量子マスター方程式の導出

中嶋 慧

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1.1　von Neumann 方程式

注目系のハミルトニアンを H_S, 熱浴のハミルトニアン H_B, 相互作用を H_1 とし、

$$H(t) \;=\; H_0 + H_1(t),\; H_0 = H_S + H_B \tag{1.1}$$

とする。全系の密度演算子 $\rho(t)$ を、計数場 χ を使って一般化したもの $\rho(\chi, t)$ は、変形された von Neumann 方程式

$$\frac{d}{dt}\rho(\chi,t) \;=\; -i\big[H_\chi(t)\rho(\chi,t) - \rho(\chi,t)H_{-\chi}(t)\big], \tag{1.2}$$

$$H_{a,\chi}(t) \overset{\text{def}}{=} e^{i\chi A/2}H_a(t)e^{-i\chi A/2} \quad (a = 0, 1, S, B, \text{無印}) \tag{1.3}$$

を満たし、初期条件は、

$$\rho(\chi, 0) \;=\; \sum_n P_n\rho(0)P_n \tag{1.4}$$

である。A は熱浴の物理量であり、P_n は A の固有値 a_n の空間への射影演算子である：

$$AP_n = a_nP_n,\; P_n^2 = P_n,\; P_n^\dagger = P_n. \tag{1.5}$$

$\mathrm{Tr}\rho(\chi, \tau)$ は、時刻 $t = \tau$ と $t = 0$ における A の測定値の差についての母関数である。もしも、$\rho(\chi, 0) = \rho(0)$ なら (これは多くの場合満たされる)、$\chi = 0$ で $\rho(\chi, t)$ は全系の密度演算子となる:

$$\rho(0, t) \;=\; \rho(t). \tag{1.6}$$

1.2　相互作用描像

超演算子

$$\hat{H}_a\bullet \overset{\text{def}}{=} H_{a,\chi}(t)\bullet - \bullet H_{a,-\chi}(t) \quad (a = 0, 1, S, B, \text{無印}) \tag{1.7}$$

を導入する ($\hat{H}_S\bullet = [H_S, \bullet]$ である)。(1.2) の解は、

$$\rho(\chi, t) \;=\; \hat{V}(t)\rho(\chi, 0), \tag{1.8}$$

$$\frac{d}{dt}\hat{V}(t) \;=\; -i\hat{H}(t)\hat{V}(t), \quad \hat{V}(0) = 1 \tag{1.9}$$

である。今、$\hat{U}(t)$ を、

$$\hat{V}(t) \;=\; e^{-i\hat{H}_0t}\hat{U}(t) \tag{1.10}$$

で定義する。これと (1.8) より、

$$\rho(\chi, t) \;=\; e^{-i\hat{H}_0t}\rho^I(\chi, t), \tag{1.11}$$

$$\rho^I(\chi, t) \overset{\text{def}}{=} \hat{U}(t)\rho(\chi, 0) \tag{1.12}$$

となる。(1.10) を微分して、

$$-i\hat{H}e^{-i\hat{H}_0t}\hat{U}(t) = -i\hat{H}_0e^{-i\hat{H}_0t}\hat{U}(t) + e^{-i\hat{H}_0t}\frac{d\hat{U}(t)}{dt},$$

$$-i\hat{H}_1e^{-i\hat{H}_0t}\hat{U}(t) = e^{-i\hat{H}_0t}\frac{d\hat{U}(t)}{dt}, \tag{1.13}$$

$$\frac{d\hat{U}(t)}{dt} = -i\hat{H}_1^I(t)\hat{U}(t) \tag{1.14}$$

を得る。初期条件は、$\hat{U}(0) = 1$ である。また、ここで、

$$\hat{H}_1^I(t) \stackrel{\text{def}}{=} e^{i\hat{H}_0t}\hat{H}_1e^{-i\hat{H}_0t} \tag{1.15}$$

である。今、

$$\hat{U}(t,s) = \hat{U}(t)\hat{U}^{-1}(s) \tag{1.16}$$

とすると、これは、

$$\frac{\partial}{\partial t}\hat{U}(t,s) = -i\hat{H}_1^I(t)\hat{U}(t,s) \tag{1.17}$$

を満たす。また、

$$\hat{U}(t,s) = \hat{U}(t,t')\hat{U}(t',s), \tag{1.18}$$

$$\hat{U}(t,t) = 1 \tag{1.19}$$

を満たす。これらより、

$$\hat{U}(s,t) = \hat{U}^{-1}(t,s) \tag{1.20}$$

である。

1.3 射影演算子法：一般論

1.3.1 近似なし

射影演算子 $\mathcal{P}$ を

$$\mathcal{P}^2 = \mathcal{P} \tag{1.21}$$

を満たす任意の演算子とし、

$$\mathcal{Q} \stackrel{\text{def}}{=} 1 - \mathcal{P} \tag{1.22}$$

とすると、

$$\mathcal{Q}^2 = (1-\mathcal{P})^2 = 1 - 2\mathcal{P} + \mathcal{P}^2 = 1 - \mathcal{P}$$

$$= \mathcal{Q}, \tag{1.23}$$

$$\mathcal{QP} = \mathcal{P} - \mathcal{P}^2 = 0, \tag{1.24}$$

$$\mathcal{PQ} = \mathcal{P} - \mathcal{P}^2 = 0 \tag{1.25}$$

が得られる。今、

$$\hat{x}(t) \stackrel{\text{def}}{=} \mathcal{Q}\hat{U}(t), \quad \hat{y}(t) \stackrel{\text{def}}{=} \mathcal{P}\hat{U}(t) \tag{1.26}$$

とする。(1.14) は、

$$\begin{aligned} \frac{d}{dt}\hat{U}(t) &= -i\hat{H}_1^I(t)[\mathcal{Q}+\mathcal{P}]\hat{U}(t) \\ &= -i\hat{H}_1^I(t)\hat{x}(t) - i\hat{H}_1^I(t)\hat{y}(t) \end{aligned} \tag{1.27}$$

または、(1.23),(1.21) を用いて、

$$\begin{aligned} \frac{d}{dt}\hat{U}(t) &= -i\hat{H}_1^I(t)[\mathcal{Q}^2+\mathcal{P}^2]\hat{U}(t) \\ &= -i\hat{H}_1^I(t)\mathcal{Q}\hat{x}(t) - i\hat{H}_1^I(t)\mathcal{P}\hat{y}(t) \end{aligned} \tag{1.28}$$

ともかける。これに左から $\mathcal{Q}$ を作用させて、

$$\frac{d}{dt}\hat{x}(t) = -i\hat{H}_{1,QQ}^I(t)\hat{x}(t) - i\hat{H}_{1,QP}^I(t)\hat{y}(t) \tag{1.29}$$

を得る。ここで、

$$\hat{H}_{1,QQ}^I(t) \stackrel{\text{def}}{=} \mathcal{Q}\hat{H}_1^I(t)\mathcal{Q}, \quad \hat{H}_{1,QP}^I \stackrel{\text{def}}{=} \mathcal{Q}\hat{H}_1^I(t)\mathcal{P} \tag{1.30}$$

である。(1.29) より、$\hat{W}(t)$ を任意の演算子として、

$$\begin{aligned} \frac{d}{dt}[\hat{W}(t)\hat{x}(t)] &= -i\hat{W}(t)[\hat{H}_{1,QQ}^I(t)\hat{x}(t) + \hat{H}_{1,QP}^I(t)\hat{y}(t)] + \frac{d\hat{W}(t)}{dt}\hat{x}(t) \\ &= \hat{W}(t)[-i\hat{H}_{1,QQ}^I(t) + \hat{W}^{-1}(t)\frac{d\hat{W}(t)}{dt}]\hat{x}(t) - i\hat{W}(t)\hat{H}_{1,QP}^I(t)\hat{y}(t) \end{aligned} \tag{1.31}$$

である。今、$\hat{W}_{QQ}(t)$ を

$$\begin{aligned} -i\hat{H}_{1,QQ}^I(t) + \hat{W}_{QQ}^{-1}(t)\frac{d\hat{W}_{QQ}(t)}{dt} &= 0, \\ \frac{d\hat{W}_{QQ}(t)}{dt} &= i\hat{W}_{QQ}(t)\hat{H}_{1,QQ}^I(t) \end{aligned} \tag{1.32}$$

を満たす、初期条件

$$\hat{W}_{QQ}(0) = 1 \tag{1.33}$$

の解とする。このとき、(1.31) より、

$$\frac{d}{dt}[\hat{W}_{QQ}(t)\hat{x}(t)] = -\hat{W}_{QQ}(t)i\hat{H}_{1,QP}^I(t)\hat{y}(t) \tag{1.34}$$

を得る。これを解くと、

$$\hat{W}_{QQ}(t)\hat{x}(t) - \hat{W}_{QQ}(0)\hat{x}(0) = -i\int_0^t ds\, \hat{W}_{QQ}(s)\hat{H}_{1,QP}^I(s)\hat{y}(s)$$

であり、(1.33) と (1.26) より $\hat{W}_{QQ}(0)\hat{x}(0) = \mathcal{Q}$ である。上式を $\hat{x}(t)$ について解いて、

$$\hat{x}(t) = \hat{W}_{QQ}^{-1}(t)\mathcal{Q} - i\int_0^t ds\, \hat{W}_{QQ}^{-1}(t)\hat{W}_{QQ}(s)\hat{H}_{1,QP}^I(s)\hat{y}(s) \tag{1.35}$$

を得る。今、

$$\hat{U}_{QQ}(t) \stackrel{\text{def}}{=} \hat{W}_{QQ}^{-1}(t), \tag{1.36}$$

$$\hat{U}_{QQ}(s,t) \stackrel{\text{def}}{=} \hat{U}_{QQ}(s)\hat{U}_{QQ}^{-1}(t) \tag{1.37}$$

とする。このとき、

$$\hat{U}_{QQ}(t,t) = 1, \tag{1.38}$$

$$\hat{U}_{QQ}(t,u)\hat{U}_{QQ}(u,s) = \hat{U}_{QQ}(t,s), \tag{1.39}$$

$$\hat{U}_{QQ}(s,t) = \hat{U}_{QQ}^{-1}(t,s) \tag{1.40}$$

となる。これより、

$$\begin{aligned}\hat{W}_{QQ}^{-1}(t)\hat{W}_{QQ}(s) &= \hat{U}_{QQ}(t,0)\hat{U}_{QQ}(0,s) \\ &= \hat{U}_{QQ}(t,s)\end{aligned} \tag{1.41}$$

である。

(1.41),(1.36) および $\hat{y}(t)$ の定義 (1.26) を使うと、(1.35) は

$$\hat{x}(t) = \hat{U}_{QQ}(t)\mathcal{Q} - i\int_0^t ds\, \hat{U}_{QQ}(t,s)\hat{H}_{1,QP}^I(s)\hat{y}(s) \tag{1.42}$$

となる。(1.42),(1.26) の $\hat{y}(t)$ の定義を、(1.27) の右辺に代入して、

$$\begin{aligned}\frac{d}{dt}\hat{U}(t) = &-i\hat{H}_1^I(t)\hat{U}_{QQ}(t)\mathcal{Q} - \int_0^t ds\, \hat{H}_1^I(t)\hat{U}_{QQ}(t,s)\hat{H}_{1,QP}^I(s)\mathcal{P}\hat{U}(s) \\ &-i\hat{H}_1^I(t)\mathcal{P}\hat{U}(t)\end{aligned} \tag{1.43}$$

を得る。

両辺を $\rho(\chi,0)$ に作用させると、

$$\begin{aligned}\frac{d}{dt}\rho^I(\chi,t) = &-i\hat{H}_1^I(t)\hat{U}_{QQ}(t)\mathcal{Q}\rho(\chi,0) - \int_0^t ds\, \hat{H}_1^I(t)\hat{U}_{QQ}(t,s)\hat{H}_{1,QP}^I(s)\mathcal{P}\rho^I(\chi,s) \\ &-i\hat{H}_1^I(t)\mathcal{P}\rho^I(\chi,t)\end{aligned} \tag{1.44}$$

となる。これに $\mathcal{P}$ を作用させて、

$$\begin{aligned}\frac{d}{dt}\mathcal{P}\rho^I(\chi,t) = &-i\mathcal{P}\hat{H}_1^I(t)\hat{U}_{QQ}(t)\mathcal{Q}\rho(\chi,0) - \int_0^t ds\, \mathcal{P}\hat{H}_1^I(t)\hat{U}_{QQ}(t,s)\hat{H}_{1,QP}^I(s)\mathcal{P}\rho^I(\chi,s) \\ &-i\mathcal{P}\hat{H}_1^I(t)\mathcal{P}\rho^I(\chi,t)\end{aligned} \tag{1.45}$$

