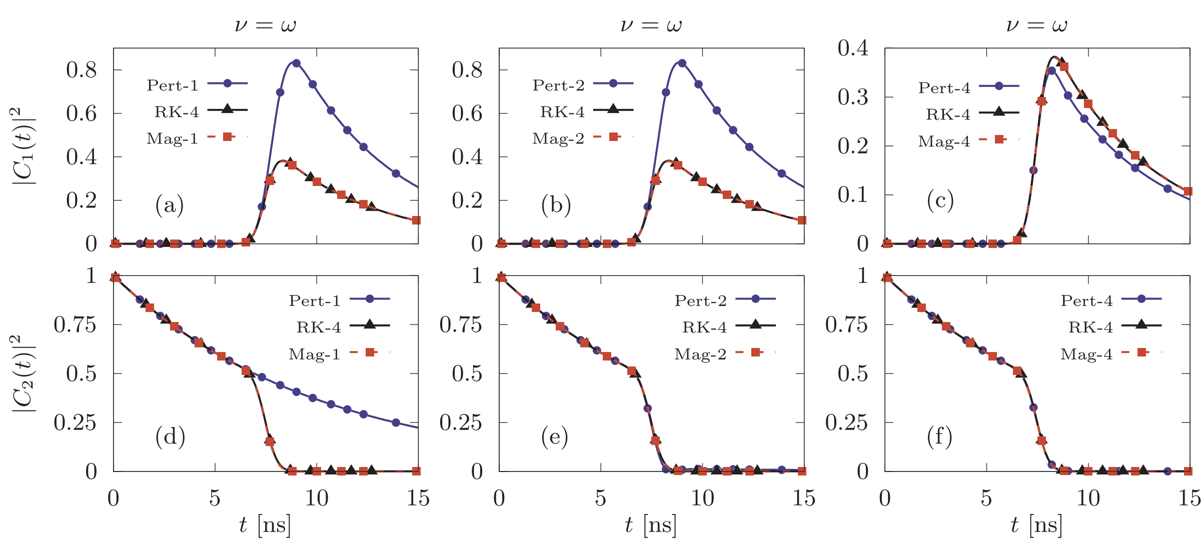

Fig. 3. Numerical results obtained by the Magnus expansion (red dashed line with rectangular nodes), standard perturbation (blue solid line with circular nodes) and fourth-order Runge-Kutta (black solid line with triangular nodes) methods. Orders of the Magnus expansion and perturbation methods are 1 for plots (a) and (d), 2 for plots (b) and (e), and 4 for plots (c) and (f). Initial state of the system is ground state. Driving field is on resonance with the two-level system and the considered pulse shape is Gaussian. Other parameters used in the calculations are the same as in Fig. 2.

Magnus series converges faster than the standard perturbation method for the Gaussian π pulse. Hence, even first-order Magnus expansion method well describes the time evolution of a two-level system in the case of resonant driving. However, if the system is perturbed by off-resonant driving or adiabatic driving where detuning Δ is much greater than pulse bandwidth (see Fig. 4), then the Magnus series is still convergent but the rate of convergence is not fast enough as the resonant driving. As a result, the fourth-order Magnus expansion is required to describe time evolution of a two-level system. Nevertheless, the Magnus expansion is still better describing the system than the standard perturbation method.

Master equation method

In order to apply Magnus expansion on the system with dephasing we consider another model of the two-level system that decays from the excited level $|1\rangle$ to the ground level $|2\rangle$ with rate Γ (see Fig. 1b). For the current model, time dynamics can be described by the standard master equation that is written in the following form [49,50]

$$\dot{\hat{\rho}}(t) = -\frac{i}{\hbar}\left[\hat{H}(t), \hat{\rho}(t)\right] - \frac{\Gamma}{2}\left(\hat{\sigma}_+\hat{\sigma}_-\hat{\rho}(t) - 2\hat{\sigma}_-\hat{\rho}(t)\hat{\sigma}_+ + \hat{\rho}(t)\hat{\sigma}_+\hat{\sigma}_-\right) \tag{20}$$

