Lindblad Equation

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I. LINDBLAD MASTER EQUATION

A. General Markovian Form

For general open quantum evolution, suppose the system and environment are separable initially: $\rho_T = \rho \otimes \rho_B$, where we assume $\rho_B = \sum_\alpha \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$. Then the evolution of system-bath is unitary: $\rho_T(t) = U(t)\rho_T U^\dagger(t)$. Trace out the environment's degrees of freedom, we have the quantum channel expression:

$$\rho(t) = \sum_{\alpha\beta} W_{\alpha\beta}\rho W^\dagger_{\alpha\beta}, \quad W_{\alpha\beta} = \sqrt{\lambda_\beta}\langle\phi_\alpha|U(t)|\phi_\beta\rangle. \tag{1}$$

In general, the evolution of an open quantum system has the form $\rho(t) = \mathcal{L}_t[\rho]$. The Lindblad equation assumes a semi-group relation: $\mathcal{L}_t = \lim_{N\to\infty} \mathcal{L}_{t/N}\cdot\mathcal{L}_{t/N}\cdots\mathcal{L}_{t/N}$. Such time decimation implies that the evolution is Markovian. We will show that Markovian approximation leads directly to the Lindblad equation. First, we choose a complete operator basis $\{F_i\}$ in N-dimensional Hilbert space, satisfying $\mathrm{Tr}[F_i^\dagger F_j] = \delta_{ij}$, where we choose $F_0 = N^{-1/2}\cdot\mathbb{I}$. For a quantum channel, the channel operator K_μ can be expanded as $K_\mu = \sum_i \mathrm{Tr}[F_i^\dagger K_\mu]F_i$. In general, we have:

$$\mathcal{L}_t[\rho] = \sum_{ij} c_{ij}(t)F_i\rho F_j^\dagger,$$

where the Hermitian coefficient $c_{ij}(t)$ is $c_{ij}(t) = \sum_\mu \mathrm{Tr}[F_i^\dagger K_\mu] \cdot \mathrm{Tr}[F_j^\dagger K_\mu]^*$. Our target is to compute the limit

$$\frac{d}{dt}\rho \equiv \lim_{t\to 0} \frac{1}{t}(\mathcal{L}_t[\rho] - \rho).$$

For this purpose, we define the (Hermitian) coefficient a_{ij} as:

$$a_{00} = \lim_{t\to 0} \frac{c_{00}(t) - N}{t}, \quad a_{ij} = \lim_{t\to 0} \frac{c_{ij}(t)}{t}.$$

The limit is then

$$\frac{d}{dt}\rho = \frac{a_{00}}{N}\rho + \frac{1}{\sqrt{N}} \sum_{i>0} \left(a_{i0} F_i \rho + a_{i0}^* \rho F_i^\dagger \right) + \sum_{i,j>0} a_{ij} F_i \rho F_j^\dagger.$$

To further simplify the expression, we define

$$F = \frac{1}{\sqrt{N}} \sum_{i=1}^{N^2-1} a_{i0} F_i, \quad G = \frac{1}{2N} a_{00}\mathbb{I} + \frac{1}{2}(F^\dagger + F), \quad H = \frac{1}{2i}(F^\dagger - F).$$

The limit can be expressed by G, H in a compact form:

$$\frac{d\rho}{dt} = -i[H, \rho] + \{G, \rho\} + \sum_{i,j=1}^{N^2-1} a_{ij} F_i \rho F_j^\dagger. \tag{2}$$

Note the $[H, \rho]$ part is the traceless part and the $\{G, \rho\}$ is the trace part. Since the quantum channel preserves the trace (for any ρ):

$$\mathrm{Tr}\left[\frac{d\rho}{dt}\right] = \mathrm{Tr}\left[\left(2G + \sum_{i,j=1}^{N^2-1} a_{ij} F_j^\dagger F_i\right)\rho\right] = 0.$$

Therefore $G = -\frac{1}{2}\sum_{i,j=1}^{N^2-1} a_{ij} F_j^\dagger F_i$. We thus obtain the Lindblad form:

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_{i,j=1}^{N^2-1} a_{ij} \left(F_i \rho F_j^\dagger - \frac{1}{2}\{F_j^\dagger F_i, \rho\} \right).$$

We can further simplify the form by diagonalizing the matrix a_{ij}. It is a convention to take the norm of a_{ij} out to indicate the strength of the system-bath coupling, and the diagonalized Lindblad equation is

$$\frac{d\rho}{dt} = -i[H, \rho] + \gamma \sum_m \left(L_m \rho L_m^\dagger - \frac{1}{2}\{L_m^\dagger L_m, \rho\} \right). \tag{3}$$

B. First Principal Deduction

In this section, we consider a general system-bath coupling:[1]

$$H_T = H + H_B + V, \quad V = \sum_k A_k \otimes B_k. \tag{4}$$

We will show under certain condition, the dynamics of the system is well approximated by the Lindblad equation. We first assume that initially, the total system is a product state

$$\rho_T(0) = \rho(0) \otimes \rho_B.$$

[1] Without loss of generality, we can also assume $\|A_k\| = 1$, $\mathrm{Tr}[\rho_B B_k] = 0$.