を得る。ここまでは恒等式で、厳密に正しい。

1.3.2 摂動論

$\hat{U}_{QQ}(t,s)$ を $\hat{H}_1^I(t)$ について展開する。まず、$\hat{U}_{QQ}(t,s)$ の従う微分方程式を求める。(1.37),(1.36) より、

$$\begin{aligned}\hat{U}_{QQ}(t,s) &= \hat{W}_{QQ}^{-1}(t)\hat{W}_{QQ}(s), \\ \frac{\partial}{\partial t}\hat{U}_{QQ}(t,s) &= \big[\frac{\partial}{\partial t}\hat{W}_{QQ}^{-1}(t)\big]\hat{W}_{QQ}(s)\end{aligned} \tag{1.46}$$

である。$\hat{W}_{QQ}(t)\hat{W}^{-1}_{QQ}(t) = 1$ を微分して、

$$
\begin{aligned}
0 &= [\frac{d}{dt}\hat{W}_{QQ}(t)]\hat{W}^{-1}_{QQ}(t) + \hat{W}_{QQ}(t)\frac{d}{dt}\hat{W}^{-1}_{QQ}(t), \qquad (1.47)\\
\frac{d}{dt}\hat{W}^{-1}_{QQ}(t) &= -\hat{W}^{-1}_{QQ}(t)\Big[\frac{d}{dt}\hat{W}_{QQ}(t)\Big]\hat{W}^{-1}_{QQ}(t)\\
&= -i\hat{W}^{-1}_{QQ}(t)i\hat{W}_{QQ}(t)\hat{H}^{I}_{1,QQ}(t)\hat{W}^{-1}_{QQ}(t)\\
&= -i\hat{H}^{I}_{1,QQ}(t)\hat{W}^{-1}_{QQ}(t) \qquad (1.48)
\end{aligned}
$$

を得る。これを (1.46) に代入して、

$$
\begin{aligned}
\frac{\partial}{\partial t}\hat{U}_{QQ}(t,s) &= -i\hat{H}^{I}_{1,QQ}(t)\hat{W}^{-1}_{QQ}(t)\hat{W}_{QQ}(s)\\
&= -i\hat{H}^{I}_{1,QQ}(t)\hat{U}_{QQ}(t,s) \qquad (1.49)
\end{aligned}
$$

を得る。これと初期条件 $\hat{U}_{QQ}(s,s) = 1$ より

$$
\hat{U}_{QQ}(t,s) = 1 - i\int_s^t du\ \hat{H}^{I}_{1,QQ}(u)\hat{U}_{QQ}(u,s) \qquad (1.50)
$$

この右辺自身を右辺の $\hat{U}_{QQ}(u,s)$ に代入して、

$$
\begin{aligned}
\hat{U}_{QQ}(t,s) &= 1 - i\int_s^t du\ \hat{H}^{I}_{1,QQ}(u) - \int_s^t du_1\int_s^{u_1} du_2\ \hat{H}^{I}_{1,QQ}(u_1)\hat{H}^{I}_{1,QQ}(u_2)\hat{U}_{QQ}(u_2,s)\\
&= 1 - i\int_s^t du\ \hat{H}^{I}_{1,QQ}(u) - \int_s^t du_1\int_s^{u_1} du_2\ \hat{H}^{I}_{1,QQ}(u_1)\hat{H}^{I}_{1,QQ}(u_2) + \mathcal{O}(\hat{H}^{I}_{1})^3 \qquad (1.51)
\end{aligned}
$$

を得る。$\mathcal{O}(\hat{H}^{I}_{1})^3$ は $\hat{H}^{I}_{1}(t)$ について 3 次以上の項である。(1.45) 右辺第 1 項は、

$$
\begin{aligned}
&-i\mathcal{P}\hat{H}^{I}_{1}(t)\hat{U}_{QQ}(t)\mathcal{Q}\rho(\chi,0)\\
&= -i\mathcal{P}\hat{H}^{I}_{1}(t)\mathcal{Q}\rho(\chi,0) - \int_0^t ds\ \mathcal{P}\hat{H}^{I}_{1}(t)\hat{H}^{I}_{1,QQ}(s)\mathcal{Q}\rho(\chi,0) + \mathcal{O}(\hat{H}^{I}_{1})^3 \qquad (1.52)
\end{aligned}
$$

右辺第 2 項は、

$$
\begin{aligned}
&-\int_0^t ds\ \mathcal{P}\hat{H}^{I}_{1}(t)\hat{U}_{QQ}(t,s)\hat{H}^{I}_{1,QP}(s)\mathcal{P}\rho^{I}(\chi,s)\\
&= -\int_0^t ds\ \mathcal{P}\hat{H}^{I}_{1}(t)\hat{H}^{I}_{1,QP}(s)\mathcal{P}\rho^{I}(\chi,s) + \mathcal{O}(\hat{H}^{I}_{1})^3\\
&= -\int_0^t ds\ \mathcal{P}\hat{H}^{I}_{1}(t)(1-\mathcal{P})\hat{H}^{I}_{1}(s)\mathcal{P}\rho^{I}(\chi,s) + \mathcal{O}(\hat{H}^{I}_{1})^3\\
&= -\int_0^t ds\ [\mathcal{P}\hat{H}^{I}_{1}(t)\hat{H}^{I}_{1}(s)\mathcal{P}\rho^{I}(\chi,s) - \mathcal{P}\hat{H}^{I}_{1}(t)\mathcal{P}\hat{H}^{I}_{1}(s)\mathcal{P}\rho^{I}(\chi,s)] + \mathcal{O}(\hat{H}^{I}_{1})^3 \qquad (1.53)
\end{aligned}
$$

となる。以上より、(1.45) は、

$$
\begin{aligned}
\frac{d}{dt}\mathcal{P}\rho^{I}(\chi,t) &= -i\mathcal{P}\hat{H}^{I}_{1}(t)\mathcal{Q}\rho(\chi,0) - \int_0^t ds\ \mathcal{P}\hat{H}^{I}_{1}(t)\hat{H}^{I}_{1,QQ}(s)\mathcal{Q}\rho(\chi,0)\\
&\quad - \int_0^t ds\ [\mathcal{P}\hat{H}^{I}_{1}(t)\hat{H}^{I}_{1}(s)\mathcal{P}\rho^{I}(\chi,s) - \mathcal{P}\hat{H}^{I}_{1}(t)\mathcal{P}\hat{H}^{I}_{1}(s)\mathcal{P}\rho^{I}(\chi,s)]\\
&\quad -i\mathcal{P}\hat{H}^{I}_{1}(t)\mathcal{P}\rho^{I}(\chi,t) + \mathcal{O}(\hat{H}^{I}_{1})^3 \qquad (1.54)
\end{aligned}
$$

となる。

1.4 量子マスター方程式

1.4.1 相互作用描像

今、$\mathcal{P}$ として、

$$\mathcal{P}\bullet = \rho_B \otimes \mathrm{Tr}_B(\bullet) \tag{1.55}$$

を選ぶ。また、

$$\rho(0) = \rho_B \otimes \rho_S(0) \tag{1.56}$$

を仮定する。このとき、(1.4) より、

$$\rho(\chi, 0) = \rho_B \otimes \rho_S(0) \tag{1.57}$$

となる。このとき、

$$\begin{aligned} \mathcal{Q}\rho(\chi,0) &= \rho(\chi,0) - \rho_B \otimes \mathrm{Tr}_B(\rho_B)\rho_S(0) \\ &= 0, \end{aligned} \tag{1.58}$$

$$\begin{aligned} \mathcal{P}\rho^I(\chi,s) &= \rho_B \otimes \mathrm{Tr}_B(\rho^I(\chi,s)) \\ &= \rho_B \otimes \rho_S^I(\chi,s) \end{aligned} \tag{1.59}$$

となる。ここで、

$$\rho_S^I(\chi,t) \stackrel{\mathrm{def}}{=} \mathrm{Tr}_B(\rho^I(\chi,t)) \tag{1.60}$$

である。(1.58) より、(1.54) の第 1,2 項は 0 になる。

ここで、

$$[A, H_B] = 0 \tag{1.61}$$

と

$$H_1 = R_\mu a_\mu \tag{1.62}$$

を仮定する。μ については和を取るものとする。a_μ は注目系の演算子、R_μ は熱浴系の演算子である。このとき、

$$\hat{H}_B\bullet = [H_B, \bullet], \tag{1.63}$$

$$\hat{H}_1\bullet = [H_1, \bullet]_\chi \equiv H_{1,\chi}\bullet - \bullet H_{1,-\chi}, \tag{1.64}$$

$$H_{1,\chi} = R_{\mu,\chi}a_\mu \tag{1.65}$$

となる。(1.63) より、演算子 X に対して

$$e^{-i\hat{H}_0 t}X = e^{-iH_0 t}Xe^{iH_0 t} \equiv X^I(-t) \tag{1.66}$$

であり、従って

$$\begin{aligned} \hat{H}_1^I(t)X &= e^{i\hat{H}_0 t}\hat{H}_1 e^{-i\hat{H}_0 t}X \\ &= e^{i\hat{H}_0 t}\hat{H}_1(e^{-iH_0 t}Xe^{iH_0 t}) \\ &= e^{i\hat{H}_0 t}[H_1, e^{-iH_0 t}Xe^{iH_0 t}]_\chi \\ &= [H_1^I(t), X]_\chi \end{aligned} \tag{1.67}$$

を得る。ここで、

$$[X,Y]_\chi = X_\chi Y - YX_{-\chi}, \quad X_\chi \equiv e^{i\chi A/2} X e^{-i\chi A/2}, \tag{1.68}$$

$$H_1^I(t) = R_\mu^I(t) a_\mu^I(t) \tag{1.69}$$

である。これらと (1.59) より、

$$\begin{aligned}
\mathcal{P}\hat{H}_1^I(s)\mathcal{P}\rho^I(\chi,s) &= \mathcal{P}[H_1^I(s), \rho_B\rho_S^I(\chi,s)]_\chi \\
&= \rho_B \mathrm{Tr}_B[H_1^I(s), \rho_B\rho_S^I(\chi,s)]_\chi \\
&= \rho_B \mathrm{Tr}_B\big(H_{1,\chi}^I(s)\rho_B\rho_S^I(\chi,s) - \rho_B\rho_S^I(\chi,s)H_{1,-\chi}^I(s)\big) \\
&= \rho_B\Big[\mathrm{Tr}_B\{R_{\mu,\chi}^I(s)\rho_B\}a_\mu^I(s)\rho_S^I(\chi,s) - \mathrm{Tr}_B\{\rho_B R_{\mu,-\chi}^I(s)\}\rho_S^I(\chi,s)a_\mu^I(s)\Big] \\
&= 0.
\end{aligned} \tag{1.70}$$

最後の等号で、

$$\langle R_{\mu,\chi}^I(t)\rangle_B = 0\,, \quad \langle\cdots\rangle_B \stackrel{\text{def}}{=} \mathrm{Tr}_B[\rho_B\cdots] \tag{1.71}$$

を仮定した。これは多くの場合に満たされる。

また、

$$\begin{aligned}
\mathcal{P}\hat{H}_1^I(t)\hat{H}_1^I(s)\mathcal{P}\rho_S^I(\chi,s) &= \mathcal{P}\hat{H}_1^I(t)[H_1^I(s), \rho_B\rho_S^I(\chi,s)]_\chi \\
&= \mathcal{P}\big[H_1^I(t), [H_1^I(s), \rho_B\rho_S^I(\chi,s)]_\chi\big]_\chi \\
&= \rho_B \mathrm{Tr}_B\big[H_1^I(t), [H_1^I(s), \rho_B\rho_S^I(\chi,s)]_\chi\big]_\chi
\end{aligned} \tag{1.72}$$

となる。以上より、(1.54) は、

$$\begin{aligned}
\rho_B\frac{d}{dt}\rho_S^I(\chi,t) &= -\rho_B\int_0^t ds\ \mathrm{Tr}_B\big[H_1^I(t), [H_1^I(s), \rho_B\rho_S^I(\chi,s)]_\chi\big]_\chi, \\
\frac{d}{dt}\rho_S^I(\chi,t) &= -\int_0^t ds\ \mathrm{Tr}_B\big[H_1^I(t), [H_1^I(s), \rho_B\rho_S^I(\chi,s)]_\chi\big]_\chi
\end{aligned} \tag{1.73}$$