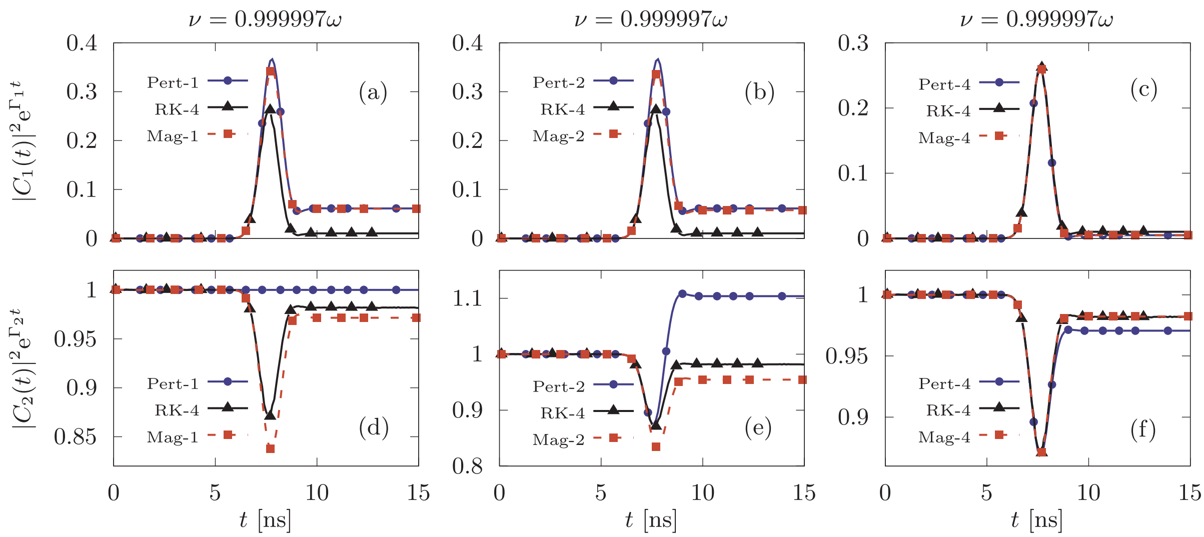

Fig. 4. The same plots as in Fig. 3 for off-resonant driving. Frequency of driving field is $\nu = 0.999997\omega$ which obeys the adiabatic condition $1/\Delta \ll FWHM$. Orders of the Magnus expansion and perturbation methods are 1 for plots (a) and (d), 2 for plots (b) and (e), and 4 for plots (c) and (f). Initial state of the system is ground state and the considered pulse shape is Gaussian. For the purpose of clarity of graphs, the exponential decay factors are omitted (see the label of vertical axis).

where $\hat{\sigma}_+$ and $\hat{\sigma}_-$ are raising and lowering operators of the two-level system. Here, Hamiltonian $\widehat{H}(t)$ is given by

$$\widehat{H}(t) = \frac{\hbar\omega}{2}\hat{\sigma}_z - \hbar\Omega(t)\hat{\sigma}_x. \tag{21}$$

With new variables $\tilde{z}(t)$, $\tilde{\rho}_{12}(t)$ and $\tilde{\rho}_{21}(t)$ that are described as

$$\begin{aligned}\tilde{z}(t) &= (\rho_{11}(t) - \rho_{22}(t))\mathrm{e}^{\Gamma t},\\ \tilde{\rho}_{12}(t) &= \rho_{12}(t)\mathrm{e}^{(i\omega+\Gamma/2)t},\\ \tilde{\rho}_{21}(t) &= \rho_{21}(t)\mathrm{e}^{-(i\omega-\Gamma/2)t}\end{aligned} \tag{22}$$

the master Eq. (20) becomes

$$\begin{aligned}\dot{\tilde{z}}(t) &= -2i\Omega(t)(\tilde{\rho}_{12}(t)\mathrm{e}^{-(i\omega-\Gamma/2)t} - \tilde{\rho}_{21}(t)\mathrm{e}^{(i\omega+\Gamma/2)t}) - \Gamma\mathrm{e}^{\Gamma t},\\ \dot{\tilde{\rho}}_{12}(t) &= -i\Omega(t)\tilde{z}(t)\mathrm{e}^{(i\omega-\Gamma/2)t},\\ \dot{\tilde{\rho}}_{21}(t) &= i\Omega(t)\tilde{z}(t)\mathrm{e}^{-(i\omega+\Gamma/2)t}.\end{aligned} \tag{23}$$

Here, $\tilde{z}(t)\mathrm{e}^{-\Gamma t}$ is population inversion. Eq. (23) can be written in compact form as follows

$$\dot{\mathbf{R}}(t) = \mathbf{M}(t)\mathbf{R}(t) + \mathbf{A}(t), \tag{24}$$

where $\mathbf{R}(t) = (\tilde{z}(t)\ \ \tilde{\rho}_{12}(t)\ \ \tilde{\rho}_{21}(t))^T$,

$$\mathbf{M}(t) = \begin{pmatrix} 0 & -2i\Omega(t)\mathrm{e}^{-(i\omega-\Gamma/2)t} & 2i\Omega(t)\mathrm{e}^{(i\omega+\Gamma/2)t}\\ -i\Omega(t)\mathrm{e}^{(i\omega-\Gamma/2)t} & 0 & 0\\ i\Omega(t)\mathrm{e}^{-(i\omega+\Gamma/2)t} & 0 & 0\end{pmatrix} \tag{25}$$

and

$$\mathbf{A}(t) = \begin{pmatrix} -\Gamma\mathrm{e}^{\Gamma t}\\ 0\\ 0\end{pmatrix}. \tag{26}$$

