Lecture 5

Dynamics and control of open quantum systems

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This lecture covers Schrieffer-Wolff perturbation theory and the Jaynes-Cummings model.

I. JAYNES-CUMMINGS HAMILTONIAN

The following Hamiltonian describes a spin$-\frac{1}{2}$ interacting with a harmonic oscillator

$$H/\hbar = \frac{\omega_a}{2}\sigma^z \otimes I_r + \omega_r I_q \otimes a^\dagger a + g(\sigma^+ \otimes a + \sigma^- \otimes a^\dagger) = \frac{\omega_a}{2}\sigma^z + \omega_r a^\dagger a + g(\sigma^+ a + \sigma^- a^\dagger). \tag{1}$$

The spin is described by the Pauli matrices σ^i, together with the identity I_q, whereas for the harmonic oscillator we have the bosonic commutation relation $[a, a^\dagger] = 1$ as before.

A. Exact diagonalization

To diagonalize this Hamiltonian, it is simplest to find a conserved quantity, i.e. an operator that commutes with it. This is the excitation number $N = a^\dagger a + \frac{1+\sigma^z}{2}$. We leave the proof that $[N, H] = 0$ as an *exercise*. Then N and H will be diagonal in the same basis.

The eigenspaces of N are $V_0 = \{|0, 0\rangle\}$, $V_1 = \{|0, 1\rangle, |1, 0\rangle\}, \ldots, V_n = \{|n-1, 1\rangle, |n, 0\rangle\}, \ldots$, where the subscript of V denotes the eigenvalue of N, and the two labels of the kets count the number of excitations in the simple harmonic oscillator and in the spin, respectively. For the one-dimensional eigenspace V_0, the eigenenergy is $E_{0,0} = -\omega_a/2$. Over V_n for $n \geq 1$,

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the Hamiltonian is represented by the two-dimensional block

$$H_n = \begin{pmatrix} \langle n-1,1|\, H\, |n-1,1\rangle & \langle n-1,1|\, H\, |n,0\rangle \\ \langle n,0|\, H\, |n-1,1\rangle & \langle n,0|\, H\, |n,0\rangle \end{pmatrix} = \begin{pmatrix} (n-1)\omega_r + \frac{\omega_a}{2} & g\sqrt{n} \\ g\sqrt{n} & n\omega_r - \frac{\omega_a}{2} \end{pmatrix} \\ = \left(n - \frac{1}{2}\right)\omega_r I_2 + \frac{\omega_a - \omega_r}{2}\tau^z + g\sqrt{n}\tau^x. \tag{2}$$

We have introduced Pauli matrices τ^i, along with the identity operator, that act on the two-dimensional subspace V_n. The full Hamiltonian is block-diagonal, i.e. we write $H = H_0 \oplus H_1 \oplus H_2 \oplus \ldots$ acting on $V = V_0 \oplus V_1 \oplus V_2 \oplus \ldots$.

We may further write

$$\begin{aligned} H_n &= \vec{r}_n \cdot \vec{\tau} + \left(n - \frac{1}{2}\right)\omega_r I_2 \\ \vec{r}_n &= (g\sqrt{n}, 0, \Delta/2) \equiv r_n(\sin\theta_n, 0, \cos\theta_n), \\ r_n &= |\vec{r}_n| = \sqrt{ng^2 + \Delta^2/4},\ \sin\theta_n = g\sqrt{n}/r_n,\ \cos\theta_n = \Delta/(2r_n). \end{aligned} \tag{3}$$

From this form, we can calculate using the previous subsection the eigenenergies and eigenvectors in the subspace V_n for $n \geq 1$

$$\begin{aligned} E_{\pm,n} &= \pm r_n, \\ |\psi_{+,n}\rangle &= \cos\left(\frac{\theta_n}{2}\right)|n,0\rangle + \sin\left(\frac{\theta_n}{2}\right)|n-1,1\rangle, \\ |\psi_{-,n}\rangle &= \sin\left(\frac{\theta_n}{2}\right)|n,0\rangle - \cos\left(\frac{\theta_n}{2}\right)|n-1,1\rangle. \end{aligned} \tag{4}$$

$\theta_n/2$ can be interpreted as a 'mixing angle'.

B. Schrieffer-Wolff Perturbation Theory

We rewrite the Jaynes-Cummings Hamiltonian Eq. (1) in the form

$$H = H_0 + \hbar g I_+, \tag{5}$$

where we define the unperturbed Hamiltonian

$$H_0 = \hbar\omega_r a^\dagger a + \hbar\omega_a \frac{\sigma_z}{2}, \tag{6}$$

and let

$$I_\pm = a^\dagger\sigma_- \pm a\sigma_+. \tag{7}$$

I_+ is the Hermitian operator that defines the perturbation, and I_- is an antihermitian operator that will enter the definition of the generator of the Schrieffer-Wolff transformation below.