となる。これが Born 方程式である。

1.4.2 シュレーディンガー描像

今、

$$\rho_S(\chi,t) \stackrel{\text{def}}{=} \mathrm{Tr}_B[\rho(\chi,t)] \tag{1.74}$$

とする。(1.8) より、

$$\begin{aligned}
\rho_S(\chi,t) &= \mathrm{Tr}_B[e^{-i\hat{H}_0 t}\rho^I(\chi,t)] \\
&= \mathrm{Tr}_B[e^{-iH_0 t}\rho^I(\chi,t)e^{iH_0 t}] \\
&= \mathrm{Tr}_B[e^{-iH_B t}e^{-iH_S t}\rho^I(\chi,t)e^{iH_S t}e^{iH_B t}]
\end{aligned} \tag{1.75}$$

である。$|n\rangle$ を熱浴系の完全系とすると、

$$\begin{aligned}
\mathrm{Tr}_B[e^{-iH_Bt}e^{-iH_St}\rho^I(\chi,t)e^{iH_St}e^{iH_Bt}] &= \sum_n \langle n|e^{-iH_Bt}e^{-iH_St}\rho^I(\chi,t)e^{iH_St}e^{iH_Bt}|n\rangle \\
&= \sum_{n,m} \langle n|e^{-iH_Bt}e^{-iH_St}\rho^I(\chi,t)e^{iH_St}|m\rangle\langle m|e^{iH_Bt}|n\rangle \\
&= \sum_{n,m} \langle m|e^{iH_Bt}|n\rangle\langle n|e^{-iH_Bt}e^{-iH_St}\rho^I(\chi,t)e^{iH_St}|m\rangle \\
&= \sum_m \langle m|e^{iH_Bt}e^{-iH_Bt}e^{-iH_St}\rho^I(\chi,t)e^{iH_St}|m\rangle \\
&= \mathrm{Tr}_B[e^{-iH_St}\rho^I(\chi,t)e^{iH_St}] \\
&= e^{-iH_St}\mathrm{Tr}_B[\rho^I(\chi,t)]e^{iH_St} \\
&= e^{-iH_St}\rho_S^I(\chi,t)e^{iH_St} \qquad (1.76)
\end{aligned}$$

となるから、

$$\rho_S(\chi,t) = e^{-iH_St}\rho_S^I(\chi,t)e^{iH_St} \qquad (1.77)$$

を得る。これと (1.73) から、

$$\begin{aligned}
i\frac{d}{dt}\rho_S(\chi,t) &= [H_S,\rho_S(\chi,t)] + ie^{-iH_St}\frac{d\rho_S^I(\chi,t)}{dt}e^{iH_St} \\
&= [H_S,\rho_S(\chi,t)] - i\int_0^t ds\, e^{-iH_St}\mathrm{Tr}_B\big[H_1^I(t),[H_1^I(s),\rho_B\rho_S^I(\chi,s)]_\chi\big]_\chi e^{iH_St} \\
&= [H_S,\rho_S(\chi,t)] - i\int_0^t ds\, e^{-iH_St}\mathrm{Tr}_B\big[H_1^I(t),[H_1^I(s),\rho_B e^{iH_Ss}\rho_S(\chi,s)e^{-iH_Ss}]_\chi\big]_\chi e^{iH_St}
\end{aligned} \qquad (1.78)$$

となる。

1.4.3 Born-Markov 近似

(1.73) で、$s=t-u$ として、

$$\frac{d}{dt}\rho_S^I(\chi,t) = -\int_0^t du\ \mathrm{Tr}_B\big[H_1^I(t),[H_1^I(t-u),\rho_B\rho_S^I(\chi,t-u)]_\chi\big]_\chi \qquad (1.79)$$

を得る。$\rho_S^I(\chi,t-u)$ を $\rho_S^I(\chi,t)$ で近似して、

$$\frac{d}{dt}\rho_S^I(\chi,t) = -\int_0^t du\ \mathrm{Tr}_B\big[H_1^I(t),[H_1^I(t-u),\rho_B\rho_S^I(\chi,t)]_\chi\big]_\chi \qquad (1.80)$$

を得る。これを Redfield 方程式という。更に、$\int_0^t du$ を $\int_0^\infty du$ で近似した、

$$\frac{d}{dt}\rho_S^I(\chi,t) = -\int_0^\infty du\ \mathrm{Tr}_B\big[H_1^I(t),[H_1^I(t-u),\rho_B\rho_S^I(\chi,t)]_\chi\big]_\chi \qquad (1.81)$$

が Born-Markov 近似である。このとき、(1.73) の対応物は、

$$\begin{aligned}
i\frac{d}{dt}\rho_S(\chi,t) &= [H_S,\rho_S(\chi,t)] + ie^{-iH_St}\frac{d\rho_S^I(\chi,t)}{dt}e^{iH_St} \\
&= [H_S,\rho_S(\chi,t)] - i\int_0^\infty du\, e^{-iH_St}\mathrm{Tr}_B\big[H_1^I(t),[H_1^I(t-u),\rho_B\rho_S^I(\chi,t)]_\chi\big]_\chi e^{iH_St} \\
&= [H_S,\rho_S(\chi,t)] - i\int_0^\infty du\, e^{-iH_St}\mathrm{Tr}_B\big[H_1^I(t),[H_1^I(t-u),\rho_B e^{iH_St}\rho_S(\chi,t)e^{-iH_St}]_\chi\big]_\chi e^{iH_St}
\end{aligned} \qquad (1.82)$$

となる。

1.5 TCL 型

1.5.1 近似なし

(1.43) は TC(time convolution) 型と言われる。TCL(time convolutionless) 型の方程式は、以下ように得られる。

(1.28) は、

$$\frac{d}{dt}\hat{U}(t) = -i\hat{H}_1^I(t)\mathcal{Q}\hat{x}(t) - i\hat{H}_1^I(t)\mathcal{P}\hat{y}(t) \tag{1.83}$$

であった。これに左から $\mathcal{Q}$ を作用させて、(1.29), すなわち、

$$\frac{d}{dt}\hat{x}(t) = -i\mathcal{Q}\hat{H}_1^I(t)\mathcal{Q}\hat{x}(t) - i\mathcal{Q}\hat{H}_1^I(t)\mathcal{P}\hat{y}(t) \tag{1.84}$$

を得る。(1.83) に左から $\mathcal{P}$ を作用させて、

$$\frac{d}{dt}\hat{y}(t) = -i\mathcal{P}\hat{H}_1^I(t)\mathcal{Q}\hat{x}(t) - i\mathcal{P}\hat{H}_1^I(t)\mathcal{P}\hat{y}(t) \tag{1.85}$$

を得る。(1.42) は、

$$\hat{x}(t) = \hat{U}_{QQ}(t)\mathcal{Q} - i\int_0^t ds\,\hat{U}_{QQ}(t,s)\hat{H}_{1,QP}^I(s)\hat{y}(s) \tag{1.86}$$

であった。上式の第 2 項で、

$$\begin{aligned}\hat{y}(s) &= \mathcal{P}\hat{U}(s)\\ &= \mathcal{P}\hat{U}^{-1}(t,s)\hat{U}(t)\\ &= \mathcal{P}\hat{U}^{-1}(t,s)[\hat{x}(t)+\hat{y}(t)]\end{aligned} \tag{1.87}$$

なので、

$$\begin{aligned}\hat{x}(t) &= \hat{U}_{QQ}(t)\mathcal{Q} - i\int_0^t ds\,\hat{U}_{QQ}(t,s)\hat{H}_{1,QP}^I(s)\mathcal{P}\hat{U}^{-1}(t,s)[\hat{x}(t)+\hat{y}(t)]\\ &= \hat{U}_{QQ}(t)\mathcal{Q} + \hat{S}(t)\hat{x}(t) + \hat{S}(t)\hat{y}(t),\end{aligned} \tag{1.88}$$

$$\hat{S}(t) \stackrel{\text{def}}{=} -i\int_0^t ds\,\hat{U}_{QQ}(t,s)\hat{H}_{1,QP}^I(s)\mathcal{P}\hat{U}^{-1}(t,s) \tag{1.89}$$

となる。(1.88) より、

$$\begin{aligned}[1-\hat{S}(t)]\hat{x}(t) &= \hat{U}_{QQ}(t)\mathcal{Q} + \hat{S}(t)\hat{y}(t),\\ \hat{x}(t) &= [1-\hat{S}(t)]^{-1}\hat{U}_{QQ}(t)\mathcal{Q} + [1-\hat{S}(t)]^{-1}\hat{S}(t)\hat{y}(t)\end{aligned} \tag{1.90}$$

を得る。これを (1.85) に代入して、

$$\begin{aligned}\frac{d}{dt}\hat{y}(t) &= -i\mathcal{P}\hat{H}_1^I(t)\mathcal{Q}[1-\hat{S}(t)]^{-1}\hat{U}_{QQ}(t)\mathcal{Q} - i\mathcal{P}\hat{H}_1^I(t)\mathcal{Q}[1-\hat{S}(t)]^{-1}\hat{S}(t)\hat{y}(t) - i\mathcal{P}\hat{H}_1^I(t)\mathcal{P}\hat{y}(t)\\ &= \hat{I}(t) + \hat{J}(t)\hat{y}(t)\end{aligned} \tag{1.91}$$

を得る。ここで、

$$\hat{I}(t) \stackrel{\text{def}}{=} -i\mathcal{P}\hat{H}_1^I(t)\mathcal{Q}[1-\hat{S}(t)]^{-1}\hat{U}_{QQ}(t)\mathcal{Q}, \tag{1.92}$$

$$\hat{J}(t) \stackrel{\text{def}}{=} -i\mathcal{P}\hat{H}_1^I(t)\mathcal{P} - i\mathcal{P}\hat{H}_1^I(t)\mathcal{Q}[1-\hat{S}(t)]^{-1}\hat{S}(t) \tag{1.93}$$

である。(1.91) が TCL 型の方程式である。

1.5.2 Born 近似

さて、

$$[1-\hat{S}(t)]^{-1} \;=\; 1+\hat{S}(t)+[\hat{S}(t)]^2+\cdots \tag{1.94}$$

であり、$\hat{S}(t)$ において、

$$\hat{U}^{-1}(t,s) \;=\; 1+i\int_s^t du\ \hat{H}_1^I(u)+\cdots \tag{1.95}$$

である。よって、

$$\begin{aligned}\hat{S}(t) \;&=\; -i\int_0^t ds\,\hat{U}_{QQ}(t,s)\hat{H}^I_{1,QP}(s)\mathcal{P}+\int_0^t ds\,\hat{U}_{QQ}(t,s)\hat{H}^I_{1,QP}(s)\mathcal{P}\int_s^t du\ \hat{H}_1^I(u)+\cdots\\ &=\; -i\int_0^t ds\ \hat{H}^I_{1,QP}(s)\mathcal{P}+\int_0^t ds\int_s^t du\,\Big[-\mathcal{Q}\hat{H}_1^I(u)\mathcal{Q}\hat{H}_1^I(s)\mathcal{P}+\mathcal{Q}\hat{H}_1^I(s)\mathcal{P}\hat{H}_1^I(u)\Big]+\cdots\\ &=\; \hat{S}^{(1)}(t)+\hat{S}^{(2)}(t)+\cdots\end{aligned} \tag{1.96}$$

となる。ここで、

$$\hat{S}^{(1)}(t) \;=\; -i\int_0^t ds\ \mathcal{Q}\hat{H}_1^I(s)\mathcal{P}, \tag{1.97}$$

$$\hat{S}^{(2)}(t) \;=\; \int_0^t ds\int_s^t du\,\Big[-\mathcal{Q}\hat{H}_1^I(u)\mathcal{Q}\hat{H}_1^I(s)\mathcal{P}+\mathcal{Q}\hat{H}_1^I(s)\mathcal{P}\hat{H}_1^I(u)\Big] \tag{1.98}$$

である。よって、

$$\begin{aligned}[1-\hat{S}(t)]^{-1} \;&=\; 1+\hat{S}^{(1)}(t)+[\hat{S}^{(1)}(t)]^2+\hat{S}^{(2)}(t)+\cdots\\ &=\; 1+\hat{S}^{(1)}(t)+\hat{S}^{(2)}(t)+\cdots\end{aligned} \tag{1.99}$$

