Rabi – II

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Section 1: SVD 分解和 C 矩阵的关系

1.1 C 矩阵到 SVD 分解

一个系综矩阵 $A_{N\times M}, (M > N)$，定义关联矩阵 $C_{M\times M} = A^T_{M\times N} A_{N\times M}$，求得 C 矩阵的特征值λ_i和对应标准正交的特征向量

$$\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r, \boldsymbol{v}_{r+1}, ..., \boldsymbol{v}_M \tag{1}$$

其中 r 是 C 矩阵的秩。可以写成正交矩阵 $V_{M\times M} = \left[V_{1_{M\times r}}, V_{2_{M\times M-r}}\right] = [\boldsymbol{v}_1, \boldsymbol{v}_2, ..., \boldsymbol{v}_r, \boldsymbol{v}_{r+1}, ..., \boldsymbol{v}_M]$，其中 V_1 是 C 矩阵的前 r 个特征向量，V_2 是 C 矩阵的后 $M-r$ 个特征向量。

根据特征值与特征向量的定义，有：

$$A^T A \boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i \quad (i = 1, 2, ..., M) \tag{2}$$

考虑 $A\boldsymbol{v}_i \quad (i = 1, 2, ..., M)$，有：

$$\langle A\boldsymbol{v}_i, A\boldsymbol{v}_j \rangle = \boldsymbol{v}_i^T A^T A \boldsymbol{v}_j = \boldsymbol{v}_i^T \lambda_j \boldsymbol{v}_j = \lambda_j \boldsymbol{v}_i^T \boldsymbol{v}_j = \begin{cases} \lambda_i, 1 \le i = j \le r \\ 0, i \ne j \end{cases} \tag{3}$$

令 $\Lambda_{M\times M} = \mathrm{diag}(\lambda_1, \lambda_2, ..., \lambda_r, 0, ..., 0) = \begin{pmatrix} \Lambda_{1_{r\times r}} & 0 \\ 0 & 0 \end{pmatrix}$，设 $\Sigma_{1_{r\times r}} = \sqrt{\Lambda_{1_{r\times r}}}$，则有：

从而有 $A^T A V_1 = V_1 \Lambda_1 = V_1 \Sigma_1^2$，进一步得到

$$\Sigma_1^{-1} V_1^T A^T A V_1 \Sigma_1^{-1} = I \tag{4}$$

令 $U_{1_{N\times r}} = A_{N\times M} V_{1_{M\times r}} {\Sigma_1^{-1}}_{r\times r}$，则有 $U_1^T U_1 = I$，即 U_1 是正交矩阵。可以选择$N-r$ 个正交矩阵 U_2，使得 $U_{N\times N} = \left[U_{1_{N\times r}}, U_{2_{N\times N-r}}\right]$ 是标准正交矩阵。

综上，

$$U^T_{N\times N} A_{N\times M} V_{M\times M} = \begin{pmatrix} U_1^T A V_1 & U_1^T A V_2 \\ U_2^T A V_1 & U_2^T A V_2 \end{pmatrix} = \begin{pmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{pmatrix} = \Sigma_{N\times M} \tag{5}$$

即 $A = U\Sigma V^T$，这就是 SVD 分解。

特征值λ_i和σ_i的关系是 $\lambda_i = \sigma_i^2$。

1.2 SVD 分解到 C 矩阵

根据 SVD 分解，有 $A = U\Sigma V^T$

$$\begin{gathered} C = A^T A = V\Sigma^T U^T U \Sigma V^T = V \Sigma^2 V^T \\ \Rightarrow CV = V\Sigma^2 \end{gathered} \tag{6}$$

对于 Σ^2 矩阵对角线上的每一项有本征方程

$$Cv_i = \lambda_i v_i = \sigma_i^2 v_i \tag{7}$$

1.3 SVD 分解到 K 矩阵

对于 $K = AA^T$ 矩阵，有

$$K = U\Sigma V^T V\Sigma^T U^T = U\Sigma\Sigma^T U^T = U\Lambda U^T \tag{8}$$

对于 Λ 矩阵对角线上的每一项有本征方程

$$Ku_i = \lambda_i u_i = \sigma_i^2 u_i \tag{9}$$

Section 2: 量子本征态

2.1 形式化定义

一个量子系统可以拆分为A和B两部分，分别表征系统A和环境B。系统A的哈密顿量为H_A，环境B的哈密顿量为H_B，系统和环境的相互作用哈密顿量为H_{AB}。系统和环境的总哈密顿量为$H = H_A + H_B + H_{AB}$，系统的基态波函数可以写为

$$|G\rangle = \sum_{\tau=0}^{M} \sum_{i=0}^{N} a_{\tau i} \left|\psi_\tau^A\right\rangle \left|\psi_i^B\right\rangle \tag{10}$$

量子系综矩阵写为

$$A = (\boldsymbol{s}_1 \ \ \boldsymbol{s}_2 \ \ \dots \ \ \boldsymbol{s}_M) \tag{11}$$

与 Eq. 10 对应，得到

$$\boldsymbol{s}_\tau = \begin{pmatrix} a_{\tau 0} \\ a_{\tau 1} \\ \vdots \\ a_{\tau N} \end{pmatrix} = \sum_{i=0}^{N} a_{\tau i} \left|\psi_i^B\right\rangle \tag{12}$$

可以定义一个关联矩阵，表示系统态τ和τ'在环境作用下的关联，即

$$\begin{aligned} C_{\tau\tau'} = \langle \boldsymbol{s}_\tau, \boldsymbol{s}_{\tau'} \rangle &= \left(\sum_i a_{\tau i} \left|\psi_i^B\right\rangle \right)^\dagger \sum_j a_{\tau' j} \left|\psi_j^B\right\rangle \\ &= \sum_i \sum_j a_{\tau i}^* a_{\tau' j} \left\langle \psi_i^B \middle| \psi_j^B \right\rangle = \sum_i \sum_j a_{\tau i}^* a_{\tau' j} \delta_{ij} \\ &= \sum_i a_{\tau i}^* a_{\tau' i} \end{aligned} \tag{13}$$