Under the assumption that $|\Delta| \equiv |\omega_a - \omega_r| \gg g$, the Hamiltonian Eq. (1) can be diagonalized by the unitary transformation

$$\mathbf{D} = e^{-\Lambda(N_q)I_-}, \tag{8}$$

with the following definitions

$$\begin{aligned} \Lambda\left(N_q\right) &= -\frac{\arctan\left(2\lambda\sqrt{N_q}\right)}{2\sqrt{N_q}}, \\ N_q &\equiv a^\dagger a + \Pi_e, \end{aligned} \tag{9}$$

where $\Pi_e = |e\rangle\langle e|$ is the projector onto the excited state of the atom $\sigma_z |e\rangle = |e\rangle$.

Under the action of $\mathbf{D}$ in Eq. (8),

$$H^{\mathbf{D}} \equiv \mathbf{D}^\dagger H \mathbf{D} = \hbar\omega_r a^\dagger a + \hbar\omega_a \frac{\sigma_z}{2} - \frac{\hbar\Delta}{2}\left(1 - \sqrt{1 + 4\lambda^2 N_q}\right)\sigma_z. \tag{10}$$

In the following subsection we derive this result. This solution draws from Boissonneault *et al.*, Phys. Rev. A **79**, 013819 (2009).

1. *Derivation*

We first define the commutator as a superoperator

$$\mathcal{C}_A B \equiv [A, B], \quad \mathcal{C}_A^m B = \overbrace{[A,[A,[A,\ldots,B]]]}^{m \text{ times}}, \tag{11}$$

whence the Baker-Campbell-Hausdorff formula becomes

$$e^A B e^{-A} = \sum_{n=0}^{\infty} \frac{1}{n!} \mathcal{C}_A^n B. \tag{12}$$

Writing the unitary that we are seeking in the form of Eq. (8)

$$\mathbf{D} = e^{-\Lambda(N_q)I_-}, \tag{13}$$

with Λ a yet unspecified function, we note that since N_q commutes with either H or $I_\pm$, then $\Lambda(N_q)$ can be treated as a scalar when considering the nested commutators of the BCH formula Eq. (12) applied with $A = H$ and $B = \Lambda(N_q)I_-$.

Since

$$\mathcal{C}_{I_-} H_0 = \hbar \Delta I_+, \tag{14}$$

we can recast the transformed Hamiltonian Eq. (5) using Eq. (12)

$$H^{\mathbf{D}} \equiv \mathbf{D}^\dagger H \mathbf{D} = H_0 + \hbar \sum_{n=0}^{\infty} \frac{(n+1)g + \Delta\Lambda}{(n+1)!} \mathcal{C}^n_{\Lambda I_-} I_+. \tag{15}$$

To evaluate the sum, we need the following identities, which can be proved by induction

$$\begin{aligned} \mathcal{C}^{2n}_{\Lambda I_-} I_+ &= (-4)^n \Lambda^{2n} N_q^n I_+, \\ \mathcal{C}^{2n+1}_{\Lambda I_-} I_+ &= -2(-4)^n \Lambda^{2n+1} N_q^{n+1} \sigma_z. \end{aligned} \tag{16}$$

This allows us to evaluate the sum in Eq. (15)

$$\begin{aligned} H^{\mathbf{D}} =& H_0 + \hbar \left\{ \frac{\Delta \sin\left(2\Lambda\sqrt{N_q}\right)}{2\sqrt{N_q}} + g\cos\left(2\Lambda\sqrt{N_q}\right) \right\} I_+ \\ & - 2\hbar N_q \sigma_z \left\{ \frac{g \sin\left(2\Lambda\sqrt{N_q}\right)}{2\sqrt{N_q}} + \frac{\Delta\left[1-\cos\left(2\Lambda\sqrt{N_q}\right)\right]}{4N_q} \right\}. \end{aligned} \tag{17}$$

Note that this expression contains both off-diagonal (second term in the equation above) and diagonal terms (first and third terms). We may now make the choice

$$\Lambda\left(N_q\right) = \frac{-\arctan\left(2\lambda\sqrt{N_q}\right)}{2\sqrt{N_q}} \tag{18}$$

that nulls the off-diagonal term, to obtain

$$H^{\mathbf{D}} = H_0 - \frac{\hbar\Delta}{2}\left(1 - \sqrt{1+4\lambda^2 N_q}\right)\sigma_z. \tag{19}$$