となる。ここで、$\mathcal{P}\mathcal{Q}=0$ より、$[\hat{S}^{(1)}(t)]^2=0$ を用いた。また、

$$[1-\hat{S}(t)]^{-1}\hat{S}(t) \;=\; \hat{S}^{(1)}(t)+\hat{S}^{(2)}(t)+\cdots \tag{1.100}$$

である。

よって、H_1^I の 2 次までで、

$$\begin{aligned}\hat{J}(t) \;&\approx\; -i\mathcal{P}\hat{H}_1^I(t)\mathcal{P}-i\mathcal{P}\hat{H}_1^I(t)\mathcal{Q}\hat{S}^{(1)}(t)\\ &=\; -i\mathcal{P}\hat{H}_1^I(t)\mathcal{P}-i\mathcal{P}\hat{H}_1^I(t)\int_0^t ds\ \mathcal{Q}\hat{H}_1^I(s)\mathcal{P}\end{aligned} \tag{1.101}$$

である。

1.5.3 TCL 型の量子マスター方程式

(1.91) を $\rho(\chi,0)$ に作用させると、

$$\frac{d}{dt}\mathcal{P}\rho^I(\chi,t) \;=\; \hat{J}(t)\mathcal{P}\rho^I(\chi,t)+\hat{I}(t)\rho(\chi,0) \tag{1.102}$$

である。$\mathcal{Q}\rho(\chi,0)=0$ を仮定すると、

$$\frac{d}{dt}\mathcal{P}\rho^I(\chi,t) \;=\; \hat{J}(t)\mathcal{P}\rho^I(\chi,t) \tag{1.103}$$

であり、H_1^I の 2 次ままで、

$$\frac{d}{dt}\mathcal{P}\rho^I(\chi,t) \;=\; -i\mathcal{P}\hat{H}_1^I(t)\mathcal{P}\rho^I(\chi,t) - i\mathcal{P}\hat{H}_1^I(t)\int_0^t ds\;\mathcal{Q}\hat{H}_1^I(s)\mathcal{P}\rho^I(\chi,t) \tag{1.104}$$

となる。ここで、

$$\mathcal{P}\hat{H}_1^I(t) = 0 \tag{1.105}$$

を仮定すると、

$$\frac{d}{dt}\mathcal{P}\rho^I(\chi,t) \;=\; -i\mathcal{P}\int_0^t ds\;\hat{H}_1^I(t)\hat{H}_1^I(s)\mathcal{P}\rho^I(\chi,t) \tag{1.106}$$

となる。これは (1.80) の Redfield 方程式に対応する。

2　量子マスター方程式の素朴な導出：Coarse-graining approximation

この pdf の以下は、ほとんど [1] からの抜粋である。

We consider system S weakly coupled to several baths. The total Hamiltonian is given by

$$H(\alpha'(t)) = H_S(\alpha_S(t)) + \sum_b [H_b(\alpha'_b(t)) + H_{Sb}(\alpha_{Sb}(t))]. \tag{2.1}$$

$H_S(\alpha_S)$ is the system Hamiltonian and α_S denotes a set of control parameters of the system. $H_b(\alpha'_b)$ is the Hamiltonian of the bath b and α'_b is a set of control parameters. $H_{Sb}(\alpha_{Sb})$ is the coupling Hamiltonian between S and the bath b, and α_{Sb} is a set of control parameters. We suppose that the states of the baths for $b = 1, 2, \cdots, n_{\mathrm{C}}$ are the canonical distributions and these for $b = n_{\mathrm{C}}+1, \cdots, n_{\mathrm{C}}+n_{\mathrm{GC}}$ are the grand canonical distributions. We denote $\{1, \cdots, n_{\mathrm{C}}\}$ and $\{n_{\mathrm{C}} + 1, \cdots, n_{\mathrm{C}} + n_{\mathrm{GC}}\}$ by $\boldsymbol{\mathcal{C}}$ and $\boldsymbol{\mathcal{G}}$. We denote the inverse temperature of the bath b by β_b and the chemical potential of the bath $b \in \boldsymbol{\mathcal{G}}$ by μ_b. α''_b denotes β_b for $b \in \boldsymbol{\mathcal{C}}$ and the set of β_b and $\beta_b\mu_b$ for $b \in \boldsymbol{\mathcal{G}}$. We symbolize the set of all control parameters $(\alpha_S,\ \{\alpha_{Sb}\}_b,\ \{\alpha'_b\}_b,\ \{\alpha''_b\}_b)$ by α, $(\alpha_S,\ \{\alpha_{Sb}\}_b,\ \{\alpha'_b\}_b)$ by α', $\{\alpha''_b\}_b$ by α'', $(\alpha'_b,\ \alpha''_b)$ by α_b, and $\{\alpha_b\}_b$ by α_B. While α' are dynamical parameters, α'' are thermodynamical parameters. We denote the set of all the linear operators of S by B.

The modified von Neumann equation is

$$\frac{d}{dt}\rho^{\chi}(t) = -i[H(t), \rho^{\chi}(t)]_{\chi}. \tag{2.2}$$

Here, $[A, B]_{\chi} \stackrel{\mathrm{def}}{=} A_{\chi}B - BA_{-\chi}$ and $A_{\chi} \stackrel{\mathrm{def}}{=} e^{i\sum_{\mu}\chi_{O_\mu}O_\mu/2}Ae^{-i\sum_{\mu}\chi_{O_\mu}O_\mu/2}$. We suppose

$$\rho(0) = \rho_S(0) \otimes \rho_B(\alpha_B(0)), \tag{2.3}$$

where

$$\rho_B(\alpha_B(0)) \stackrel{\mathrm{def}}{=} \bigotimes_b \rho_b(\alpha_b(0)) \tag{2.4}$$

であり、$b \in \boldsymbol{\mathcal{C}}$ に対しては、

$$\rho_b(\alpha_b(0)) \stackrel{\mathrm{def}}{=} e^{-\beta_b(0)H_b(\alpha'_b(0))}/Z_b(\alpha_b(0)), \tag{2.5}$$

$$Z_b(\alpha_b) \stackrel{\mathrm{def}}{=} \mathrm{Tr}_b[e^{-\beta_b H_b(\alpha'_b)}] \tag{2.6}$$

であり、 $b \in \boldsymbol{\mathcal{G}}$ に対しては、

$$\rho_b(\alpha_b(0)) \stackrel{\mathrm{def}}{=} e^{-\beta_b(0)[H_b(\alpha'_b(0))-\mu_b(0)N_b]}/\Xi_b(\alpha_b(0)), \tag{2.7}$$

$$\Xi_b(\alpha_b) \stackrel{\mathrm{def}}{=} \mathrm{Tr}_b[e^{-\beta_b[H_b(\alpha'_b)-\mu_b N_b]}] \tag{2.8}$$

である。Tr_b denotes the trace of the bath b and N_b ($b \in \boldsymbol{\mathcal{G}}$) is the total number operator of the bath b. Then,

$$\rho^{\chi}(0) = \rho_S(0) \otimes \sum_{\{o_\nu\}} P_{\{o_\nu\}}\rho_B(\alpha_B(0))P_{\{o_\nu\}}, \tag{2.9}$$

obeys. We suppose $[H_b, N_b] = 0$. We suppose that O_μ commute with H_b and N_b:

$$[O_\mu, H_b] = 0,\ [O_\mu, N_b] = 0. \tag{2.10}$$

Then, $P_{\{o_\nu\}}$ commutes with $\rho_B(\alpha_B(0))$ and

$$\rho^\chi(0) = \rho_S(0) \otimes \rho_B(\alpha_B(0)), \tag{2.11}$$

holds.

We defined

$$\rho_S^\chi(t) \stackrel{\text{def}}{=} \text{Tr}_B[\rho^\chi(t)], \tag{2.12}$$

which provides the generating function

$$Z_\tau(\chi) = \text{Tr}_S[\rho_S^\chi(t=\tau)]. \tag{2.13}$$

Tr_B denotes the trace over all baths' degrees of freedom. We assume $\rho(t) \approx \rho_S(t) \otimes \rho_B(\alpha_B(t))$ $(0 < t \leq \tau)$, where

$$\rho_B(\alpha_B(t)) \stackrel{\text{def}}{=} \bigotimes_b \rho_b(\alpha_b(t)), \tag{2.14}$$

$$\rho_b(\alpha_b(t)) \stackrel{\text{def}}{=} \begin{cases} e^{-\beta_b(t)H_b(\alpha_b'(t))}/Z_b(\alpha_b(t)) & b \in \boldsymbol{\mathcal{C}} \\ e^{-\beta_b(t)[H_b(\alpha_b'(t))-\mu_b(t)N_b]}/\Xi_b(\alpha_b(t)) & b \in \boldsymbol{\mathcal{G}} \end{cases}. \tag{2.15}$$

and

$$\rho_S(t) \stackrel{\text{def}}{=} \text{Tr}_B[\rho(t)]. \tag{2.16}$$

First, we introduce the coarse-graining approximation (CGA). An operator in the interaction picture corresponding to $A(t)$ is defined by

$$A^I(t) = U_0^\dagger(t) A(t) U_0(t), \tag{2.17}$$

with

$$\frac{dU_0(t)}{dt} = -i[H_S(\alpha_S(t)) + \sum_b H_b(\alpha_b'(t))]U_0(t), \tag{2.18}$$

and $U_0(0) = 1$. The system reduced density operator in the interaction picture is given by

$$\rho_S^{I,\chi}(t) = \text{Tr}_B[\rho^{I,\chi}(t)], \tag{2.19}$$

where

$$\rho^{I,\chi}(t) = U_0^\dagger(t)\rho^\chi(t)U_0(t). \tag{2.20}$$

$\rho^{I,\chi}(t)$ is governed by

$$\frac{d\rho^{I,\chi}(t)}{dt} = -i[H_{\text{int}}^I(t), \rho^{I,\chi}(t)]_\chi, \tag{2.21}$$

with

$$H_{\text{int}} \stackrel{\text{def}}{=} \sum_b H_{Sb}. \tag{2.22}$$

Up to the second order perturbation in $H_{\rm int}$, we obtain

$$\begin{aligned}\rho^{I,\chi}(t+\tau_{\rm CG}) &= \rho^{I,\chi}(t) \\ &\quad - \int_t^{t+\tau_{\rm CG}} du \int_t^u ds \ {\rm Tr}_B\{[H^I_{\rm int}(u),[H^I_{\rm int}(s),\rho^{I,\chi}(t)\rho_B(\alpha_B(t))]_\chi]_\chi\} \\ &\equiv \rho^{I,\chi}(t) + \tau_{\rm CG}\hat{L}^\chi_{\tau_{\rm CG}}(t)\rho^{I,\chi}(t),\end{aligned} \tag{2.23}$$

using the large-reservoir approximation

$$\rho^{I,\chi}(t) \approx \rho^{I,\chi}(t) \otimes \rho_B(\alpha_B(t)), \tag{2.24}$$

and supposing

$${\rm Tr}_B[H^I_{\rm int}(u)\rho_B(\alpha_B(t))] = 0. \tag{2.25}$$

The arbitrary parameter $\tau_{\rm CG}$ (> 0) is called the coarse-graining time. The CGA [2, 3] is defined by

$$\frac{d}{dt}\rho^{I,\chi}(t) = \hat{L}^\chi_{\tau_{\rm CG}}(t)\rho^{I,\chi}(t). \tag{2.26}$$

In the Schrödinger picture, (2.26) is described as

$$\frac{d\rho^\chi(t)}{dt} = -i[H_S(\alpha_S(t)),\rho^\chi(t)] + \sum_b \mathcal{L}^\chi_{b,\tau_{\rm CG}}(\alpha_t)\rho^\chi(t). \tag{2.27}$$

At $\chi = 0$, this is the Lindblad type. If $\tau_{\rm CG} \ll \tau$, the super-operator $\mathcal{L}^\chi_{b,\tau_{\rm CG}}$ is described as a function of the set of control parameters at time t. $\alpha_t = \alpha(t)$ is the value of α at time t. In this thesis, we suppose

$$\tau_{\rm CG} \ll \tau. \tag{2.28}$$

Moreover, $\tau_{\rm CG}$ should be much shorter than the relaxation time of the system, τ_S:

$$\tau_{\rm CG} \ll \tau_S. \tag{2.29}$$

For the adiabatic modulation, $\tau_S \ll \tau$ should hold, then $\tau_{\rm CG} \ll \tau_S \ll \tau$ holds.