根据 SVD 分解分解($A = U \Sigma V^\dagger$)，得到本征态的形式为

$$\begin{aligned} E &= U\Sigma = AV \\ \Rightarrow E_k &= \sum_{\tau=0}^{M} V_{\tau k} \boldsymbol{s}_\tau = \sum_{\tau=0}^{M} V_{\tau k} \sum_{i=0}^{N} a_{\tau i} \left|\psi_i^B\right\rangle \end{aligned} \tag{14}$$

2.2 Rabi 模型为例

Rabi 模型的哈密顿量为

$$\hat{H} = \omega \hat{a}^\dagger \hat{a} + \frac{\Omega}{2} \hat{\sigma}_x + g\left(\hat{a}^\dagger + \hat{a}\right) \hat{\sigma}_z \tag{15}$$

其中ω是振子的频率，Ω是自旋的频率，g是耦合系数。根据算符关系$\hat{x} = \frac{1}{\sqrt{2\omega}}\left(\hat{a}^\dagger + \hat{a}\right)$ 和 $\hat{p} = -i\sqrt{\frac{\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right)$，可以得到

$$\begin{aligned} \hat{p}^2 &= -\frac{\omega}{2}\left(\hat{a}^{\dagger 2} + \hat{a}^2 - \hat{a}^\dagger \hat{a} - \hat{a}\hat{a}^\dagger\right) = -\frac{\omega}{2}\left(\hat{a}^{\dagger 2} + \hat{a}^2 - 2\hat{a}^\dagger \hat{a} + 1\right) \\ \hat{x}^2 &= \frac{1}{2\omega}\left(\hat{a}^{\dagger 2} + \hat{a}^2 + \hat{a}^\dagger \hat{a} + \hat{a}\hat{a}^\dagger\right) = \frac{1}{2\omega}\left(\hat{a}^{\dagger 2} + \hat{a}^2 + 2\hat{a}^\dagger \hat{a} - 1\right) \end{aligned} \tag{16}$$

进一步可以得到

$$
\begin{aligned}
\frac{2}{\omega}\hat{p}^2 + 2\omega\hat{x}^2 &= 4\hat{a}^\dagger\hat{a} - 2 \\
\hat{a}^\dagger\hat{a} &= \frac{1}{2}\left(\frac{\hat{p}^2}{\omega} + \omega\hat{x}^2 + 1\right)
\end{aligned}
\tag{17}
$$

哈密顿量可以写为

$$
\begin{aligned}
\hat{H} &= \frac{1}{2}(\hat{p}^2 + \omega^2\hat{x}^2 + \omega) + \frac{\Omega}{2}\hat{\sigma}_x + \sqrt{2\omega}g\hat{x}\hat{\sigma}_z \\
\hat{H}_r &= \frac{\hat{H}}{\Omega/2} = \frac{1}{\Omega}(\hat{p}^2 + \omega^2\hat{x}^2 + \omega) + \hat{\sigma}_x + 2\frac{\sqrt{2\omega}}{\Omega}g\hat{x}\hat{\sigma}_z
\end{aligned}
\tag{18}
$$

令 $y^2 \equiv \frac{\omega^2}{\Omega}\hat{x}^2$，Eq. 18 可以写为

$$
\begin{aligned}
\hat{H}_r &= \frac{\hat{p}^2}{\Omega} + y^2 + \frac{\omega}{\Omega} + \hat{\sigma}_x + 2\frac{\sqrt{2\omega}}{\Omega}g\frac{\sqrt{\Omega}}{\omega}y\hat{\sigma}_z \\
&= -\frac{1}{\Omega}\frac{\partial^2}{\partial x^2} + y^2 + \frac{\omega}{\Omega} + \hat{\sigma}_x + 2g\sqrt{\frac{2}{\omega\Omega}}y\hat{\sigma}_z \\
&= -\frac{\omega^2}{\Omega^2}\frac{\partial^2}{\partial y^2} + y^2 + \frac{\omega}{\Omega} + \hat{\sigma}_x + 2g\sqrt{\frac{2}{\omega\Omega}}y\hat{\sigma}_z
\end{aligned}
\tag{19}
$$

令 $\eta \equiv \frac{\Omega}{\omega}$和 $R \equiv \frac{2g}{\sqrt{\omega\Omega}}$，则有

$$
\hat{H}_r = -\frac{1}{\eta}\frac{\partial^2}{\partial y^2} + y^2 + \frac{1}{\eta} + \hat{\sigma}_x + \sqrt{2}Ry\hat{\sigma}_z \tag{20}
$$

当 $\eta \to \infty$ 时，哈密顿量可以写为

$$
\begin{aligned}
\hat{H}_r(y) &= \lim_{\eta\to\infty}\hat{H}_r = y^2 + \hat{\sigma}_x + \sqrt{2}Ry\hat{\sigma}_z \\
&= \begin{pmatrix} y^2 + \sqrt{2}Ry & 1 \\ 1 & y^2 - \sqrt{2}Ry \end{pmatrix}
\end{aligned}
\tag{21}
$$

哈密顿量的本征值为

$$
E_\pm = y^2 \pm \sqrt{1 + 2R^2y^2} \tag{22}
$$

函数性质可知，$E_$对应的基态位置，当 $R \le 1$ 时，基态在 $y = 0$ 处，当 $R > 1$ 时，基态在

$$
y = \pm\frac{\sqrt{R^4 - 1}}{\sqrt{2}R} \tag{23}
$$

处

首先分析 $R \le 1$ 的情况，此时哈密顿量写为

$$
\hat{H}_r = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{24}
$$

对应的本征值和本征波函数为

$$
\begin{aligned}
&\lambda_{\pm} = \pm 1 \\
&\psi_{\pm} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)
\end{aligned} \tag{25}
$$