We can now define Lamb and ac Stark shift operators as follows

$$\begin{aligned} \delta_L &\equiv H^{\mathbf{D}}(0,1) - H^{\mathbf{D}}(0,-1) - \hbar\omega_a = -\frac{\hbar\Delta}{2}\left(1-\sqrt{1+4\lambda^2}\right) \\ \delta_S\left(a^\dagger a\right) &\equiv H^{\mathbf{D}}\left(a^\dagger a, 1\right) - H^{\mathbf{D}}\left(a^\dagger a, -1\right) - \delta_L - \hbar\omega_a \\ &= \frac{\hbar\Delta}{2}\left(\sqrt{1+4\lambda^2\left(a^\dagger a+1\right)} + \sqrt{1+4\lambda^2 a^\dagger a} - 1 - \sqrt{1+4\lambda^2}\right). \end{aligned} \tag{20}$$

Note that the unitary operator redefines the excitations in the problem. We have for the operators that were previously diagonal in the eigenbases of the atom and oscillator, respectively

$$\begin{aligned} \sigma_z^{\mathbf{D}} &= \sigma_z\left(\frac{1}{\sqrt{1+4\lambda^2 N_q}}\right) - \frac{2\lambda}{\sqrt{1+4\lambda^2 N_q}} I_+, \\ \left(a^\dagger a\right)^{\mathbf{D}} &= a^\dagger a + \frac{\sigma_z}{2} + \frac{\left(\lambda I_+ - \sigma_z/2\right)}{\sqrt{1+4N_q\lambda^2}}, \end{aligned} \tag{21}$$

and

$$\begin{aligned} a^{\mathbf{D}} &\approx a\left[1+\frac{\lambda^2\sigma_z}{2}\right]+\lambda\left[1-3\lambda^2\left(a^\dagger a+\frac{1}{2}\right)\right]\sigma_- +\lambda^3 a^2\sigma_+ \\ \sigma_-^{\mathbf{D}} &\approx \sigma_-\left[1-\lambda^2\left(a^\dagger a+\frac{1}{2}\right)\right]+\lambda a\sigma_z-\lambda^2 a^2\sigma_+ \end{aligned} \tag{22}$$

Finally, the Hamiltonian up to cubic order in λ is

$$H^{\mathbf{D}} \approx \hbar\left(\omega_r+\zeta\right)a^\dagger a+\hbar\left[\omega_a+2\chi\left(a^\dagger a+\frac{1}{2}\right)\right]\frac{\sigma_z}{2}+\hbar\zeta\left(a^\dagger a\right)^2\sigma_z, \tag{23}$$

where we have introduced

$$\begin{aligned} \chi &= g^2\left(1-\lambda^2\right)/\Delta, \\ \zeta &= -g^4/\Delta^3. \end{aligned} \tag{24}$$

C. Coupling to environment

Suppose that the system described by H in Eq. (5) is coupled to a bath via the operator $A = a + a^\dagger$ via $H_{SB} = A \otimes B$ with B some bath operator as introduced in earlier lectures on the Lindblad master equation. Can we use the Schrieffer-Wolff approach to compute the so-called Purcell relaxation rate? We assume zero temperature throughout this subsection.

First, the system-bath coupling would be written in the interaction picture with respect to H, so we need to evaluate the time-evolution operator $U(t,0)$. First we reexpress it as follows using the unitarity of $\mathbf{D}$

$$e^{-iHt} = \mathbf{D}e^{-iH^{\mathbf{D}}t}\mathbf{D}^\dagger. \tag{25}$$

Then we note that under $\mathbf{D}$ the system operator coupling to the bath transforms as (according to Eq. (22))

$$\begin{aligned} a+a^\dagger \to a^{\mathbf{D}}+a^{\dagger\mathbf{D}} &\approx a\left[1+\frac{\lambda^2\sigma_z}{2}\right]+\lambda\left[1-3\lambda^2\left(a^\dagger a+\frac{1}{2}\right)\right]\sigma_-+\lambda^3a^2\sigma_+ +\text{H.c.} \\ &\approx a+\lambda\sigma_- +\text{H.c.}, \end{aligned} \tag{26}$$

where we have kept the lowest-order contribution linear in λ.

We now need to recall how the Lindblad master equation is derived. We first need to express the system-bath coupling Hamiltonian in the interaction picture with respect to the uncoupled system and bath Hamiltonians, that is, we need

$$A(t) \equiv e^{iHt}(a+a^\dagger)e^{-iHt} = \mathbf{D}e^{iH^{\mathbf{D}}t}\mathbf{D}^\dagger(a+a^\dagger)\mathbf{D}e^{-iH^{\mathbf{D}}t}\mathbf{D}^\dagger = \mathbf{D}e^{iH^{\mathbf{D}}t}(a^{\mathbf{D}}+a^{\dagger\mathbf{D}})e^{-iH^{\mathbf{D}}t}\mathbf{D}^\dagger, \tag{27}$$

or equivalently

$$A^{\mathbf{D}}(t) \equiv \mathbf{D}^{\dagger} A(t) \mathbf{D} = e^{iH^{\mathbf{D}}t}(a^{\mathbf{D}} + a^{\dagger \mathbf{D}}) e^{-iH^{\mathbf{D}}t} \equiv \sum_{\omega} A^{\mathbf{D}}(\omega) e^{-i\omega t}. \tag{28}$$

This suggests it is more convenient to write the Lindblad master equation in the frame rotated by $\mathbf{D}$.