In general, the FCS-QME is given by

$$\frac{d\rho^\chi_S(t)}{dt} = -i[H_S(\alpha_S(t)),\rho^\chi_S(t)] + \sum_b \mathcal{L}^\chi_b(t)\rho^\chi_S(t), \tag{2.30}$$

with the initial condition

$$\rho^\chi_S(0) = \rho_S(0). \tag{2.31}$$

$\mathcal{L}^\chi_b(t)$ describes the coupling effects between S and the bath b and depends on used approximations. In this thesis, we suppose

$$\mathcal{L}^\chi_b(t) = \mathcal{L}^\chi_b(\alpha_t). \tag{2.32}$$

The Born-Markov approximation without or within the RWA and the CGA satisfy this equation. Then, the FCS-QME is given by

$$\frac{d\rho^\chi_S(t)}{dt} = \hat{K}^\chi(\alpha_t)\rho^\chi_S(t). \tag{2.33}$$

Here,

$$\hat{K}^{\chi}(\alpha)\bullet = -i[H_S(\alpha_S), \bullet] + \sum_b \mathcal{L}_b^{\chi}(\alpha)\bullet, \tag{2.34}$$

is the Liouvillian. Here and in the following, $\bullet$ denotes an arbitrary liner operator of the system.

In general, the interaction Hamiltonian is given by

$$H_{Sb}(\alpha_{Sb}) = \sum_\mu s_{b\mu} R_{b,\mu}(\alpha_{Sb}) = \sum_\mu R_{b,\mu}^\dagger(\alpha_{Sb}) s_{b\mu}^\dagger. \tag{2.35}$$

Here, $s_{b\mu}$ is an operator of the system and $R_{b,\mu}(\alpha_{Sb})$ is an operator of the bath b. We suppose

$$\mathrm{Tr}_b[\rho_b(\alpha_b(t)) R_{b,\mu}(\alpha_{Sb}(s))] = 0, \tag{2.36}$$

corresponding to (2.25). Then,

$$\begin{aligned}
&\mathrm{Tr}_B\Big\{[H_{\mathrm{int}}^I(u), [H_{\mathrm{int}}^I(s), \rho_S^{I,\chi}(t)\rho_B(\alpha_B(t))]_\chi]_\chi\Big\} \\
&= \sum_b \sum_{\mu,\nu} \Big(s_{b\nu}^{I\dagger}(u) s_{b\mu}^I(s) \rho_S^{I,\chi}(t) \mathrm{Tr}_b[R_{b,\nu,\chi}^{I\dagger}(u) R_{b,\mu,\chi}^I(s) \rho_b(\alpha_b(t))] \\
&\quad - s_{b\mu}^I(s) \rho_S^{I,\chi}(t) s_{b\nu}^{I\dagger}(u) \mathrm{Tr}_b[R_{b,\mu,\chi}^I(s) \rho_b(\alpha_b(t)) R_{b,\nu,-\chi}^{I\dagger}(u)] \\
&\quad - s_{b\nu}^I(u) \rho_S^{I,\chi}(t) s_{b\mu}^{I\dagger}(s) \mathrm{Tr}_b[R_{b,\nu,\chi}^I(u) \rho_b(\alpha_b(t)) R_{b,\mu,-\chi}^{I\dagger}(s)] \\
&\quad + \rho_S^{I,\chi}(t) s_{b\mu}^{I\dagger}(s) s_{b\nu}^I(u) \mathrm{Tr}_b[\rho_b(\alpha_b(t)) R_{b,\mu,-\chi}^{I\dagger}(s) R_{b,\nu,-\chi}^I(u)] \Big),
\end{aligned} \tag{2.37}$$

holds. In the calculation of $\mathrm{Tr}_b[R_{b,\nu,\chi}^{I\dagger}(u) R_{b,\mu,\chi}^I(s) \rho_b(\alpha_b(t))]$, the values of the control parameters can be approximated by α_t. Then, we obtain

$$\mathrm{Tr}_b[R_{b,\nu,\chi}^{I\dagger}(u) R_{b,\mu,\chi}^I(s) \rho_b] \approx \mathrm{Tr}_b[\rho_b R_{b,\nu}^\dagger(u-s) R_{b,\mu}] \equiv C_{b,\nu\mu}(u-s), \tag{2.38}$$

$$\mathrm{Tr}_b[R_{b,\mu,\chi}^I(s) \rho_b R_{b,\nu,-\chi}^{I\dagger}(u)] \approx \mathrm{Tr}_b[\rho_b R_{b,\nu,-2\chi}^\dagger(u-s) R_{b,\mu}] \equiv C_{b,\nu\mu}^\chi(u-s), \tag{2.39}$$

$$\mathrm{Tr}_b[R_{b,\nu,\chi}^I(u) \rho_b R_{b,\mu,-\chi}^{I\dagger}(s)] \approx \mathrm{Tr}_b[\rho_b R_{b,\mu,-2\chi}^\dagger(s-u) R_{b,\nu}] = C_{b,\mu\nu}^\chi(s-u), \tag{2.40}$$

$$\mathrm{Tr}_b[\rho_b R_{b,\mu,-\chi}^{I\dagger}(s) R_{b,\nu,-\chi}^I(u)] \approx \mathrm{Tr}_b[\rho_b R_{b,\mu}^\dagger(s-u) R_{b,\nu}] = C_{b,\mu\nu}(s-u), \tag{2.41}$$

with

$$R_{b,\nu}^\dagger(v) = e^{iH_b(\alpha_b(t))v} R_{b,\nu}^\dagger(\alpha_{Sb}(t)) e^{-iH_b(\alpha_b(t))v}. \tag{2.42}$$

Here, $\rho_b = \rho_b(\alpha_b(t))$ and $R_{b,\mu} = R_{b,\mu}(\alpha_b(t))$. Then, (2.37) becomes

$$\begin{aligned}
&\mathrm{Tr}_B\Big\{[H_{\mathrm{int}}^I(u), [H_{\mathrm{int}}^I(s), \rho_S^{I,\chi}(t)\rho_B(\alpha_B(t))]_\chi]_\chi\Big\} \\
&= \sum_b \sum_{\mu,\nu} \Big(s_{b\nu}^{I\dagger}(u) s_{b\mu}^I(s) \rho_S^{I,\chi}(t) C_{b,\nu\mu}(u-s) - s_{b\mu}^I(s) \rho_S^{I,\chi}(t) s_{b\nu}^{I\dagger}(u) C_{b,\nu\mu}^\chi(u-s) \\
&\quad - s_{b\nu}^I(u) \rho_S^{I,\chi}(t) s_{b\mu}^{I\dagger}(s) C_{b,\mu\nu}^\chi(s-u) + \rho_S^{I,\chi}(t) s_{b\mu}^{I\dagger}(s) s_{b\nu}^I(u) C_{b,\mu\nu}(s-u) \Big),
\end{aligned} \tag{2.43}$$

and

$$\begin{aligned}
&\mathcal{L}_{b,\tau_{\mathrm{CG}}}^\chi(\alpha_t)\bullet \\
&= -\frac{1}{\tau_{\mathrm{CG}}} \int_t^{t+\tau_{\mathrm{CG}}} du \int_t^u ds \sum_{\mu,\nu} \Big(s_{b\nu}^{I\dagger}(u,t) s_{b\mu}^I(s,t) \bullet C_{b,\nu\mu}(u-s) \\
&\quad - s_{b\mu}^I(s,t) \bullet s_{b\nu}^{I\dagger}(u,t) C_{b,\nu\mu}^\chi(u-s) \\
&\quad - s_{b\nu}^I(u,t) \bullet s_{b\mu}^{I\dagger}(s,t) C_{b,\mu\nu}^\chi(s-u) + \bullet s_{b\mu}^{I\dagger}(s,t) s_{b\nu}^I(u,t) C_{b,\mu\nu}(s-u) \Big),
\end{aligned} \tag{2.44}$$

holds. Here,

$$s_{b\mu}^I(s,t) \;=\; U_S(t)U_S^\dagger(s)s_{b\mu}U_S(s)U_S^\dagger(t). \tag{2.45}$$

and $U_S(t)$ is the solution of $\frac{dU_S(t)}{dt} = -iH_S(\alpha_S(t))U_S(t)$ for $U_S(0)=1$. In the calculation of $s_{b\mu}^I(s,t)$, the values of the control parameters can be approximated by α_t. Then, we obtain

$$s_{b\mu}^I(s,t) \;=\; \sum_\omega e^{-i\omega(s-t)}s_{b\mu}(\omega), \tag{2.46}$$

$$s_{b\nu}^{I\dagger}(u,t) \;=\; \sum_\omega e^{i\omega(u-t)}[s_{b\nu}(\omega)]^\dagger. \tag{2.47}$$

Here, the eigenoperator $s_{b\mu}(\omega)$ is defined by

$$s_{b\mu}(\omega) \;=\; \sum_{n,m,r,s}\delta_{\omega_{mn},\omega}|E_n,r\rangle\langle E_n,r|s_{b\mu}|E_m,s\rangle\langle E_m,s|, \tag{2.48}$$

with $\omega_{mn}=E_m-E_n$ and

$$H_S|E_n,r\rangle = E_n|E_n,r\rangle. \tag{2.49}$$

r denotes the label of the degeneracy. ω is one of the elements of
$\{\omega_{mn}|\ \langle E_n,r|s_{b\mu}|E_m,s\rangle \neq 0\ \ ^\exists\mu\}$. $s_{b\mu}(\omega)$ and ω depend on α_S. The eigenoperators satisfy

$$\sum_\omega s_{b\mu}(\omega) = s_{b\mu}, \tag{2.50}$$

and

$$[H_S, s_{b\mu}(\omega)] = -\omega s_{b\mu}(\omega). \tag{2.51}$$

Then, we obtain

$$\begin{aligned}\mathcal{L}^\chi_{b,\tau_{\rm CG}}(\alpha)\bullet \;=\; & -\frac{1}{\tau_{\rm CG}}\int_t^{t+\tau_{\rm CG}}du\int_t^{t+\tau_{\rm CG}}ds\ \sum_{\mu,\nu}\sum_{\omega,\omega'}\theta(u-s)\\ &\times\Big(\Big\{[s_{b\nu}(\omega')]^\dagger s_{b\mu}(\omega)\bullet C_{b,\nu\mu}(u-s)\\ &-s_{b\mu}(\omega)\bullet[s_{b\nu}(\omega')]^\dagger C^\chi_{b,\nu\mu}(u-s)\Big\}e^{-i\omega(s-t)}e^{i\omega'(u-t)}\\ &+\Big\{-s_{b\mu}(\omega)\bullet[s_{b\nu}(\omega')]^\dagger C^\chi_{b,\nu\mu}(s-u)\\ &+\bullet[s_{b\nu}(\omega')]^\dagger s_{b\mu}(\omega)C_{b,\nu\mu}(s-u)\Big\}e^{i\omega'(s-t)}e^{-i\omega(u-t)}\Big).\end{aligned} \tag{2.52}$$

In last two terms, we swapped μ and ν. $\theta(u-s)$ is the step function.