Eq. (24) is a first-order inhomogeneous linear matrix differential equation. Hence, we can treat the homogeneous part of Eq. (24) with the use of Magnus expansion to find homogeneous solution $\mathbf{R}_{\mathrm{hom}}(t)$. A way to obtain a complete solution of Eq. (24) is to sum the homogeneous solution and the particular solution of the inhomogeneous equation.

As we mention above, the homogeneous equation $\dot{\mathbf{R}}_{\mathrm{hom}}(t) = \mathbf{M}(t)\mathbf{R}_{\mathrm{hom}}(t)$ can be solved using the first-order Magnus expansion as follows

$$\mathbf{R}_{\mathrm{hom}}(t) = \mathbf{O}(t)\mathbf{R}_{\mathrm{hom}}(0), \tag{27}$$

where

$$\mathbf{O}(t) = \begin{pmatrix} \cosh\eta & -\frac{\theta_1\sinh\eta}{\eta} & \frac{\theta_2\sinh\eta}{\eta}\\ -\frac{\theta_3\sinh\eta}{\eta} & \frac{(\theta_2\theta_4+\theta_1\theta_3\cosh\eta)}{\eta^2} & \frac{(1-\cosh\eta)\theta_2\theta_3}{\eta^2}\\ \frac{\theta_4\sinh\eta}{\eta} & \frac{(1-\cosh\eta)\theta_1\theta_4}{\eta^2} & \frac{(\theta_1\theta_3+\theta_2\theta_4\cosh\eta)}{\eta^2}\end{pmatrix}. \tag{28}$$

In the above equation, time dependence of functions $\theta_1(t)$, $\theta_2(t)$, $\theta_3(t)$, $\theta_4(t)$ and $\eta(t)$ is not presented for the sake of simplicity and explicit forms of the functions are determined as

$$\begin{aligned}\theta_1(t) &= 2i\int_0^t \mathrm{d}t_1\Omega(t_1)\mathrm{e}^{-(i\omega-\Gamma/2)t_1},\\ \theta_2(t) &= 2i\int_0^t \mathrm{d}t_1\Omega(t_1)\mathrm{e}^{(i\omega+\Gamma/2)t_1},\\ \theta_3(t) &= i\int_0^t \mathrm{d}t_1\Omega(t_1)\mathrm{e}^{(i\omega-\Gamma/2)t_1},\\ \theta_4(t) &= i\int_0^t \mathrm{d}t_1\Omega(t_1)\mathrm{e}^{-(i\omega+\Gamma/2)t_1},\\ \eta(t) &= \sqrt{\theta_1(t)\theta_3(t)+\theta_2(t)\theta_4(t)}.\end{aligned} \tag{29}$$

In order to solve inhomogeneous Eq. (24) we need a particular solution of it. It is obtained as

$$\mathbf{R}_{\mathrm{inhom}}(t) = \mathbf{O}(t)\int_0^t \mathrm{d}t_1\mathbf{O}^{-1}(t_1)\mathbf{A}(t_1) = \mathbf{O}(t)\begin{pmatrix} -\Gamma\int_0^t \mathrm{d}t_1\cosh\eta(t_1)\mathrm{e}^{\Gamma t_1}\\ -\Gamma\int_0^t \mathrm{d}t_1\frac{\theta_3(t_1)\sinh\eta(t_1)}{\eta(t_1)}\mathrm{e}^{\Gamma t_1}\\ \Gamma\int_0^t \mathrm{d}t_1\frac{\theta_4(t_1)\sinh\eta(t_1)}{\eta(t_1)}\mathrm{e}^{\Gamma t_1}\end{pmatrix}. \tag{30}$$

Finally, general solution is the sum of the solutions of the homogeneous and inhomogeneous equations

$$\mathbf{R}(t) = \mathbf{O}(t)\mathbf{R}(0) + \mathbf{R}_{\mathrm{inhom}}(t). \tag{31}$$