If the von Neumann equation is

$$\dot{\rho} = -i[H_{total}, \rho], \tag{29}$$

then in the rotated frame

$$\dot{\rho}^{\mathbf{D}} = -i[H^{\mathbf{D}}_{total}, \rho^{\mathbf{D}}]. \tag{30}$$

Therefore the equation for the reduced density matrix $\rho^{\mathbf{D}}$ (abuse of notation) is

$$\dot{\rho}^{\mathbf{D}} = -i[H^{\mathbf{D}}, \rho^{\mathbf{D}}] + \sum_{\omega} \gamma(\omega) \mathcal{D}[A^{\mathbf{D}}(\omega)] \rho^{\mathbf{D}}, \tag{31}$$

with $\gamma(\omega)$ being related to the bilateral power spectral density of the bath modes as in Eq. (43) of Lecture 2 with $\alpha = \beta$. Then all that remains is then to evaluate Eq. (28). To get our answer we will do this using the order-λ result of Eq. (26), and use $H^{\mathbf{D}}$ of Eq. (32) up to order order λ, i.e.

$$H^{\mathbf{D}} = \hbar\omega_r a^{\dagger} a + \hbar(\omega_a + \chi)\frac{\sigma_z}{2} + \hbar\chi a^{\dagger} a \sigma_z + O(\lambda^2) \tag{32}$$

In evaluating Eq. (28) we furthermore neglect terms of order χ in $H^{\mathbf{D}}$, ultimately using its order-λ^0 contributions only. Then we find

$$A^{\mathbf{D}}(\omega_a) = \lambda\sigma_-, A^{\mathbf{D}}(-\omega_a) = \lambda\sigma_+, A^{\mathbf{D}}(\omega_r) = a, A^{\mathbf{D}}(-\omega_r) = a^{\dagger}, \tag{33}$$

leading to

$$\dot{\rho}^{\mathbf{D}} = -i[H^{\mathbf{D}}, \rho^{\mathbf{D}}] + \gamma(\omega_r)\mathcal{D}[a]\rho^{\mathbf{D}} + \lambda^2\gamma(\omega_a)\mathcal{D}[\sigma_-]\rho^{\mathbf{D}}. \tag{34}$$

Assuming that the bath power spectral density is flat with $\gamma(\omega) = \kappa$, we get the result

$$\dot{\rho}^{\mathbf{D}} = -i[H^{\mathbf{D}}, \rho^{\mathbf{D}}] + \kappa\mathcal{D}[a]\rho^{\mathbf{D}} + \lambda^2\kappa\mathcal{D}[\sigma_-]\rho^{\mathbf{D}}, \tag{35}$$

leading to the formula for the Purcell decay rate of the qubit (rate of radiative decay of an atom coupled to a detuned lossy cavity)

$$\gamma_P = \left(\frac{g}{\Delta}\right)^2 \kappa. \tag{36}$$

Note that this is primarily due to the 'hybridization' of the qubit with the cavity, given by the hybridization coefficient $\lambda \ll 1$, and that therefore this is an apparently weak effect on the qubit $\gamma_P \ll \kappa$, which however turns out to be important in practice.

II. ORDER-BY-ORDER ROTATING-WAVE APPROXIMATION FROM SCHRIEFFER-WOLFF PERTURBATION THEORY

Note for Fall 2023 course: This material was not covered in class, so it will not be on the exam. Below we consider a generic Schrieffer-Wolff perturbation theory for time-dependent Hamiltonians. Let us consider a generic Baker-Campbell-Hausdorff expansion of the form

$$e^{-\hat{G}_\mathrm{I}(t)}(\hat{H}_\mathrm{I} - i\partial_t)e^{\hat{G}_\mathrm{I}(t)} = \hat{H}_\mathrm{I} - i\dot{\hat{G}}_\mathrm{I} + [\hat{H}_\mathrm{I}, \hat{G}_\mathrm{I}] - \frac{i}{2}[\dot{\hat{G}}_\mathrm{I}, \hat{G}_\mathrm{I}] + \frac{1}{2!}[[\hat{H}_\mathrm{I}, \hat{G}_\mathrm{I}], \hat{G}_\mathrm{I}] - \frac{i}{3!}[[\dot{\hat{G}}_\mathrm{I}, \hat{G}_\mathrm{I}], \hat{G}_\mathrm{I}]$$
$$+\frac{1}{3!}[[[\hat{H}_\mathrm{I}, \hat{G}_\mathrm{I}], \hat{G}_\mathrm{I}], \hat{G}_\mathrm{I}] - i\partial_t + ...$$