显然基态(环境)的本征值和本征波函数对应为

$$
\begin{aligned}
&\lambda_{-} = -1 \\
&\psi_{-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)
\end{aligned} \tag{26}
$$

基态的波函数可以写为

$$
\begin{aligned}
|G\rangle &= \sum_{\tau}\sum_{i} a_{\tau i}|\psi_{\tau}^{A}\rangle|\psi_{i}^{B}\rangle = \sum_{i}\left(a_{-i}|-\rangle|\psi_{i}^{B}\rangle + a_{+i}|+\rangle|\psi_{i}^{B}\rangle\right) \\
&= \psi(0)\left(a_{-0}|-\rangle + a_{+0}|+\rangle\right) \\
&= \psi(0)\left(-\frac{1}{\sqrt{2}}|-\rangle + \frac{1}{\sqrt{2}}|+\rangle\right) \\
&= \frac{\psi(0)}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}
\end{aligned} \tag{27}
$$

其中 $\psi(0)$ 是系统的基态波函数。

根据 Eq. 13 可以得到量子本征微观态的关联矩阵为

$$
C^{Q}_{\tau\tau'} = \sum_{i} a^{*}_{\tau i} a_{\tau' i} = a_{\tau 0} a_{\tau' 0} \tag{28}
$$

写成矩阵形式为

$$
\begin{aligned}
C^{Q} &= \begin{pmatrix} a_{-0}^{2} & a_{-0}a_{+0} \\ a_{+0}a_{-0} & a_{+0}^{2} \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}
\end{aligned} \tag{29}
$$

对应的量子本征态为

$$
\begin{aligned}
&|\pm\rangle_{x} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \\
&\Rightarrow V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = (v_{+} \;\; v_{-})
\end{aligned} \tag{30}
$$

与相应的本征值

$$
\lambda_{-} = 1, \lambda_{+} = 0 \tag{31}
$$

可能的量子本征微观态为

$$\begin{aligned}E_k &= \sum_{\tau=0}^{M} V_{\tau k} \sum_{i=0}^{N} a_{\tau i} |\psi_i^B\rangle \\ &= \sum_{\tau=0}^{M} V_{\tau k} a_{\tau 0} \psi(0) \\ &= \psi(0)(V_{-k} a_{-0} + V_{+k} a_{+0}) \\ &= \psi(0) \frac{V_{+k} - V_{-k}}{\sqrt{2}} \\ \Rightarrow E_{\pm} &= \psi(0) \frac{V_{+\pm} - V_{-\pm}}{\sqrt{2}} = \psi(0) \frac{1 \mp 1}{\sqrt{2}}\end{aligned} \tag{32}$$

当 $R > 1$ 时，哈密顿量写为

$$\hat{H}_r(y_{\pm}) = \frac{1}{2}(R^2 - R^{-2}) + \begin{pmatrix} \pm\sqrt{R^4-1} & 1 \\ 1 & \mp\sqrt{R^4-1} \end{pmatrix} \tag{33}$$

对应的本征值为

$$\begin{aligned}\left(\lambda \mp \sqrt{R^4-1}\right)\left(\lambda \pm \sqrt{R^4-1}\right) - 1 = 0 \\ \lambda^2 - (R^4 - 1) - 1 = 0 \\ \lambda^2 - R^4 = 0 \\ \Rightarrow \lambda_{\pm} = \pm R^2\end{aligned} \tag{34}$$

基态能对应本征值为 $\lambda_{\_} = -R^2$.

考虑基态对应的本征波函数，首先考虑 y_+，有

$$\hat{H}_r(y_+) = \frac{1}{2}(R^2 - R^{-2}) + \begin{pmatrix} \sqrt{R^4-1} & 1 \\ 1 & -\sqrt{R^4-1} \end{pmatrix} \tag{35}$$

设 $y_{\pm}$对应的本征态为

$$|\pm\rangle^{(y)} = \begin{pmatrix} \pm\alpha \\ \pm\beta \end{pmatrix} \tag{36}$$

则有

$$\begin{pmatrix} \pm\sqrt{R^4-1} & 1 \\ 1 & \mp\sqrt{R^4-1} \end{pmatrix} \begin{pmatrix} \pm\alpha \\ \pm\beta \end{pmatrix} = -R^2 \begin{pmatrix} \alpha_{\pm} \\ \beta_{\pm} \end{pmatrix} \tag{37}$$

为 y_+，有

$$
\begin{gathered}
\begin{cases}
\sqrt{R^4-1}\alpha_+ + \beta_+ = -R^2\alpha_+ \\
\alpha_+ - \sqrt{R^4-1}\beta_+ = -R^2\beta_+
\end{cases} \\
\Rightarrow \\
\begin{cases}
(R^4-1)\alpha_+ + \sqrt{R^4-1}\beta_+ = -R^2\sqrt{R^4-1}\alpha_+ \\
\alpha_+ - \sqrt{R^4-1}\beta_+ = -R^2\beta_+
\end{cases} \\
\Rightarrow \\
R^4\alpha_+ = -R^2\sqrt{R^4-1}\alpha_+ - R^2\beta_+ \\
\Rightarrow \\
\left(R^2+\sqrt{R^4-1}\right)\alpha_+ = -\beta_+ \\
\Rightarrow \\
\beta_+ = -\left(R^2+\sqrt{R^4-1}\right)\alpha_+
\end{gathered}
\tag{38}
$$