When two-level system is initially in the ground state $|2\rangle$, namely $\tilde{z}(0) = -1$ and $\tilde{\rho}_{12}(0) = \tilde{\rho}_{21}(0) = 0$, the solution for $\tilde{z}(t)$ is

$$\begin{aligned}\tilde{z}(t) =& -\cosh\eta(t) - \Gamma\cosh\eta(t)\int_0^t \mathrm{d}t_1\cosh\eta(t_1)\mathrm{e}^{\Gamma t_1}\\ &+ \Gamma\frac{\theta_1(t)\sinh\eta(t)}{\eta(t)}\int_0^t \mathrm{d}t_1\frac{\theta_3(t_1)\sinh\eta(t_1)}{\eta(t_1)}\mathrm{e}^{\Gamma t_1}\\ &+ \Gamma\frac{\theta_2(t)\sinh\eta(t)}{\eta(t)}\int_0^t \mathrm{d}t_1\frac{\theta_4(t_1)\sinh\eta(t_1)}{\eta(t_1)}\mathrm{e}^{\Gamma t_1}.\end{aligned} \tag{32}$$

Excited-state and ground-state probabilities are easily deduced from $\tilde{z}(t)$ using equation $\rho_{11}(t) = (1+\tilde{z}(t)\mathrm{e}^{-\Gamma t})/2$. Solution for $\tilde{\rho}_{12}(t)$ is obtained as

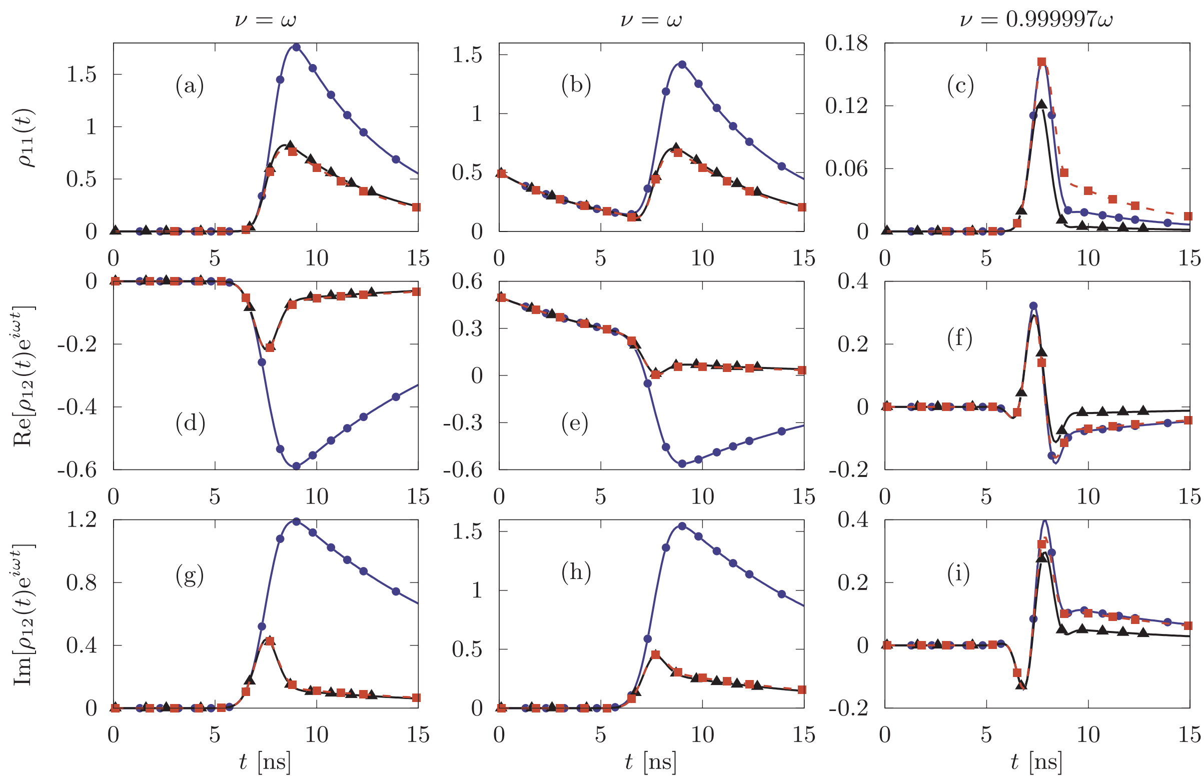

Fig. 5. Numerical results obtained by the first-order Magnus expansion (red dashed line with rectangular nodes), second-order standard perturbation (blue solid line with circular nodes) and fourth-order Runge-Kutta (black solid line with triangular nodes) methods. Driving field is on resonance with the two-level system for the first and second columns and off resonance for the third column ($\nu = 0.999997\omega$). Initial state of the system is ground state for the first and third columns and coherent superposition state ($\rho_{11}(0) = \rho_{12}(0) = \rho_{21}(0) = 1/2$) for the second column. Pulse shape is Gaussian for all cases. Decay rate is $\Gamma = 2 \times 10^8$ 1/s and other parameters used in the calculations are the same as in Fig. 2.