Let us assume that the generator can be expanded as follows:

$$\hat{G}_\mathrm{I}(t) = \lambda \hat{G}_\mathrm{I}^{(1)}(t) + \lambda^2 \hat{G}_\mathrm{I}^{(2)}(t) + ... \tag{37}$$

We can rewrite (37) up to contributions of order λ^3 as follows

$$\begin{aligned}
&e^{-\hat{G}_\mathrm{I}}(\hat{H}_\mathrm{I} - i\partial_t)e^{\hat{G}_\mathrm{I}} = \\
&\hat{H}_\mathrm{I} - i\lambda\dot{\hat{G}}_\mathrm{I}^{(1)} \\
&+[\hat{H}_\mathrm{I}, \lambda\hat{G}_\mathrm{I}^{(1)}] - \frac{i}{2}[\lambda\dot{\hat{G}}_\mathrm{I}^{(1)}, \lambda\hat{G}_\mathrm{I}^{(1)}] - i\lambda^2\dot{\hat{G}}_\mathrm{I}^{(2)} \\
&+[\hat{H}_\mathrm{I}, \lambda^2\hat{G}_\mathrm{I}^{(2)}] - \frac{i}{2}[\lambda^2\dot{\hat{G}}_\mathrm{I}^{(2)}, \lambda\hat{G}_\mathrm{I}^{(1)}] - \frac{i}{2}[\lambda\dot{\hat{G}}_\mathrm{I}^{(1)}, \lambda^2\hat{G}_\mathrm{I}^{(2)}] + \frac{1}{2!}[[\hat{H}_\mathrm{I}, \lambda\hat{G}_\mathrm{I}^{(1)}], \lambda\hat{G}_\mathrm{I}^{(1)}] - \frac{i}{3!}[[\lambda\dot{\hat{G}}_\mathrm{I}^{(1)}, \lambda\hat{G}_\mathrm{I}^{(1)}], \lambda\hat{G}_\mathrm{I}^{(1)}] \\
&\qquad -i\lambda^3\dot{\hat{G}}_\mathrm{I}^{(3)} \\
&-i\partial_t + O(\lambda^4) \\
\equiv\ &\lambda\hat{H}_\mathrm{I}^{(1)}(t) - i\lambda\dot{\hat{G}}_\mathrm{I}^{(1)} \\
&+\lambda^2\hat{H}_\mathrm{I}^{(2)}(t) - i\lambda^2\dot{\hat{G}}_\mathrm{I}^{(2)} \\
&+\lambda^3\hat{H}_\mathrm{I}^{(3)}(t) - i\lambda^3\dot{\hat{G}}_\mathrm{I}^{(3)} \\
&-i\partial_t + O(\lambda^4).
\end{aligned} \tag{38}$$

The first, second, and third row contain terms that are first-order, second-order and third-order in λ, respectively. We needed to introduce the following notation:

$$\hat{H}_{\rm I}(t) \equiv \lambda \hat{H}_{\rm I}^{(1)}(t) \equiv \lambda \overline{\hat{H}}_I^{(1)} + \lambda \widetilde{\hat{H}}_I^{(1)}(t), \tag{39}$$

and moreover let us define more generally for $k > 1$ integer a separation over constant and oscillatory terms:

$$\lambda^k \hat{H}_{\rm I}^{(k)}(t) \equiv \lambda^k \overline{\hat{H}}_I^{(k)} + \lambda^k \widetilde{\hat{H}}_I^{(k)}(t). \tag{40}$$

Definition (DC and AC parts of a time-dependent operator). The definitions above involved the DC part of a time-dependent operator $\hat{O}(t)$, defined as:

$$\overline{\hat{O}} \equiv \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \hat{O}(t). \tag{41}$$

Moreover, we may define the AC, or oscillatory part, of the operator, according to

$$\widetilde{\hat{O}}(t) \equiv \hat{O}(t) - \overline{\hat{O}}. \tag{42}$$

Properties. The operations $\overline{\hat{O}}$ and $\widetilde{\hat{O}}(t)$ are linear, in the sense that $\widetilde{\hat{O}_1 + \hat{O}_2(t)} = \widetilde{\hat{O}}_1(t) + \widetilde{\hat{O}}_2(t)$, and $\overline{\hat{O}_1 + \hat{O}_2(t)} = \overline{\hat{O}}_1(t) + \overline{\hat{O}}_2(t)$. Moreover, they are idempotent: $\overline{\overline{\hat{O}}} = \overline{\hat{O}}$, and $\widetilde{\widetilde{\hat{O}}} = \widetilde{\hat{O}}$, but application of one after another gives zero: $\overline{\widetilde{\hat{O}}} = 0$, and $\widetilde{\overline{\hat{O}}} = 0$. Thus, they appear to share properties with a pair of projectors onto complementary Hilbert subspaces.