为 y_-，有

$$
\begin{gathered}
\begin{cases}
-\sqrt{R^4-1}\alpha_- + \beta_- = -R^2\alpha_- \\
\alpha_- + \sqrt{R^4-1}\beta_- = -R^2\beta_-
\end{cases} \\
\Rightarrow \\
\begin{cases}
(R^4-1)\alpha_- - \sqrt{R^4-1}\beta_- = R^2\sqrt{R^4-1}\alpha_- \\
\alpha_- + \sqrt{R^4-1}\beta_- = -R^2\beta_-
\end{cases} \\
\Rightarrow \\
R^4\alpha_- = R^2\sqrt{R^4-1}\alpha_- - R^2\beta_- \\
\Rightarrow \\
\left(R^2-\sqrt{R^4-1}\right)\alpha_- = -\beta_- \\
\Rightarrow \\
\beta_- = -\left(R^2-\sqrt{R^4-1}\right)\alpha_-
\end{gathered}
\tag{39}
$$

所以

$$
\beta_\pm = -\left(R^2 \pm \sqrt{R^4-1}\right)\alpha_\pm \tag{40}
$$

同时，为了满足归一化条件$\alpha_\pm^2+\beta_\pm^2=1$，有

$$
\begin{aligned}
(\alpha_\pm)^2 + (\beta_\pm)^2 &= 1 \\
\alpha_\pm^2 + \left(\left(R^2 - \sqrt{R^4-1}\right)\alpha_\pm\right)^2 &= 1 \\
\alpha_\pm^2 + \left(R^4 \pm 2R^2\sqrt{R^4-1} + R^4 - 1\right)\alpha_\pm^2 &= 1 \\
\left(2R^4 \pm 2R^2\sqrt{R^4-1}\right)\alpha_\pm^2 &= 1 \\
\alpha_\pm^2 &= \frac{1}{2R^4 \pm 2R^2\sqrt{R^4-1}} \\
&\Rightarrow \\
\beta_\pm^2 &= \frac{R^2 \pm \sqrt{R^4-1}}{2R^2} \\
&\Rightarrow \\
\begin{pmatrix}\alpha_\pm \\ \beta_\pm\end{pmatrix} &= \begin{pmatrix}\frac{1}{\sqrt{2}R\sqrt{R^2\pm\sqrt{R^4-1}}} \\ -\frac{\sqrt{R^2\pm\sqrt{R^4-1}}}{\sqrt{2}R}\end{pmatrix}
\end{aligned}
\tag{41}
$$

因此，基态波函数为

$$
\begin{aligned}
|G\rangle &= \sum_\tau \sum_i a_{\tau i}|\psi_\tau^A\rangle|\psi_i^B\rangle = \sum_i \left(a_{-i}|-\rangle|\psi_i^B\rangle + a_{+i}|+\rangle|\psi_i^B\rangle\right) \\
&= a_{-y_-}|-\rangle|y_-\rangle + a_{-y_+}|-\rangle|y_+\rangle + a_{+y_-}|+\rangle|y_-\rangle + a_{+y_+}|+\rangle|y_+\rangle \\
&= \frac{\psi(y-y_+)}{\sqrt{2}}\begin{pmatrix}\alpha_+ \\ \beta_+\end{pmatrix} + \frac{\psi(y-y_-)}{\sqrt{2}}\begin{pmatrix}\alpha_- \\ \beta_-\end{pmatrix}
\end{aligned}
\tag{42}
$$

其中 $\psi(y-y_+)$ 和 $\psi(y-y_-)$ 是系统的基态局域波函数，且$a_{-y_-} = \frac{1}{\sqrt{2}}\beta_-, a_{-y_+} = \frac{1}{\sqrt{2}}\beta_+, a_{+y_-} = \frac{1}{\sqrt{2}}\alpha_-, a_{+y_+} = \frac{1}{\sqrt{2}}\alpha_+$。

Eq. 42 可以得到量子本征微观态的关联矩阵为

$$
C_{\tau\tau'}^Q = \sum_i a_{\tau i}^* a_{\tau' i} = a_{\tau y_-}a_{\tau' y_-} + a_{\tau y_+}a_{\tau' y_+}
\tag{43}
$$

写成矩阵形式为

$$
\begin{aligned}
C^Q &= \begin{pmatrix} a_{-y_-}^2 + a_{-y_+}^2 & a_{-y_-}a_{+y_-} + a_{-y_+}a_{+y_+} \\ a_{-y_-}a_{+y_-} + a_{-y_+}a_{+y_+} & a_{+y_-}^2 + a_{+y_+}^2 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} \alpha_-^2 + \beta_-^2 & \alpha_-\beta_- + \alpha_+\beta_+ \\ \alpha_-\beta_- + \alpha_+\beta_+ & \alpha_+^2 + \beta_+^2 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & -\frac{1}{R^2} \\ -\frac{1}{R^2} & 1 \end{pmatrix}
\end{aligned}
\tag{44}
$$

对应的本征值

$$
\lambda_\pm = \frac{1}{2}\left(1 \pm \frac{1}{R^2}\right)
\tag{45}
$$

和本征态为

$$
\begin{aligned}
v_\pm &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm 1\end{pmatrix}\\
\Rightarrow V &= \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = \begin{pmatrix}v_+ & v_-\end{pmatrix}
\end{aligned}
\tag{46}
$$

可能的量子本征微观态为

$$
\begin{aligned}
E_k &= \sum_{\tau=0}^{M} V_{\tau k}\sum_{i=0}^{N} a_{\tau i}\left|\psi_i^B\right\rangle\\
&= \sum_{\tau=0}^{M}\left(V_{\tau k}a_{\tau y_-}\psi(y-y_-) + V_{\tau k}a_{\tau y_+}\psi(y-y_+)\right)\\
&= V_{-k}a_{-y_-}\psi(y-y_-) + V_{-k}a_{-y_+}\psi(y-y_+) + V_{+k}a_{+y_-}\psi(y-y_-) + V_{+k}a_{+y_+}\psi(y-y_+)\\
\Rightarrow E_\pm &= \frac{1}{2}\left(\alpha_-\psi(y-y_-) + \alpha_+\psi(y-y_+) \pm \beta_-\psi(y-y_-) \pm \beta_+\psi(y-y_+)\right)
\end{aligned}
\tag{47}
$$