$$\begin{aligned}\tilde{\rho}_{12}(t)=&\frac{\theta_3(t)\sinh\eta(t)}{\eta(t)}+\Gamma\frac{\theta_3(t)\sinh\eta(t)}{\eta(t)}\int_0^t \mathrm{d}t_1\cosh\eta(t_1)\mathrm{e}^{\Gamma t_1}\\ &-\Gamma\frac{\theta_2(t)\theta_4(t)+\theta_1(t)\theta_3(t)\cosh\eta(t)}{\eta^2(t)}\int_0^t \mathrm{d}t_1\frac{\theta_3(t_1)\sinh\eta(t_1)}{\eta(t_1)}\mathrm{e}^{\Gamma t_1}\\ &+\Gamma\frac{(1-\cosh\eta(t))\theta_2(t)\theta_3(t)}{\eta^2(t)}\int_0^t \mathrm{d}t_1\frac{\theta_4(t_1)\sinh\eta(t_1)}{\eta(t_1)}\mathrm{e}^{\Gamma t_1}.\end{aligned} \tag{33}$$

Next, we examine Eqs. (32) and (33) by numerical simulations.

Numerical analysis

As the probability amplitude method, we also perform numerical calculation in the case of Gaussian π pulse. In Fig. 5, the excited-state probability $\rho_{11}(t)$, as well as the real and imaginary parts of the coherence term $\rho_{12}(t)$ are plotted as a function of time for the resonant and off-resonant cases, and also for different initial conditions. Notice that Eqs. (32) and (33) are expressed in terms of double integrals even it is a result of the first-order Magnus expansion. Therefore, we compare the numerical results of the first-order Magnus expansion with the results of the second-order perturbation method. In the case of resonant driving, the Magnus expansion describes adequately the dynamics of the two-level system if the initial state is the ground state or the coherent state $\rho_{11}(0) = \rho_{12}(0) = \rho_{21}(0) = 1/2$ (see the first and second columns of Fig. 5) whereas the second-order perturbation method does not well describe the time evolution since it results in the values of ρ_{11} and ρ_{12} that goes out of the acceptable physical range, for instance $\rho_{11} > 1$, $\mathrm{Re}(\rho_{12}) < -0.5$ and $\mathrm{Im}(\rho_{12}) > 0.5$ at some time between 7 ns and 9 ns. On the other hand, the third column of Fig. 5 exhibits a dynamics of a two-level system interacting with the off-resonant driving which satisfies the adiabatic condition $1/\Delta \ll FWHM$. We observe that the Magnus expansion does not exhibit any advantage over the second-order perturbation method, and both first-order Magnus and second-order perturbation methods do not well describe the time evolution of a two-level system in the adiabatic regime.

Conclusions

In summary, analytical solution obtained by the first-order Magnus expansion method is examined with Gaussian and hyperbolic secant π pulses. In both cases, the approximate analytical solution is well consistent with the results of numerical calculations. This analytical solutions could be potentially useful for design of the qubit control when the dissipation is considered.

Furthermore, numerical simulation of a dissipative two-level system interacting with a time-dependent π pulse is carried out using the first-, second-, and the fourth-order Magnus expansion. Despite the π pulse does not obey the well-known convergence condition given by Refs. [37,38], convergence of the Magnus expansion of our model is fast enough and that permits to use only the first-order Magnus expansion when the frequency of the field is on resonance with the two-level system. Additionally, when the dissipative two-level system is off-resonant with the driving pulse i.e. in adiabatic regime, Magnus expansion is convergent, however the rate of convergence is not as fast as the case of the resonant driving. In that situation, we found that the fourth-order and higher-order Magnus expansions are required to obtain a reasonable solution of the dynamics.

We also show that the Magnus expansion is applicable for the master equation. Unlike the second-order standard perturbation method, the approximate solution obtained by the first-order Magnus expansion well matches the "exact" numerical solution obtained by the fourth-order Runge-Kutta method.

CRediT authorship contribution statement

Tuguldur Kh. Begzjav: Methodology, Software, Resources, Writing

- original draft. **Hichem Eleuch:** Conceptualization, Writing - review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, athttps://doi.org/10.1016/j.rinp.2020.103098.

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