Having introduced these notations, we are equipped to write the iterative procedure to derive the RWA Hamiltonian. The condition for removing non-RWA terms at order λ^k:

$$\lambda^k \hat{H}_{\rm I}^{(k)}(t) - i\lambda^k \dot{\hat{G}}_I^{(k)}(t) = \lambda^k \overline{\hat{H}}_I^{(k)}, \tag{43}$$

Note that $\lambda^k \hat{H}_{\rm I}^{(k)}(t)$ for $k \geq 2$ is generally dependent on $\hat{G}_{\rm I}^{(1)}, ..., \hat{G}_{\rm I}^{(k-1)}$, which means that this is an iterated procedure: Equation (43) must be solved in order for $k = 1, 2, 3, ...$ Once the first k equations have been solved, we can write down the RWA Hamiltonian in the following form

$$e^{-\hat{G}_{\rm I}(t)}(\hat{H}_{\rm I} - i\partial_t)e^{\hat{G}_{\rm I}(t)} = \sum_{l=1}^{k} \lambda^l \overline{\hat{H}}_I^{(l)} + O(\lambda^{k+1}), \tag{44}$$

where terms of order λ^{k+1} are time-dependent, but terms of order $\leq k$ are stationary.

A. First-order RWA

In the first iteration we write Eq. (43) for $k=1$:

$$\lambda \hat{H}_{\mathrm{I}}^{(1)}(t) - i\lambda \dot{\hat{G}}_{I}^{(1)}(t) = \lambda \overline{\hat{H}}_{I}^{(1)}, \tag{45}$$

which yields, upon recalling the separation of $\lambda \hat{H}_{\mathrm{I}}^{(1)}(t)$, Eq. (40):

$$\begin{aligned} \lambda \widetilde{\hat{H}}_{I}^{(1)} - i\lambda \dot{\hat{G}}_{I}^{(1)} = 0 \quad \leftrightarrow \quad \lambda \hat{G}_{\mathrm{I}}^{(1)}(t) &= \frac{\lambda}{i}\int^{t} dt' \widetilde{\hat{H}}_{I}^{(1)}(t') + \lambda \hat{G}_{\mathrm{I},0}^{(1)} \\ &\equiv \lambda \widetilde{\hat{G}}_{\mathrm{I}}^{(1)}(t) + \lambda \overline{\hat{G}}_{\mathrm{I}}^{(1)} \end{aligned} \tag{46}$$

Note that the integral is indefinite, so that the first term is oscillatory, and we can set $\frac{\lambda}{i}\int^{t} dt' \widetilde{\hat{H}}_{I}^{()}(1)(t') \equiv \lambda \widetilde{\hat{G}}_{\mathrm{I}}^{(1)}(t)$, while the second term is the integration constant, which sets the DC part of the order-λ generator $\lambda \hat{G}_{\mathrm{I},0}^{(1)} \equiv \lambda \overline{\hat{G}}_{\mathrm{I}}^{(1)}$. Imposing the equation above, we rewrite Eq. (38) where to $O(\lambda)$ we have obtained a stationary Hamiltonian:

$$e^{-\hat{G}_{\mathrm{I}}}(\hat{H}_{\mathrm{I}} - i\partial_t)e^{\hat{G}_{\mathrm{I}}} = \lambda \overline{\hat{H}}_{I}^{()}(1) + O(\lambda^2), \tag{47}$$

where we recall that, from the definition (39), $\lambda \overline{\hat{H}}_{I}^{()}(1) = \overline{\hat{H}_{\mathrm{I}}}$. This is the standard RWA approximation.