Section 3: Quantum Phase Transition and Universal Dynamics in the Rabi

3.1 SECTION A : LOW-ENERGY EFFECTIVE HAMILTONIANS

3.1.a Schrieffer-Wolff (SW) transformation

推导基于文献[1, p.201~204]，一个哈密顿量 H 可以分为两部分 $H = H_0 + H'$，其中 H_0 是我们感兴趣的部分，H' 是扰动。

我们考虑一个幺正变换$U = e^S$，其中生成元S应该是反厄密$S^\dagger = -S$的。变换后的哈密顿量可以写为

$$H' = U^\dagger H U = H + [H, S] + \frac{1}{2!}[[H, S], S] + \dots \tag{48}$$

做幺正变换的目的是让哈密顿量对角化，即

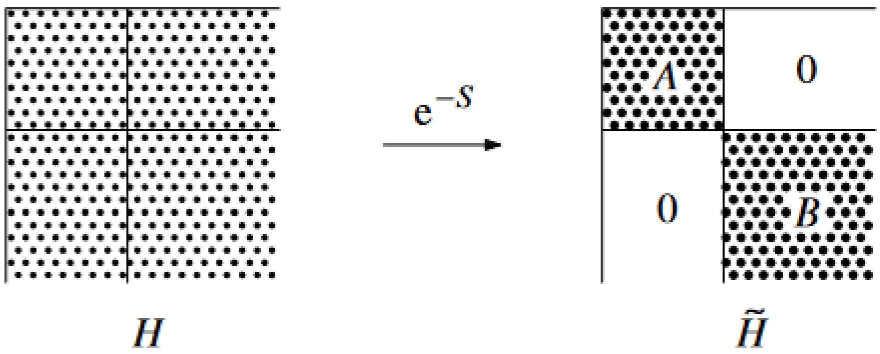

Fig. B.1. Removal of off-diagonal elements of H

而原始哈密顿量可以分为三个部分，分别是对角线部分H_0，块对角部分H_1和反对称部分H_2。

$$H = H_0 + H_1 + H_2 \tag{49}$$

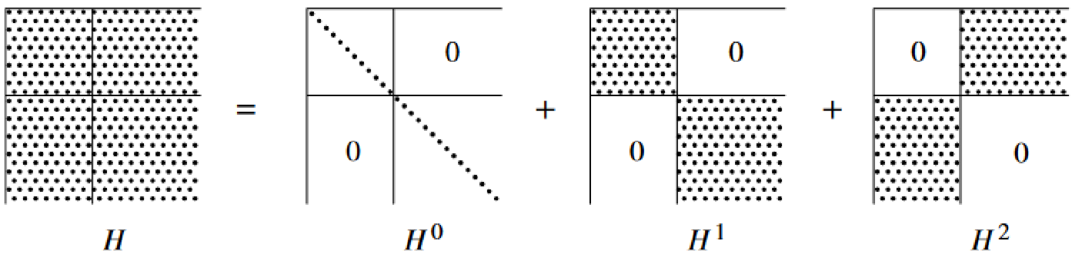

Fig. B.2. Representation of H as $H^0 + H^1 + H^2$

因为 S 必须是非块对角的，像 H^2 一样，所以 H 的块对角部分 $\tilde{H}_d$ 包含了 $[H^0 + H^1, S]^{(j)}$ 奇数项 和 $[H^2, S]^{(j)}$ 的偶数项

$$\tilde{H}_d = \sum_{j=0}^{\infty} \frac{1}{(2j)!}[H^0 + H^1, S]^{(2j)} + \sum_{j=0}^{\infty} \frac{1}{(2j+1)!}[H^2, S]^{(2j+1)} \tag{50}$$

同理，H 的非块对角部分 $\tilde{H}_n$ 包含了 $[H^0 + H^1, S]^{(j)}$ 偶数项 和 $[H^2, S]^{(j)}$ 的奇数项

$$\tilde{H}_n = \sum_{j=0}^{\infty} \frac{1}{(2j+1)!} [H^0 + H^1, S]^{(2j+1)} + \sum_{j=0}^{\infty} \frac{1}{(2j)!} [H^2, S]^{(2j)} \tag{51}$$

由于我们的目的是让 H 对角化，所以非对角部分 $\tilde{H}_n$ 必须为零，即

$$\begin{gathered} \tilde{H}_n = 0 \\ \Rightarrow \sum_{j=0}^{\infty} \frac{1}{(2j+1)!} [H^0 + H^1, S]^{(2j+1)} + \sum_{j=0}^{\infty} \frac{1}{(2j)!} [H^2, S]^{(2j)} = 0 \end{gathered} \tag{52}$$

将 S 展开为 $S = S^{(1)} + S^{(2)} + \ldots$，我们可以逐次逼近$S^{(j)}$到$S$：

为了对应阶数,，同时方便计算，我们重新将哈密顿量写为

$$H = H_0 - \lambda V \tag{53}$$

其中 λ 是一个小量, H^0 是低阶对角的哈密顿量，V 是非对角的哈密顿量。

而 S 也可以写为

$$S = \lambda S^{(1)} + \lambda^2 S^{(2)} + \ldots \tag{54}$$

根据 Eq. 52，我们可以得到

$$[H_0, S] + \lambda V - \frac{1}{2} \lambda [[V, S], S] + \cdots = 0 \tag{55}$$

将 λ 展开到 1 阶

$$\left[H_0, S^{(1)}\right] = V \tag{56}$$

将 λ 展开到 2 阶

$$\left[H_0, S^{(2)}\right] = 0 \tag{57}$$

将 λ 展开到 3 阶

$$\begin{gathered} \left[H_0, S^{(3)}\right] - \frac{1}{2} \left[\left[V, S^{(1)}\right], S^{(1)}\right] + \frac{1}{3!} \left[\left[\left[H_0, S^{(1)}\right], S^{(1)}\right], S^{(1)}\right] = 0 \\ \Rightarrow \left[H_0, S^{(3)}\right] = \frac{1}{3} \left[\left[V, S^{(1)}\right], S^{(1)}\right] \end{gathered} \tag{58}$$