Now, we introduce

$$\Phi^\chi_{b,\nu\mu}(\Omega) \overset{\rm def}{=} \int_{-\infty}^\infty du\ C^\chi_{b,\nu\mu}(u)e^{i\Omega u}. \tag{2.53}$$

Then,

$$\begin{aligned}\int_{-\infty}^\infty du\ C^\chi_{b,\nu\mu}(u)\theta(u)e^{i\omega u} \;&=\; \frac{1}{2\pi}\int_0^\infty du\int_{-\infty}^\infty d\Omega\ \Phi^\chi_{b,\nu\mu}(\Omega)e^{-i\Omega u}e^{i\omega u}\\ &= \frac{1}{2\pi}\int_{-\infty}^\infty d\Omega\ \Big[\pi\delta(\Omega-\omega)-i\frac{\rm P}{\Omega-\omega}\Big]\Phi^\chi_{b,\nu\mu}(\Omega)\\ &= \frac{1}{2}\Phi^\chi_{b,\nu\mu}(\omega)-\frac{i}{2}\Psi^\chi_{b,\nu\mu}(\omega) = \Phi^{(+)\chi}_{b,\nu\mu}(\omega),\end{aligned} \tag{2.54}$$

holds. Here, P denotes the Cauchy principal value and

$$\Psi^{\chi}_{b,\nu\mu}(\omega) \stackrel{\rm def}{=} \frac{\rm P}{\pi}\int_{-\infty}^{\infty} d\Omega\ \frac{\Phi^{\chi}_{b,\nu\mu}(\Omega)}{\Omega-\omega}, \tag{2.55}$$

$$\Phi^{(\pm)\chi}_{b,\nu\mu}(\Omega) \stackrel{\rm def}{=} \frac{1}{2}\Phi^{\chi}_{b,\nu\mu}(\omega) \mp \frac{i}{2}\Psi^{\chi}_{b,\nu\mu}(\omega). \tag{2.56}$$

(2.54) leads

$$C^{\chi}_{b,\nu\mu}(u-s)\theta(u-s) = \int_{-\infty}^{\infty} d\Omega\ \frac{\Phi^{(+)\chi}_{b,\nu\mu}(\Omega)}{2\pi}e^{-i\Omega(u-s)}. \tag{2.57}$$

Similarly,

$$C^{\chi}_{b,\nu\mu}(s-u)\theta(u-s) = \int_{-\infty}^{\infty} d\Omega\ \frac{\Phi^{(-)\chi}_{b,\nu\mu}(\Omega)}{2\pi}e^{i\Omega(u-s)}, \tag{2.58}$$

holds. Then, we obtain

$$\begin{aligned}\mathcal{L}^{\chi}_{b,\tau_{\rm CG}}(\alpha)\bullet = &-\frac{1}{\tau_{\rm CG}}\int_t^{t+\tau_{\rm CG}} du \int_t^{t+\tau_{\rm CG}} ds \int_{-\infty}^{\infty}\frac{d\Omega}{2\pi}\ \sum_{\mu,\nu}\sum_{\omega,\omega'}\\ &\times\Big(\Big\{[s_{b\nu}(\omega')]^{\dagger}s_{b\mu}(\omega)\bullet\Phi^{(+)}_{b,\nu\mu}(\Omega)\\ &-s_{b\mu}(\omega)\bullet[s_{b\nu}(\omega')]^{\dagger}\Phi^{(+)\chi}_{b,\nu\mu}(\Omega)\Big\}e^{-i\Omega(u-s)}e^{-i\omega(s-t)}e^{i\omega'(u-t)}\\ &+\Big\{-s_{b\mu}(\omega)\bullet[s_{b\nu}(\omega')]^{\dagger}\Phi^{(-)\chi}_{b,\nu\mu}(\Omega)\\ &+\bullet[s_{b\nu}(\omega')]^{\dagger}s_{b\mu}(\omega)\Phi^{(-)}_{b,\nu\mu}(\Omega)\Big\}e^{i\Omega(u-s)}e^{i\omega'(s-t)}e^{-i\omega(u-t)}\Big),\end{aligned} \tag{2.59}$$

with $\Phi^{(\pm)}_{b,\nu\mu} = \Phi^{(\pm)\chi}_{b,\nu\mu}\big|_{\chi=0}$. The integrals for u and s are performed as

$$\int_t^{t+\tau_{\rm CG}} du\ e^{-i\Omega u}e^{i\omega'(u-t)} = \tau_{\rm CG}e^{-i\Omega t-i[\Omega-\omega']\tau_{\rm CG}/2}{\rm sinc}([\Omega-\omega']\tau_{\rm CG}/2), \tag{2.60}$$

$$\int_t^{t+\tau_{\rm CG}} ds\ e^{i\Omega s}e^{-i\omega(s-t)} = \tau_{\rm CG}e^{i\Omega t+i[\Omega-\omega]\tau_{\rm CG}/2}{\rm sinc}([\Omega-\omega]\tau_{\rm CG}/2), \tag{2.61}$$

then

$$\begin{aligned}\mathcal{L}^{\chi}_{b,\tau_{\rm CG}}(\alpha)\bullet = &-\sum_{\mu,\nu}\sum_{\omega,\omega'}\frac{e^{-i(\omega-\omega')/\tau_{\rm CG}}}{2\pi}\int_{-\infty}^{\infty} d\Omega\ \Big([s_{b\nu}(\omega')]^{\dagger}s_{b\mu}(\omega)\bullet\Phi^{(+)}_{b,\nu\mu}(\Omega)\\ &-s_{b\mu}(\omega)\bullet[s_{b\nu}(\omega')]^{\dagger}\Phi^{(+)\chi}_{b,\nu\mu}(\Omega)\\ &-s_{b\mu}(\omega)\bullet[s_{b\nu}(\omega')]^{\dagger}\Phi^{(-)\chi}_{b,\nu\mu}(\Omega)+\bullet[s_{b\nu}(\omega')]^{\dagger}s_{b\mu}(\omega)\Phi^{(-)}_{b,\nu\mu}(\Omega)\Big)\\ &\times\tau_{\rm CG}{\rm sinc}\frac{[\Omega-\omega']\tau_{\rm CG}}{2}{\rm sinc}\frac{[\Omega-\omega]\tau_{\rm CG}}{2},\end{aligned} \tag{2.62}$$

holds. Here, ${\rm sinc}(x) = \sin x/x$. The above equation can be rewritten as

$$\mathcal{L}^{\chi}_{b,\tau_{\rm CG}}(\alpha)\bullet = -i[h_{b,\tau_{\rm CG}}(\alpha),\bullet] + \Pi^{\chi}_{b,\tau_{\rm CG}}(\alpha)\bullet, \tag{2.63}$$

$$\begin{aligned}\Pi^{\chi}_{b,\tau_{\rm CG}}(\alpha)\bullet = &\sum_{\omega,\omega'}\sum_{\mu,\nu}\Big[\Phi^{\chi}_{b,\mu\nu}(\tau_{\rm CG},\omega,\omega')s_{b\nu}(\omega')\bullet[s_{b\mu}(\omega)]^{\dagger}\\ &-\frac{1}{2}\Phi_{b,\mu\nu}(\tau_{\rm CG},\omega,\omega')\bullet[s_{b\mu}(\omega)]^{\dagger}s_{b\nu}(\omega')\\ &-\frac{1}{2}\Phi_{b,\mu\nu}(\tau_{\rm CG},\omega,\omega')[s_{b\mu}(\omega)]^{\dagger}s_{b\nu}(\omega')\bullet\Big],\end{aligned} \tag{2.64}$$

with

$$h_{b,\tau_{\rm CG}}(\alpha) \;=\; -\frac{1}{2}\sum_{\omega,\omega'}\sum_{\mu,\nu}\Psi_{b,\mu\nu}(\tau_{\rm CG},\omega,\omega')[s_{b\mu}(\omega)]^\dagger s_{b\nu}(\omega'). \tag{2.65}$$

Here,

$$\begin{aligned}&X^\chi(\tau_{\rm CG},\omega,\omega')\\ &\;=\;\frac{e^{i(\omega-\omega')\tau_{\rm CG}/2}}{2\pi}\int_{-\infty}^{\infty}d\Omega\, X^\chi(\Omega)\tau_{\rm CG}{\rm sinc}\big(\frac{\tau_{\rm CG}(\Omega-\omega)}{2}\big){\rm sinc}\big(\frac{\tau_{\rm CG}(\Omega-\omega')}{2}\big),\end{aligned} \tag{2.66}$$

with $X = \Phi_{b,\mu\nu}, \Psi_{b,\mu\nu}$. $\Pi_{b,\tau_{\rm CG}} = \Pi^\chi_{b,\tau_{\rm CG}}\big|_{\chi=0}$ is the Lindblad type. By the way, from

$$[C_{b,\mu\nu}(t)]^* \;=\; C_{b,\nu\mu}(-t), \tag{2.67}$$

relations

$$[\Phi_{b,\mu\nu}(\Omega)]^* \;=\; \Phi_{b,\nu\mu}(\Omega), \tag{2.68}$$

and $[\Psi_{\mu\nu}(\Omega)]^* = \Psi_{\nu\mu}(\Omega)$ hold. Then,

$$[\Phi_{b,\mu\nu}(\tau_{\rm CG},\omega,\omega')]^* \;=\; \Phi_{b,\nu\mu}(\tau_{\rm CG},\omega',\omega), \tag{2.69}$$

holds.

3 回転波近似 (RWA)

Born-Markov 近似の量子マスター方程式は、相互作用描像で、

$$\frac{d\rho_S^{I,\chi}(t)}{dt} = -\int_0^\infty ds\ \mathrm{Tr}_B\Big\{[H_{\mathrm{int}}^I(t), [H_{\mathrm{int}}^I(t-s), \rho_S^{I,\chi}(t)\rho_B(\alpha_B(t))]_\chi]_\chi\Big\} \tag{3.1}$$

である。注目系のハミルトニアンが時間によらない場合、この右辺を eigenoperator を使って書き、

$$e^{i(\omega-\omega')t} \approx \delta_{\omega,\omega'} \tag{3.2}$$

と近似したものが、相互作用描像での回転波近似 (RWA) である。それをシュレーディンガー描像に移したものが RWA である。注目系のハミルトニアンが時間による場合の RWA とは何だろうか。注目系のハミルトニアンが時間によらない場合には、RWA は CGA で $\tau_{\mathrm{CG}} \to \infty$ としたものと一致する。よって、注目系のハミルトニアンが時間による場合の RWA を、CGA で $\tau_{\mathrm{CG}} \to \infty$ ($\tau_{\mathrm{CG}} \cdot \min_{\omega\neq\omega'} |\omega-\omega'| \gg 1$) としたものとして定義する。In this limit,

$$\Phi_{b,\mu\nu}^\chi(\tau_{\mathrm{CG}},\omega,\omega') \approx \Phi_{b,\mu\nu}^\chi(\omega)\delta_{\omega,\omega'},\ \Psi_{b,\mu\nu}^\chi(\tau_{\mathrm{CG}},\omega,\omega') \approx \Psi_{b,\mu\nu}^\chi(\omega)\delta_{\omega,\omega'}, \tag{3.3}$$

hold because of the fact that

$$\lim_{\tau_{\mathrm{CG}}\to\infty} \tau_{\mathrm{CG}}\mathrm{sinc}\frac{\tau_{\mathrm{CG}}(\Omega-\omega)}{2}\mathrm{sinc}\frac{\tau_{\mathrm{CG}}(\Omega-\omega')}{2} = 2\pi\delta_{\omega,\omega'}\delta(\Omega-\omega). \tag{3.4}$$

If H_S is time independent, this RWA is equivalent to usual RWA. $\mathcal{L}_b^\chi(\alpha)$ is given by

$$\mathcal{L}_b^\chi(\alpha)\bullet = \Pi_b^\chi(\alpha)\bullet - i[h_b(\alpha),\bullet], \tag{3.5}$$

where $h_b(\alpha)$ is a Hermitian operator describing the Lamb shift. $H_{\mathrm{L}}(\alpha) \stackrel{\mathrm{def}}{=} \sum_b h_b(\alpha)$ is called the Lamb shift Hamiltonian. $\Pi_b^\chi(\alpha)$ and $h_b(\alpha)$ are given by

$$\begin{aligned}\Pi_b^\chi(\alpha)\bullet &= \sum_\omega\sum_{\mu,\nu}\Big[\Phi_{b,\mu\nu}^\chi(\omega)s_{b\nu}(\omega)\bullet[s_{b\mu}(\omega)]^\dagger \\ &\quad -\frac{1}{2}\Phi_{b,\mu\nu}(\omega)\bullet[s_{b\mu}(\omega)]^\dagger s_{b\nu}(\omega) - \frac{1}{2}\Phi_{b,\mu\nu}(\omega)[s_{b\mu}(\omega)]^\dagger s_{b\nu}(\omega)\bullet\Big], \qquad (3.6)\\ h_b(\alpha) &= -\frac{1}{2}\sum_\omega\sum_{\mu,\nu}\Psi_{b,\mu\nu}(\omega)[s_{b\mu}(\omega)]^\dagger s_{b\nu}(\omega). \qquad (3.7)\end{aligned}$$

Because of (2.51), $h_b(\alpha)$ commutes with $H_S(\alpha_S)$:

$$[h_b(\alpha), H_S(\alpha_S)] = 0. \tag{3.8}$$

4 Born-Markov 近似

We denote $\mathcal{L}_b^\chi$ in the Born-Markov approximation by $\mathcal{L}_{b(\mathrm{BM})}^\chi$. From (3.1) and (2.43), we obtain

$$\mathcal{L}_{b(\mathrm{BM})}^\chi \bullet = -\int_0^\infty ds \sum_{\mu,\nu} \Big(s_{b\nu}^\dagger s_{b\mu}^I(t-s,t) \bullet C_{b,\nu\mu}(s) - s_{b\mu}^I(t-s,t) \bullet s_{b\nu}^\dagger C_{b,\nu\mu}^\chi(s)$$
$$- s_{b\nu} \bullet s_{b\mu}^{I\dagger}(t-s,t) C_{b,\mu\nu}^\chi(-s) + \bullet s_{b\mu}^{I\dagger}(t-s,t) s_{b\nu} C_{b,\mu\nu}(-s) \Big). \quad (4.1)$$