B. Second-order RWA

We move on to second order in λ. The second-order terms were:

$$\begin{aligned} \lambda^2 \hat{H}_{\mathrm{I}}^{(2)}(t) - i\lambda^2 \dot{\hat{G}}_{\mathrm{I}}^{(2)} &= [\hat{H}_{\mathrm{I}}(t), \lambda \hat{G}_{\mathrm{I}}^{(1)}(t)] - \frac{i}{2}[\lambda \dot{\hat{G}}_{\mathrm{I}}^{(1)}(t), \lambda \hat{G}_{\mathrm{I}}^{(1)}(t)] - i\lambda^2 \dot{\hat{G}}_{\mathrm{I}}^{(2)} \\ &= [\hat{H}_{\mathrm{I}}(t) - \frac{i}{2}\lambda \dot{\hat{G}}_{\mathrm{I}}^{(1)}(t), \lambda \hat{G}_{\mathrm{I}}^{(1)}(t)] - i\lambda^2 \dot{\hat{G}}_{\mathrm{I}}^{(2)} \\ &\overset{\text{Eq. (45)}}{=} [\lambda \overline{\hat{H}}_{I}^{(1)} + \frac{i}{2}\lambda \dot{\hat{G}}_{\mathrm{I}}^{(1)}(t), \lambda \hat{G}_{\mathrm{I}}^{(1)}(t)] - i\lambda^2 \dot{\hat{G}}_{\mathrm{I}}^{(2)} \end{aligned} \tag{48}$$

Condition (43) for $k=2$ implies the following equation for $\hat{G}_{\mathrm{I}}^{(2)}(t)$:

$$[\lambda \overline{\hat{H}}_{I}^{(1)} + \frac{i}{2}\lambda \dot{\hat{G}}_{\mathrm{I}}^{(1)}(t), \lambda \hat{G}_{\mathrm{I}}^{(1)}(t)] - i\lambda^2 \dot{\hat{G}}_{\mathrm{I}}^{(2)} = \lambda^2 \overline{\hat{H}}_{I}^{(2)}, \tag{49}$$

where the second-order RWA Hamiltonian is

$$\lambda^2 \overline{\hat{H}}_{I}^{(2)} \equiv \overline{[\lambda \overline{\hat{H}}_{I}^{(1)} + \frac{i}{2}\lambda \dot{\hat{G}}_{\mathrm{I}}^{(1)}(t), \lambda \hat{G}_{\mathrm{I}}^{(1)}(t)]} \tag{50}$$

We can simplify this form by using the separation of $\hat{G}_{\mathrm{I}}^{(1)}(t)$ into DC and AC components:

$$\begin{aligned}\lambda^2\overline{\hat{H}_I}^{(2)} &\equiv \overline{[\lambda\overline{\hat{H}_I}^{(1)} + \frac{i}{2}\lambda\dot{\hat{G}}_{\mathrm{I}}^{(1)}(t), \lambda\widetilde{\hat{G}_{\mathrm{I}}}^{(1)}(t) + \lambda\overline{\hat{G}_{\mathrm{I}}}^{(1)}]} \\ &= [\lambda\overline{\hat{H}_I}^{(1)}, \lambda\overline{\hat{G}_{\mathrm{I}}}^{(1)}] + \overline{[\frac{i}{2}\lambda\dot{\hat{G}}_{\mathrm{I}}^{(1)}(t), \lambda\widetilde{\hat{G}_{\mathrm{I}}}^{(1)}(t)]}. \end{aligned} \tag{51}$$

Remark that the cross terms vanished under time-averaging. We may wish to express this in terms of the Hamiltonian, so we can write

$$\begin{aligned}\lambda^2\overline{\hat{H}_I}^{(2)} &= [\lambda\overline{\hat{H}_I}^{(1)}, \lambda\overline{\hat{G}_{\mathrm{I}}}^{(1)}] + \frac{1}{2i}\overline{\left[\lambda\widetilde{\hat{H}_I}^{(1)}(t), \int^t \lambda\widetilde{\hat{H}_I}^{(1)}(t')dt'\right]} \\ &= [\lambda\overline{\hat{H}_I}^{(1)}, \lambda\overline{\hat{G}_{\mathrm{I}}}^{(1)}] + \frac{1}{2i}\overline{\left[\hat{H}_{\mathrm{I}}(t) - \lambda\overline{\hat{H}_I}^{(1)}, \int^t \left(\hat{H}_{\mathrm{I}}(t') - \lambda\overline{\hat{H}_I}^{(1)}\right) dt'\right]}. \end{aligned} \tag{52}$$

Note the first term, which corresponds to the boundary condition, and hence the DC part, of the generator.

For further use in the third-order RWA, recall that the generator obeys the equation

$$\begin{aligned}\lambda^2\widetilde{\hat{H}_I}^{(2)} - i\lambda^2\dot{\hat{G}}_I^{(2)} = 0 \quad \leftrightarrow \quad \lambda^2\hat{G}_{\mathrm{I}}^{(2)}(t) &= \frac{\lambda^2}{i}\int^t dt'\widetilde{\hat{H}_I}^{(2)}(t') + \lambda^2\hat{G}_{\mathrm{I},0}^{(2)} \\ &\equiv \lambda\widetilde{\hat{G}_{\mathrm{I}}}^{(2)}(t) + \lambda\overline{\hat{G}_{\mathrm{I}}}^{(2)}, \end{aligned} \tag{53}$$

where we write the oscillating part of the Hamiltonian at second-order in λ as follows:

$$\lambda^2\widetilde{\hat{H}_I}^{(2)}(t) = \lambda^2\hat{H}_{\mathrm{I}}^{(2)}(t) - \lambda^2\overline{\hat{H}_I}^{(2)}. \tag{54}$$