3.1.b 求解 S 的矩阵元

对于 S 的矩阵元 S_{ij}，我们可以通过逐次求解的方式得到。首先我们可以得到 S_{ij} 的一阶解

$$\begin{aligned} \langle i | \left[H_0, S^{(1)}\right] | j \rangle &= \langle i | V | j \rangle \\ \langle i | H_0 S^{(1)} | j \rangle - \langle i | S^{(1)} H_0 | j \rangle &= V_{ij} \\ E_i \langle i | S^{(1)} | j \rangle - E_j \langle i | S^{(1)} | j \rangle &= V_{ij} \\ S_{ij}^{(1)} &= \frac{V_{ij}}{E_i - E_j} \end{aligned} \tag{59}$$

然后我们可以得到 S_{ij} 的三阶解

$$
\begin{aligned}
\langle i|[H_0,S^{(3)}]|j\rangle &= \frac{1}{3}\left[\left[V,S^{(1)}\right],S^{(1)}\right]_{ij} \\
\langle i|H_0S^{(3)}|j\rangle - \langle i|S^{(3)}H_0|j\rangle &= \frac{1}{3}\left[\left[V,S^{(1)}\right],S^{(1)}\right]_{ij} \\
E_i\langle i|S^{(3)}|j\rangle - E_j\langle i|S^{(3)}|j\rangle &= \frac{1}{3}\left[\left[V,S^{(1)}\right],S^{(1)}\right]_{ij} \\
S^{(3)}_{ij} &= \frac{1}{3}\frac{\left[\left[V,S^{(1)}\right],S^{(1)}\right]_{ij}}{E_i-E_j}
\end{aligned}
\tag{60}
$$

以此类推，我们可以得到 S_{ij} 的所有阶数的解。

3.1.c 计算 Rabi 模型的 $S^{(1)}$

对于 Rabi 模型，哈密顿量写为

$$
H = \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + g\left(\hat{a}^\dagger+\hat{a}\right)\hat{\sigma}_z \tag{61}
$$

计算前四个能级
$|-,0\rangle, |+,0\rangle, |-,1\rangle, |+,1\rangle$，可以得到 $H_0=\omega\hat{a}^\dagger\hat{a}+\frac{\Omega}{2}\hat{\sigma}_x$ 的矩阵形式为

$$
H_0 = \begin{pmatrix} -\frac{\Omega}{2} & 0 & 0 & 0 \\ 0 & \frac{\Omega}{2} & 0 & 0 \\ 0 & 0 & \omega-\frac{\Omega}{2} & 0 \\ 0 & 0 & 0 & \omega+\frac{\Omega}{2} \end{pmatrix} \tag{62}
$$

非对角部分 $gV=g\left(\hat{a}^\dagger+\hat{a}\right)\hat{\sigma}_z$ 的矩阵形式为

$$
V = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{63}
$$

因此 $S^{(1)}$ 的矩阵形式为

$$
\begin{aligned}
S^{(1)}_{ij} &= \frac{V_{ij}}{E_i-E_j} \\
&= \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{\omega+\Omega} \\ 0 & 0 & \frac{1}{\Omega-\omega} & 0 \\ 0 & \frac{1}{\omega-\Omega} & 0 & 0 \\ \frac{1}{\omega+\Omega} & 0 & 0 & 0 \end{pmatrix}
\end{aligned}
\tag{64}
$$

3.1.d A systematic method for Schrieffer-Wolff transformation and its generalizations

上文 SW 变换推导过于繁琐，经过查阅文献发现更加通用（但合理性待定）的方法，来自文献[2].

SW 变换是一种幺正变换。因此，人们选择适当的幺正算子，它既可以使哈密顿完全对角化，又可以使哈密顿达到某种期望的阶。通常这种变换的一个要求是将非对角项消去到一阶，从而满足下面的条件。

$$[S, H_0] = -H_v \tag{65}$$

其中H_0是哈密顿量的对角部分，H_v是哈密顿量的非对角部分，S是反厄米算子。那么 SW 变换可以写成

$$\begin{aligned} H' &= e^S H e^{-S} \\ &= H_0 + H_v + [S, H_0] + [S, H_v] + \frac{1}{2!}[S, [S, H_0]] + \frac{1}{2!}[S, [S, H_v]] + \cdots \\ &= H_0 + H_v - H_v + [S, H_v] + \frac{1}{2!}[S, -H_v] + \frac{1}{2!}[S, [S, H_v]] + \cdots \\ &= H_0 + \frac{1}{2}[S, H_v] + \frac{1}{3}[S, [S, H_v]] + \cdots \end{aligned} \tag{66}$$

因此对角化的有效哈密顿量可以写成

$$H_{\text{eff}} = H_0 + \frac{1}{2}[S, H_v] \tag{67}$$

进行 SW 变换最关键的步骤就是获得S，但是如上文所述，S的求解只能通过微扰的方式逐次求解，这样的方法在求解高阶的S时会变得非常复杂。因此，文献[2]提出了一种更加通用的方法。

1. 首先，我们可以获取对角线哈密顿量H_0和非对角线哈密顿量H_v的对易子 η

$$\eta = [H_0, H_v] \tag{68}$$

2. 在第二步中，我们将在η上施加去掉非对角部分直到一阶的条件。要做到这一点，我们将不得不保持待定系数，它们将由上面的条件决定。
3. 最后计算η满足关系 $[\eta, H_0] = -H_v$，确定η的系数，就可以得到S。

以上方法的优势在于，它可以直接得到S，而不需要逐次求解。

3.1.d.i JC 模型

以 JC 模型为例，其哈密顿量写为

$$H = \omega \hat{a}^\dagger \hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + g\left(\hat{a}^\dagger \hat{\sigma}_- + \hat{a}\hat{\sigma}_+\right) \tag{69}$$