$C_{b,\mu\nu}(s)$ damps exponentially as $e^{-|s|/\tau_b}$ where τ_b is the relaxation time of the bath b. Then, in the calculations of $s_{b\mu}^I(t-s,t)$ and $s_{b\mu}^{I\dagger}(t-s,t)$, the values of the control parameters can be approximated by $\alpha_S(t)$. Then, we obtain

$$s_{b\mu}^I(t-s,t) = \sum_\omega e^{i\omega s} s_{b\mu}(\omega),\ \ s_{b\mu}^{I\dagger}(t-s,t) = \sum_\omega e^{-i\omega s} [s_{b\mu}(\omega)]^\dagger, \quad (4.2)$$

and

$$\mathcal{L}_{b(\mathrm{BM})}^\chi \bullet = -\int_0^\infty ds \sum_{\mu,\nu}\sum_\omega \Big(\Big\{ s_{b\nu}^\dagger s_{b\mu}(\omega) \bullet C_{b,\nu\mu}(s) - s_{b\mu}(\omega) \bullet s_{b\nu}^\dagger C_{b,\nu\mu}^\chi(s) \Big\} e^{i\omega s}$$
$$+ \Big\{ - s_{b\nu} \bullet [s_{b\mu}(\omega)]^\dagger C_{b,\mu\nu}^\chi(-s) + \bullet [s_{b\mu}(\omega)]^\dagger s_{b\nu} C_{b,\mu\nu}(-s) \Big\} e^{-i\omega s} \Big). \quad (4.3)$$

Here,

$$\begin{aligned}\int_0^\infty ds\ C_{b,\nu\mu}^\chi(s) e^{i\omega s} &= \int_0^\infty ds \int_{-\infty}^\infty d\Omega\ \frac{1}{2\pi} \Phi_{b,\nu\mu}^\chi(\Omega) e^{i(\omega-\Omega)s} \\ &= \int_{-\infty}^\infty d\Omega\ \frac{1}{2\pi} \Big[\pi\delta(\Omega-\omega) - i\mathrm{P}\frac{1}{\Omega-\omega} \Big] \Phi_{b,\nu\mu}^\chi(\Omega) \\ &= \Phi_{b,\nu\mu}^{(+)\chi}(\omega), \end{aligned} \quad (4.4)$$

and

$$\int_0^\infty ds\ C_{b,\mu\nu}^\chi(-s) e^{-i\omega s} = \Phi_{b,\mu\nu}^{(-)\chi}(\omega), \quad (4.5)$$

hold. Then, we get

$$\begin{aligned}\mathcal{L}_{b(\mathrm{BM})}^\chi \bullet &= -\sum_{\mu,\nu}\sum_\omega \Big(s_{b\mu}^\dagger s_{b\nu}(\omega) \bullet \Phi_{b,\mu\nu}^{(+)}(\omega) - s_{b\nu}(\omega) \bullet s_{b\mu}^\dagger \Phi_{b,\mu\nu}^{(+)\chi}(\omega) \\ &\quad - s_{b\nu} \bullet [s_{b\mu}(\omega)]^\dagger \Phi_{b,\mu\nu}^{(-)\chi}(\omega) + \bullet [s_{b\mu}(\omega)]^\dagger s_{b\nu} \Phi_{b,\mu\nu}^{(-)}(\omega) \Big) \\ &= \mathcal{L}_{b(\mathrm{BM})}^{\Phi,\chi} \bullet + \mathcal{L}_{b(\mathrm{BM})}^{\Phi,\chi} \bullet . \end{aligned} \quad (4.6)$$

Here,

$$\begin{aligned}\mathcal{L}_{b(\mathrm{BM})}^{\Phi,\chi} \bullet &= -\frac{1}{2}\sum_{\mu,\nu}\sum_\omega \Big(\Phi_{b,\mu\nu}(\omega) s_{b\mu}^\dagger s_{b\nu}(\omega) \bullet - \Phi_{b,\mu\nu}^\chi(\omega) s_{b\nu}(\omega) \bullet s_{b\mu}^\dagger \\ &\quad - \Phi_{b,\mu\nu}^\chi(\omega) s_{b\nu} \bullet [s_{b\mu}(\omega)]^\dagger + \Phi_{b,\mu\nu}(\omega) \bullet [s_{b\mu}(\omega)]^\dagger s_{b\nu} \Big), \end{aligned} \quad (4.7)$$

$$\begin{aligned}\mathcal{L}_{b(\mathrm{BM})}^{\Psi,\chi} \bullet &= \frac{i}{2}\sum_{\mu,\nu}\sum_\omega \frac{1}{2} \Big(\Psi_{b,\mu\nu}(\omega) s_{b\mu}^\dagger s_{b\nu}(\omega) \bullet - \Psi_{b,\mu\nu}^\chi(\omega) s_{b\nu}(\omega) \bullet s_{b\mu}^\dagger \\ &\quad + \Psi_{b,\mu\nu}^\chi(\omega) s_{b\nu} \bullet [s_{b\mu}(\omega)]^\dagger - \bullet \Psi_{b,\mu\nu}(\omega) [s_{b\mu}(\omega)]^\dagger s_{b\nu} \Big). \end{aligned} \quad (4.8)$$

5 具体的な系

In this section, we consider $b = n_\mathrm{C}+1, \cdots, n_\mathrm{C}+n_\mathrm{GC}$. Now we suppose

$$H_{Sb}(\alpha_{Sb}) = \sum_\alpha a_\alpha^\dagger B_{b\alpha} + \mathrm{h.c.},\ B_{b\alpha} = \sum_{k,\sigma} V_{bk\sigma,\alpha}(\alpha_{Sb}) c_{bk\sigma}\ (b \in \boldsymbol{\mathcal{G}}), \tag{5.1}$$

where a_α and $c_{bk\sigma}$ are single-particle annihilation operators of the system and of the bath b.

5.1 CGA

Using

$$\mathrm{Tr}_b[\rho_b B^I_{b\alpha}(t') B^I_{b\beta}(t'')] = 0 = \mathrm{Tr}_b[\rho_b B^{I\dagger}_{b\alpha}(t') B^{I\dagger}_{b\beta}(t'')], \tag{5.2}$$

we obtain

$$\begin{aligned}
\mathcal{L}^\chi_{b,\tau_\mathrm{CG}}(\alpha)\bullet &= -i[h_{b,\tau_\mathrm{CG}}(\alpha), \bullet] + \Pi^\chi_{b,\tau_\mathrm{CG}}(\alpha)\bullet, \\
\Pi^\chi_{b,\tau_\mathrm{CG}}(\alpha)\bullet &= \sum_{\omega,\omega'}\sum_{\alpha,\beta}\Big[\Phi^{-,\chi}_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega') a_\beta(\omega') \bullet [a_\alpha(\omega)]^\dagger \\
&\quad -\frac{1}{2}\Phi^-_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega') \bullet [a_\alpha(\omega)]^\dagger a_\beta(\omega') \\
&\quad -\frac{1}{2}\Phi^-_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega') [a_\alpha(\omega)]^\dagger a_\beta(\omega') \bullet \\
&\quad +\Phi^{+,\chi}_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega') [a_\beta(\omega')]^\dagger \bullet a_\alpha(\omega) \\
&\quad -\frac{1}{2}\Phi^+_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega') \bullet a_\alpha(\omega) [a_\beta(\omega')]^\dagger \\
&\quad -\frac{1}{2}\Phi^+_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega') a_\alpha(\omega) [a_\beta(\omega')]^\dagger \bullet \Big],
\end{aligned} \tag{5.3}$$

and

$$\begin{aligned}
h_{b,\tau_\mathrm{CG}}(\alpha) &= \sum_{\omega,\omega'}\sum_{\alpha,\beta}\Big[-\frac{1}{2}\Psi^-_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega')[a_\alpha(\omega)]^\dagger a_\beta(\omega') \\
&\quad +\frac{1}{2}\Psi^+_{b,\alpha\beta}(\tau_\mathrm{CG},\omega,\omega') a_\alpha(\omega)[a_\beta(\omega')]^\dagger\Big].
\end{aligned} \tag{5.4}$$

The eigenoperators $a_\alpha(\omega)$ are given by

$$a_\alpha(\omega) = \sum_{n,m,r,s} \delta_{\omega_{mn},\omega} |E_n, r\rangle\langle E_n, r|a_\alpha|E_m, s\rangle\langle E_m, s|. \tag{5.5}$$

ω is one of the elements of $\{\omega_{mn}|\ \langle E_n, r|a_\alpha|E_m, s\rangle \neq 0\ {}^\exists\alpha\}$. $a_\alpha(\omega)$ satisfy

$$\sum_\omega a_\alpha(\omega) = a_\alpha, \tag{5.6}$$

and

$$[H_S, a_\alpha(\omega)] = -\omega a_\alpha(\omega),\ [N_S, a_\alpha(\omega)] = -a_\alpha(\omega). \tag{5.7}$$

N_S is total number operator of the system. Here and in the following, we suppose

$$[N_S, H_S] = 0. \tag{5.8}$$

If $n_{\rm GC} = 0$, existence of N_S and the above equation are not required. In (5.3) and (5.4),

$$X^{\pm,\chi}(\tau_{\rm CG},\omega,\omega') = \frac{e^{\pm i(\omega-\omega')\tau_{\rm CG}/2}}{2\pi}\int_{-\infty}^{\infty} d\Omega\, X^{\pm,\chi}(\Omega)\tau_{\rm CG}{\rm sinc}\big(\frac{\tau_{\rm CG}(\Omega-\omega)}{2}\big){\rm sinc}\big(\frac{\tau_{\rm CG}(\Omega-\omega')}{2}\big), \tag{5.9}$$

and $X^{\pm}(\tau_{\rm CG},\omega,\omega') = X^{\pm,\chi}(\tau_{\rm CG},\omega,\omega')\big|_{\chi=0}$. Here, $X^{\pm,\chi}(\Omega)$ denotes one of $\Phi^{\pm,\chi}_{b,\alpha,\beta}(\Omega)$, $\Psi^{\pm,\chi}_{b,\alpha\beta}(\Omega)$, where

$$\Phi^{-,\chi}_{b,\alpha\beta}(\Omega) = \int_{-\infty}^{\infty} du\ {\rm Tr}_b[\rho_b B^I_{b\alpha,-2\chi}(u)B^\dagger_{b\beta}]e^{i\Omega u}, \tag{5.10}$$

$$\Phi^{+,\chi}_{b,\alpha\beta}(\Omega) = \int_{-\infty}^{\infty} du\ {\rm Tr}_b[\rho_b B^{\dagger I}_{b\alpha,-2\chi}(u)B_{b\beta}]e^{-i\Omega u}, \tag{5.11}$$

$$\Psi^{\pm,\chi}_{b,\alpha\beta}(\Omega) \stackrel{\rm def}{=} \frac{\rm P}{\pi}\int_{-\infty}^{\infty} d\Omega'\ \frac{\Phi^{\pm,\chi}_{b,\alpha\beta}(\Omega')}{\Omega'-\Omega}. \tag{5.12}$$