C. Third-order RWA

The third-order terms are

$$\begin{aligned}&+[\hat{H}_{\mathrm{I}}, \lambda^2\hat{G}_{\mathrm{I}}^{(2)}] - \frac{i}{2}[\lambda^2\dot{\hat{G}}_{\mathrm{I}}^{(2)}, \lambda\hat{G}_{\mathrm{I}}^{(1)}] - \frac{i}{2}[\lambda\dot{\hat{G}}_{\mathrm{I}}^{(1)}, \lambda^2\hat{G}_{\mathrm{I}}^{(2)}] + \frac{1}{2!}[[\hat{H}_{\mathrm{I}}, \lambda\hat{G}_{\mathrm{I}}^{(1)}], \lambda\hat{G}_{\mathrm{I}}^{(1)}] - \frac{i}{3!}[[\lambda\dot{\hat{G}}_{\mathrm{I}}^{(1)}, \lambda\hat{G}_{\mathrm{I}}^{(1)}], \lambda\hat{G}_{\mathrm{I}}^{(1)}] \\ &\qquad - i\lambda^3\dot{\hat{G}}_{\mathrm{I}}^{(3)} \\ &= \lambda^3\hat{H}_{\mathrm{I}}^{(3)}(t) - i\lambda^3\dot{\hat{G}}_{\mathrm{I}}^{(3)} \equiv \lambda^3\overline{\hat{H}_I}^{(3)} + \lambda^3\widetilde{\hat{H}_I}^{(3)}(t) - i\lambda^3\dot{\hat{G}}_{\mathrm{I}}^{(3)} = \lambda^3\overline{\hat{H}_I}^{(3)} \end{aligned} \tag{55}$$

The third-order RWA Hamiltonian is

$$\begin{aligned}\lambda^3\overline{\hat{H}_I}^{(3)} = &\underbrace{\overline{[\hat{H}_{\mathrm{I}}, \lambda^2\hat{G}_{\mathrm{I}}^{(2)}]}}_{\text{term 1}} \underbrace{- \frac{i}{2}\overline{[\lambda^2\dot{\hat{G}}_{\mathrm{I}}^{(2)}, \lambda\hat{G}_{\mathrm{I}}^{(1)}]}}_{\text{term 2}} \underbrace{- \frac{i}{2}\overline{[\lambda\dot{\hat{G}}_{\mathrm{I}}^{(1)}, \lambda^2\hat{G}_{\mathrm{I}}^{(2)}]}}_{\text{term 3}} \\ &\underbrace{+ \frac{1}{2!}\overline{[[\hat{H}_{\mathrm{I}}, \lambda\hat{G}_{\mathrm{I}}^{(1)}], \lambda\hat{G}_{\mathrm{I}}^{(1)}]}}_{\text{term 4}} \underbrace{- \frac{i}{3!}\overline{[[\lambda\dot{\hat{G}}_{\mathrm{I}}^{(1)}, \lambda\hat{G}_{\mathrm{I}}^{(1)}], \lambda\hat{G}_{\mathrm{I}}^{(1)}]}}_{\text{term 5}} \end{aligned} \tag{56}$$

D. RWA Hamiltonian up to third-order assuming no DC part to generator

We collect here the simpler expressions under the assumption $\overline{\hat{G}}_I^{(k)} = 0$. We will test the validity of this assumption by checking this RWA transformation against some simple test cases.

$$\begin{aligned}
\lambda\overline{\hat{H}}_I^{()}(1) &= \overline{\hat{H}_{\mathrm{I}}} \\
\lambda^2\overline{\hat{H}}_I^{()}(2) &= \frac{1}{2}\overline{\left[\lambda\widetilde{\hat{H}}_I^{()}(1), \lambda\widetilde{\hat{G}}_I^{(1)}(t)\right]} \\
\lambda^3\overline{\hat{H}}_I^{()}(3) &= +\frac{1}{2}\overline{[[\lambda\overline{\hat{H}}_I^{()}(1), \lambda\widetilde{\hat{G}}_I^{(1)}(t)], \lambda\widetilde{\hat{G}}_I^{(1)}(t)]} + \frac{1}{3}\overline{[[\lambda\widetilde{\hat{H}}_I^{()}(1), \lambda\widetilde{\hat{G}}_I^{(1)}(t)], \lambda\widetilde{\hat{G}}_I^{(1)}(t)]}.
\end{aligned} \tag{57}$$