对角部分H_0为

$$H_0 = \omega \hat{a}^\dagger \hat{a} + \frac{\Omega}{2}\hat{\sigma}_x \tag{70}$$

非对角部分H_v为

$$H_v = g\left(\hat{a}^\dagger \hat{\sigma}_- + \hat{a}\hat{\sigma}_+\right) \tag{71}$$

则对易子η为

$$
\begin{aligned}
\eta = [H_0, H_v] &= \left[\omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x, g\big(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\big)\right] \\
&= g\left[\omega\big[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\big] + \frac{\Omega}{2}\big[\hat{\sigma}_x, \hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\big]\right] \\
&= g\big[\omega\big(\hat{a}^\dagger\hat{\sigma}_- - \hat{a}\hat{\sigma}_+\big) + \Omega\big[\hat{a}^\dagger\hat{\sigma}_- - \hat{a}\hat{\sigma}_+\big]\big] \\
&= g\big[(\omega+\Omega)\hat{a}^\dagger\hat{\sigma}_- - (\omega+\Omega)\hat{a}\hat{\sigma}_+\big]
\end{aligned} \tag{72}
$$

其中用到对易关系有 $\big[\hat{a}^\dagger\hat{a}, \hat{a}^\dagger\big] = \hat{a}^\dagger$, $\big[\hat{a}^\dagger\hat{a}, \hat{a}\big] = -\hat{a}$, $[\hat{\sigma}_x, \hat{\sigma}_+] = -2\hat{\sigma}_+$, $[\hat{\sigma}_x, \hat{\sigma}_-] = 2\hat{\sigma}_-$.

待定η的系数为

$$
\eta = A\hat{a}^\dagger\hat{\sigma}_- + B\hat{a}\hat{\sigma}_+ \tag{73}
$$

它满足关系$[\eta, H_0] = -H_v$，即

$$
\begin{gathered}
[\eta, H_0] = -H_v \\
\Rightarrow \left[A\hat{a}^\dagger\hat{\sigma}_- + B\hat{a}\hat{\sigma}_+, \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x\right] = -g\big(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\big) \\
\Rightarrow A\omega\big[\hat{a}^\dagger\hat{\sigma}_-, \hat{a}^\dagger\hat{a}\big] + B\omega\big[\hat{a}\hat{\sigma}_+, \hat{a}^\dagger\hat{a}\big] + \frac{A\Omega}{2}\big[\hat{a}^\dagger\hat{\sigma}_-, \hat{\sigma}_x\big] + \frac{B\Omega}{2}\big[\hat{a}\hat{\sigma}_+, \hat{\sigma}_x\big] = -g\big(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\big) \\
\Rightarrow A\omega\big(-\hat{a}^\dagger\hat{\sigma}_-\big) + B\omega\big(\hat{a}\hat{\sigma}_+\big) - A\Omega\hat{a}^\dagger\hat{\sigma}_- + B\Omega\hat{a}\hat{\sigma}_+ = -g\big(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\big) \\
\Rightarrow \begin{cases} A(\omega+\Omega) = g \\ B(\omega+\Omega) = -g \end{cases}
\end{gathered} \tag{74}
$$

得到

$$
A = -B = \frac{g}{\omega+\Omega} \tag{75}
$$

则 S 为

$$
S = \frac{g}{\omega+\Omega}\big(\hat{a}^\dagger\hat{\sigma}_- - \hat{a}\hat{\sigma}_+\big) \tag{76}
$$

根据 Eq. 67，可以得到低能有效哈密顿量为

$$
\begin{aligned}
H_{\text{eff}} &= H_0 + \frac{1}{2}[S, H_v] \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{1}{2}\left[\frac{g}{\omega+\Omega}\left(\hat{a}^\dagger\hat{\sigma}_- - \hat{a}\hat{\sigma}_+\right), g\left(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\right)\right] \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{1}{2}\frac{g^2}{\omega+\Omega}\left[\hat{a}^\dagger\hat{\sigma}_- - \hat{a}\hat{\sigma}_+, \hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+\right] \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{1}{2}\frac{g^2}{\omega+\Omega}\left[\hat{a}^\dagger\hat{\sigma}_-, \hat{a}\hat{\sigma}_+\right] - \frac{1}{2}\frac{g^2}{\omega+\Omega}\left[\hat{a}\hat{\sigma}_+, \hat{a}^\dagger\hat{\sigma}_-\right] \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{g^2}{\omega+\Omega}\left[\hat{a}^\dagger\hat{\sigma}_-, \hat{a}\hat{\sigma}_+\right] \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{g^2}{\omega+\Omega}\left(\hat{a}^\dagger\hat{\sigma}_-\hat{a}\hat{\sigma}_+ - \hat{a}\hat{\sigma}_+\hat{a}^\dagger\hat{\sigma}_-\right) \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{g^2}{\omega+\Omega}\left(\hat{a}^\dagger\hat{a}\hat{\sigma}_-\hat{\sigma}_+ - \hat{a}\hat{a}^\dagger\hat{\sigma}_+\hat{\sigma}_-\right) \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{g^2}{\omega+\Omega}\left(\hat{a}^\dagger\hat{a}\hat{\sigma}_-\hat{\sigma}_+ - \left(1+\hat{a}^\dagger\hat{a}\right)\hat{\sigma}_+\hat{\sigma}_-\right) \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{g^2}{\omega+\Omega}\left(\hat{a}^\dagger\hat{a}[\hat{\sigma}_-, \hat{\sigma}_+] - \hat{\sigma}_+\hat{\sigma}_-\right) \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{g^2}{\omega+\Omega}\left(\hat{a}^\dagger\hat{a}\hat{\sigma}_x + \frac{\hat{\sigma}_x}{2} - \frac{1}{2}\right)
\end{aligned}
\tag{77}
$$