We set $\{O_\mu\} = \{N_b\}_{b\in\boldsymbol{\mathcal{G}}} + \{H_b\}_b$, where

$$N_b = \sum_{k,\sigma} c^\dagger_{bk\sigma}c_{bk\sigma}. \tag{5.13}$$

Whenever H_b is an element of $\{O_\mu\}$, we suppose α'_b are fixed. We introduce the eigenoperator

$$B_{b\alpha}(\Omega_b) = \sum_{n,m,r,s} \delta_{\Omega_{b,mn},\Omega_b}|E_{b,n},r\rangle\langle E_{b,n},r|B_{b\alpha}|E_{b,m},s\rangle\langle E_{b,m},s|, \tag{5.14}$$

with $\Omega_{b,mn} = E_{b,m} - E_{b,n}$ and $H_b|E_{b,n},r\rangle = E_{b,n}|E_{b,n},r\rangle$. r denotes the label of the degeneracy. Ω_b is one of the elements of $\{\Omega_{b,mn}|\ \langle E_{b,n},r|B_{b\alpha}|E_{b,m},s\rangle \neq 0\ \ ^\exists\alpha\}$. The relations

$$\sum_{\Omega_b} B_{b\alpha}(\Omega_b) = B_{b\alpha}, \tag{5.15}$$

and

$$[H_b, B_{b\alpha}(\Omega_b)] = -\Omega_b B_{b\alpha}(\Omega_b),\ [N_b, B_{b\alpha}(\Omega_b)] = -B_{b\alpha}(\Omega_b) \tag{5.16}$$

hold. Then, we obtain

$$B^I_{b\alpha,-2\chi}(u) = \sum_{\Omega_b} B_{b\alpha}(\Omega_b)e^{-i\Omega_b u + i\chi_{H_b}\Omega_b + i\chi_{N_b}}, \tag{5.17}$$

$$B^{\dagger I}_{b\alpha,-2\chi}(u) = \sum_{\Omega_b}[B_{b\alpha}(\Omega_b)]^\dagger e^{i\Omega_b u - i\chi_{H_b}\Omega_b - i\chi_{N_b}}, \tag{5.18}$$

and

$$\begin{aligned}\Phi^{-,\chi}_{b,\alpha\beta}(\Omega) &= 2\pi\sum_{\Omega_b}\delta(\Omega-\Omega_b)e^{i\chi_{H_b}\Omega_b+i\chi_{N_b}}{\rm Tr}_b(\rho_b B_{b\alpha}(\Omega_b)B^\dagger_{b\beta}) \\ &= e^{i\chi_{H_b}\Omega+i\chi_{N_b}}2\pi\sum_{\Omega_b}\delta(\Omega-\Omega_b){\rm Tr}_b(\rho_b B_{b\alpha}(\Omega_b)[B_{b\beta}(\Omega_b)]^\dagger),\end{aligned} \tag{5.19}$$

$$\begin{aligned}\Phi^{+,\chi}_{b,\alpha\beta}(\Omega) &= 2\pi\sum_{\Omega_b}\delta(\Omega-\Omega_b)e^{-i\chi_{H_b}\Omega_b-i\chi_{N_b}}{\rm Tr}_b(\rho_b [B_{b\alpha}(\Omega_b)]^\dagger B_{b\beta}) \\ &= e^{-i\chi_{H_b}\Omega-i\chi_{N_b}}2\pi\sum_{\Omega_b}\delta(\Omega-\Omega_b){\rm Tr}_b(\rho_b[B_{b\alpha}(\Omega_b)]^\dagger B_{b\beta}(\Omega_b)).\end{aligned} \tag{5.20}$$

Here, we used (5.15) and $\mathrm{Tr}_b(\rho_b B_{b\alpha}(\Omega_b)[B_{b\beta}(\Omega'_b)]^\dagger)=0$ and $\mathrm{Tr}_b(\rho_b [B_{b\alpha}(\Omega_b)]^\dagger B_{b\beta}(\Omega'_b))=0$ for $\Omega_b\neq\Omega'_b$. Then, we obtain

$$\Phi^{\pm,\chi}_{b,\alpha\beta}(\Omega)=e^{\mp(i\chi_{H_b}\Omega+i\chi_{N_b})}\Phi^{\pm}_{b,\alpha\beta}(\Omega), \tag{5.21}$$

with $\Phi^{\pm}_{b,\alpha\beta}(\Omega)=\Phi^{\pm,\chi}_{b,\alpha\beta}(\Omega)\big|_{\chi=0}$ and

$$\Psi^{-}_{b,\alpha\beta}(\Omega) = 2\sum_{\Omega_b}\mathrm{P}\frac{1}{\Omega_b-\Omega}\mathrm{Tr}_b(\rho_b B_{b\alpha}(\Omega_b)[B_{b\beta}(\Omega_b)]^\dagger), \tag{5.22}$$

$$\Psi^{+}_{b,\alpha\beta}(\Omega) = 2\sum_{\Omega_b}\mathrm{P}\frac{1}{\Omega_b-\Omega}\mathrm{Tr}_b(\rho_b [B_{b\alpha}(\Omega_b)]^\dagger B_{b\beta}(\Omega_b)). \tag{5.23}$$

$\Phi^{\pm}_{b,\alpha\beta}(\Omega)$ satisfy

$$[\Phi^{\pm}_{b,\alpha\beta}(\Omega)]^* = \Phi^{\pm}_{b,\beta\alpha}(\Omega), \tag{5.24}$$

$$\Phi^{+}_{b,\alpha\beta}(\Omega) = e^{-\beta_b(\Omega-\mu_b)}\Phi^{-}_{b,\beta\alpha}(\Omega). \tag{5.25}$$

The latter is the Kubo-Martin-Schwinger (KMS) condition. (5.25) is derived from $\rho_b B_{b\alpha}(\Omega_b)=e^{\beta_b(\Omega_b-\mu)}B_{b\alpha}(\Omega_b)\rho_b$ (derived from (5.16)) and (5.19) and (5.20).

Here, we suppose the free Hamiltonian of the bath b:

$$H_b(\alpha'_b)=\sum_{k,\sigma}\varepsilon_{bk\sigma}(\alpha'_b)c^\dagger_{bk\sigma}c_{bk\sigma}, \tag{5.26}$$

and $\{O_\mu\}=\{N_{b\sigma}\}_{b\sigma}$ with

$$N_{b\sigma} = \sum_k c^\dagger_{bk\sigma}c_{bk\sigma}. \tag{5.27}$$

In this case, α'_b can depend on time and

$$\Phi^{-,\chi}_{b,\alpha\beta}(\Omega) = 2\pi\sum_{k,\sigma}V_{bk\sigma,\alpha}V^*_{bk\sigma,\beta}F^-_b(\varepsilon_{bk\sigma})e^{i\chi_{b\sigma}}\delta(\varepsilon_{bk\sigma}-\Omega), \tag{5.28}$$

$$\Phi^{+,\chi}_{b,\alpha\beta}(\Omega) = 2\pi\sum_{k,\sigma}V^*_{bk\sigma,\alpha}V_{bk\sigma,\beta}F^+_b(\varepsilon_{bk\sigma})e^{-i\chi_{b\sigma}}\delta(\varepsilon_{bk\sigma}-\Omega), \tag{5.29}$$

$$\Psi^{-,\chi}_{b,\alpha\beta}(\Omega) = 2\sum_{k,\sigma}V_{bk\sigma,\alpha}V^*_{bk\sigma,\beta}F^-_b(\varepsilon_{bk\sigma})e^{i\chi_{b\sigma}}\mathrm{P}\frac{1}{\varepsilon_{bk\sigma}-\Omega}, \tag{5.30}$$

$$\Psi^{+,\chi}_{b,\alpha\beta}(\Omega) = 2\sum_{k,\sigma}V^*_{bk\sigma,\alpha}V_{bk\sigma,\beta}F^+_b(\varepsilon_{bk\sigma})e^{-i\chi_{b\sigma}}\mathrm{P}\frac{1}{\varepsilon_{bk\sigma}-\Omega}, \tag{5.31}$$

hold. $\chi_{b\sigma}$ denotes the counting fields for $N_{b\sigma}$. If the baths are fermions, $F^+_b(\varepsilon)=f_b(\varepsilon)\stackrel{\text{def}}{=}[\exp(\beta_b(\varepsilon-\mu_b))+1]^{-1}$ and $F^-_b(\varepsilon)=1-f_b(\varepsilon)$. If the baths are bosons, $F^+_b(\varepsilon)=n_b(\varepsilon)\stackrel{\text{def}}{=}[\exp(\beta_b(\varepsilon-\mu_b))-1]^{-1}$ and $F^-_b(\varepsilon)=1+n_b(\varepsilon)$.

5.2 RWA

For (5.1), $\Pi_b^\chi(\alpha)$ in (3.5) is given by

$$\begin{aligned}\Pi_b^\chi(\alpha)\bullet \;=\; \sum_\omega\sum_{\alpha,\beta}\Big[&\Phi^{-,\chi}_{b,\alpha\beta}(\omega)a_\beta(\omega)\bullet[a_\alpha(\omega)]^\dagger-\frac{1}{2}\Phi^{-}_{b,\alpha\beta}(\omega)\bullet[a_\alpha(\omega)]^\dagger a_\beta(\omega)\\ &-\frac{1}{2}\Phi^{-}_{b,\alpha\beta}(\omega)[a_\alpha(\omega)]^\dagger a_\beta(\omega)\bullet+\Phi^{+,\chi}_{b,\alpha\beta}(\omega)[a_\beta(\omega)]^\dagger\bullet a_\alpha(\omega)\\ &-\frac{1}{2}\Phi^{+}_{b,\alpha\beta}(\omega)\bullet a_\alpha(\omega)[a_\beta(\omega)]^\dagger-\frac{1}{2}\Phi^{+}_{b,\alpha\beta}(\omega)a_\alpha(\omega)[a_\beta(\omega)]^\dagger\bullet\Big].\end{aligned}\tag{5.32}$$

The Lamb shift is given by

$$h_b(\alpha) \;=\; \sum_\omega\sum_{\alpha,\beta}\Big(-\frac{1}{2}\Psi^{-}_{b,\alpha\beta}(\omega)[a_\alpha(\omega)]^\dagger a_\beta(\omega)+\frac{1}{2}\Psi^{+}_{b,\alpha\beta}(\omega)a_\alpha(\omega)[a_\beta(\omega)]^\dagger\Big).\tag{5.33}$$

The second equation of (5.7) leads

$$[h_b(\alpha),N_S]=0.\tag{5.34}$$

5.3 Born-Markov 近似

For (5.1), we obtain

$$\begin{aligned}\mathcal{L}^{\Phi,\chi}_{b(\mathrm{BM})}\bullet \;=\; -\frac{1}{2}\sum_{\alpha,\beta}\sum_\omega\Big(&\Phi^{-}_{b,\alpha\beta}(\omega)a_\alpha^\dagger a_\beta(\omega)\bullet-\Phi^{-,\chi}_{b,\alpha\beta}(\omega)a_\beta(\omega)\bullet a_\alpha^\dagger\\ &-\Phi^{-,\chi}_{b,\alpha\beta}(\omega)a_\beta\bullet[a_\alpha(\omega)]^\dagger+\Phi^{-}_{b,\alpha\beta}(\omega)\bullet[a_\alpha(\omega)]^\dagger a_\beta\\ &+\Phi^{+}_{b,\alpha\beta}(\omega)a_\alpha[a_\beta(\omega)]^\dagger\bullet-\Phi^{+,\chi}_{b,\alpha\beta}(\omega)[a_\beta(\omega)]^\dagger\bullet a_\alpha\\ &-\Phi^{+,\chi}_{b,\alpha\beta}(\omega)a_\beta^\dagger\bullet a_\alpha(\omega)+\Phi^{+}_{b,\alpha\beta}(\omega)\bullet a_\alpha(\omega)a_\beta^\dagger\Big),\end{aligned}\tag{5.35}$$

and

$$\begin{aligned}\mathcal{L}^{\Psi,\chi}_{b(\mathrm{BM})}\bullet \;=\; \frac{i}{2}\sum_{\alpha,\beta}\sum_\omega\Big(&\Psi^{-}_{b,\alpha\beta}(\omega)a_\alpha^\dagger a_\beta(\omega)\bullet-\Psi^{-,\chi}_{b,\alpha\beta}(\omega)a_\beta(\omega)\bullet a_\alpha^\dagger\\ &+\Psi^{-,\chi}_{b,\alpha\beta}(\omega)a_\beta\bullet[a_\alpha(\omega)]^\dagger-\Psi^{-}_{b,\alpha\beta}(\omega)\bullet[a_\alpha(\omega)]^\dagger a_\beta\\ &-\Psi^{+}_{b,\alpha\beta}(\omega)a_\alpha[a_\beta(\omega)]^\dagger\bullet+\Psi^{+,\chi}_{b,\alpha\beta}(\omega)[a_\beta(\omega)]^\dagger\bullet a_\alpha\\ &-\Psi^{+,\chi}_{b,\alpha\beta}(\omega)a_\beta^\dagger\bullet a_\alpha(\omega)+\Psi^{+}_{b,\alpha\beta}(\omega)\bullet a_\alpha(\omega)a_\beta^\dagger\Big).\end{aligned}\tag{5.36}$$

6　特異摂動と量子マスター方程式

これまで射影演算子法や、素朴な摂動論から量子マスター方程式を導出してきたが、これがどうゆう近似で何をやっているのかよく分からない。久木田 [4, 5] によると、回転波近似の量子マスター方程式は、特異摂動論で理解できる。私のノート [6] ではそれについて解説を試みた。

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