可以看到有效哈密顿量已经被对角化。

3.1.d.ii Rabi 模型

对于 Rabi 模型，哈密顿量写为

$$
H = \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + g\hat{\sigma}_z\left(\hat{a}^\dagger + \hat{a}\right) \tag{78}
$$

对角部分H_0为

$$
H_0 = \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x \tag{79}
$$

非对角部分H_v为

$$
H_v = g\hat{\sigma}_z\left(\hat{a}^\dagger + \hat{a}\right) \tag{80}
$$

则对易子η为

$$
\begin{aligned}
\eta = [H_0, H_v] &= \left[\omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x, g\hat{\sigma}_z\left(\hat{a}^\dagger + \hat{a}\right)\right] \\
&= g\omega\hat{\sigma}_z\left[\hat{a}^\dagger\hat{a}, \left(\hat{a}^\dagger + \hat{a}\right)\right] + g\frac{\Omega}{2}\left(\hat{a}^\dagger + \hat{a}\right)[\hat{\sigma}_x, \hat{\sigma}_z] \\
&= g\omega\hat{\sigma}_z\left(\hat{a}^\dagger - \hat{a}\right) - ig\Omega\left(\hat{a}^\dagger + \hat{a}\right)\hat{\sigma}_y
\end{aligned}
\tag{81}
$$

待定η的系数为

$$
\eta = A\hat{\sigma}_z\hat{a}^\dagger + B\hat{\sigma}_z\hat{a} + C\hat{a}^\dagger\hat{\sigma}_y + D\hat{a}\hat{\sigma}_y \tag{82}
$$

它满足关系$[\eta, H_0] = -H_v$，即

$$
\begin{aligned}
&[\eta, H_0] = -H_v \\
\Rightarrow &\left[A\hat{\sigma}_z\hat{a}^\dagger + B\hat{\sigma}_z\hat{a} + C\hat{a}^\dagger\hat{\sigma}_y + D\hat{a}\hat{\sigma}_y, \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x\right] = -g\hat{\sigma}_z(\hat{a}^\dagger + \hat{a}) \\
&\omega(A\hat{\sigma}_z\hat{a}^\dagger - B\hat{\sigma}_z\hat{a} + C\hat{a}^\dagger\hat{\sigma}_y - D\hat{a}\hat{\sigma}_y) \\
&+\frac{\Omega}{2}(A(2i\hat{\sigma}_y)\hat{a}^\dagger + B(2i\hat{\sigma}_y)\hat{a} + C\hat{a}^\dagger(-2i\hat{\sigma}_z) + D\hat{a}(-2i\hat{\sigma}_z)) \\
&= -g\hat{\sigma}_z(\hat{a}^\dagger + \hat{a}) \\
&\omega(A\hat{\sigma}_z\hat{a}^\dagger - B\hat{\sigma}_z\hat{a} + C\hat{a}^\dagger\hat{\sigma}_y - D\hat{a}\hat{\sigma}_y) \\
&+i\Omega(A\hat{\sigma}_y\hat{a}^\dagger + B\hat{\sigma}_y\hat{a} - C\hat{a}^\dagger\hat{\sigma}_z - D\hat{a}\hat{\sigma}_z) \\
&= -g\hat{\sigma}_z(\hat{a}^\dagger + \hat{a})
\end{aligned}
\tag{83}
$$

合并同类项，得到

$$
\begin{aligned}
(\omega A - i\Omega C)\hat{a}^\dagger\hat{\sigma}_z &= -g\hat{a}^\dagger\hat{\sigma}_z \\
(-\omega B - i\Omega D)\hat{a}\hat{\sigma}_z &= -g\hat{a}\hat{\sigma}_z \\
(\omega C + i\Omega A)\hat{a}^\dagger\hat{\sigma}_y &= 0 \\
(-\omega D + i\Omega B)\hat{a}\hat{\sigma}_y &= 0
\end{aligned}
\tag{84}
$$

后两式推导得到

$$
\begin{aligned}
C &= -i\Omega\frac{A}{\omega} \\
D &= i\Omega\frac{B}{\omega}
\end{aligned}
\tag{85}
$$

代入前两式得到

$$
\begin{aligned}
\omega A - \Omega^2\frac{A}{\omega} &= -g \\
-\omega B + \Omega^2\frac{B}{\omega} &= -g \\
\Rightarrow A = -B &= \frac{g\omega}{\Omega^2 - \omega^2}
\end{aligned}
\tag{86}
$$

则 S 为

$$
\begin{aligned}
S &= A\hat{\sigma}_z\hat{a}^\dagger + B\hat{\sigma}_z\hat{a} + C\hat{a}^\dagger\hat{\sigma}_y + D\hat{a}\hat{\sigma}_y \\
&= \frac{g\omega}{\Omega^2 - \omega^2}(\hat{a}^\dagger - \hat{a})\hat{\sigma}_z - i\frac{g\Omega}{\Omega^2 - \omega^2}(\hat{a}^\dagger + \hat{a})\hat{\sigma}_y
\end{aligned}
\tag{87}
$$

根据 Eq. 87，可以得到低能有效哈密顿量为

$$
\begin{aligned}
H_{\text{eff}} &= H_0 + \frac{1}{2}[S, H_v] \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x + \frac{1}{2}\left[\frac{g\omega}{\Omega^2 - \omega^2}(\hat{a}^\dagger - \hat{a})\hat{\sigma}_z - i\frac{g\Omega}{\Omega^2 - \omega^2}(\hat{a}^\dagger + \hat{a})\hat{\sigma}_y, g\hat{\sigma}_z(\hat{a}^\dagger + \hat{a})\right] \\
&= \omega\hat{a}^\dagger\hat{a} + \frac{\Omega}{2}\hat{\sigma}_x - \frac{g^2\omega}{\Omega^2 - \omega^2} + \frac{g^2\Omega}{\Omega^2 - \omega^2}(\hat{a}^\dagger + \hat{a})^2\hat{\sigma}_x
\end{aligned}
\tag{88}
$$

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