In the following, we will adopt the interacting picture, where the density operator evolves as

$$\partial_t \rho_T(t) = -i[V(t), \rho_T(t)] \equiv -i\mathcal{V}(t)|\rho_T(t)\rangle.$$

Note that in the last equality, ρ_T is expressed as a ket in the Hilbert space of linear operator, and the commutator with V is expressed as a superoperator $\mathcal{V}$. This notation can simplify the expression. For example, the inner product in the operator space is the trace, so the partial trace operation can be denoted as $|\rho\rangle = \langle \mathbb{I}_B|\rho_T\rangle$. The evolution of the system is then

$$\begin{aligned}\frac{d}{dt}|\rho(t)\rangle &= -i\langle \mathbb{I}_B|\mathcal{V}(t)|\rho_T(t)\rangle = -i\langle \mathbb{I}_B|\mathcal{V}(t)|\rho_T(0)\rangle - \int_0^t \langle \mathbb{I}_B|\mathcal{V}(t)\mathcal{V}(\tau)|\rho_T(\tau)\rangle d\tau \\ &= -\int_0^t \langle \mathbb{I}_B|\mathcal{V}(t)\mathcal{V}(\tau)|\rho_T(\tau)\rangle d\tau.\end{aligned}$$

Now we are taking the **Born approximation**, which states when the coupling is weak enough compared with the energy scale of the system and the bath, the total density matrix is approximated by the product state $|\rho_T(t)\rangle \approx |\rho(t)\rangle \otimes |\rho_B\rangle$. The evolution is now

$$\begin{aligned}\frac{d}{dt}\rho(t) &\approx \int_0^t \mathrm{Tr}_B\left[V(t)\rho_T(\tau)V(\tau) - \rho_T(\tau)V(\tau)V(t)\right] d\tau + h.c. \\ &= \sum_{kl}\int_0^t d\tau\ C_{lk}(\tau - t)\left[A_k(t)\rho(\tau)A_l(\tau) - \rho(\tau)A_l(\tau)A_k(t)\right] + h.c.,\end{aligned}$$

where $C_{kl}(t) \equiv \mathrm{Tr}_B[\rho_B B_k(t) B_l]$ is the correlation function of B_k's. We then take the **Markovian approximation** which assumes that the correlations of the bath decay fast in time. We can thus make the substitution $\rho(\tau) \to \rho(t)$, the result equation of motion is Markovian:

$$\begin{aligned}\frac{d}{dt}\rho(t) &\approx \sum_{kl}\int_0^t dt' C_{lk}(-t')\left[A_k(t)\rho(t)A_l(t-t') - \rho(t)A_l(t-t')A_k(t)\right] + h.c. \\ &= \sum_k \int_0^t dt\left[A_k\rho B_k - \rho B_k A_k + h.c.\right],\end{aligned}$$

where we have defined $B_k(t) = \sum_l \int_0^\infty dt' A_l(t-t')C_{lk}(-t')$. Now we switch to the frequency domain,

$$A_k(t) = \sum_\omega A_k(\omega)e^{-i\omega t}, \quad B_k(t) = \sum_{l,\omega} e^{-i\omega t}A_l(\omega)\Gamma_{lk}(\omega), \quad \Gamma_{kl}(\omega) = \int_0^\infty dt\ e^{i\omega t}C_{kl}(t).$$

We then take the **rotating wave approximation**, where we only keep the contributions from canceling frequency of operator A and B,

$$\begin{aligned}\frac{d}{dt}\rho(t) &= \sum_\omega \left[\Gamma_{lk}(\omega)A_k(\omega)\rho A_l(\omega) - \Gamma_{lk}(\omega)\rho A_l(\omega)A_k(\omega) + h.c.\right] \\ &= \sum_\omega \gamma_{kl}(\omega)(A_{l,\omega}\rho A_{k,\omega}^\dagger - \frac{1}{2}\{\rho, A_{k,\omega}^\dagger A_{l,\omega}\}) - i\left[\sum_\omega S_{kl}(\omega)A_{k,\omega}^\dagger A_{l,\omega}, \rho\right],\end{aligned} \tag{5}$$

where we defined

$$\gamma_{kl}(\omega) = \Gamma_{kl}(\omega) + \Gamma_{lk}^*(\omega), \quad S_{kl}(\omega) = \frac{\Gamma_{kl}(\omega) - \Gamma_{lk}^*(\omega)}{2i}.$$

The matrices $\gamma(\omega)$ are positive, we can then take the square root of them. The jump operator is then

$$L_{i,\omega} = \sum_j \sqrt{\gamma_{ij}(\omega)}A_{j,\omega}.$$

The evolution is then in the Lindblad form.

C. Stochastic Schrödinger Equation

The Lindblad form Eq. (3) is equivalent to the stochastic Schrödinger equation (SSE):

$$d|\psi\rangle = -iH|\psi\rangle + A[\psi]dt + B[\psi]dW, \tag{6}$$

where dW is a stochastic infinitesimal element. The expectation value is then the average over all possible evolution path (trajectory): $\langle O(t)\rangle = \overline{\langle\psi(t)|O|\psi(t)\rangle}$.

1. Poisson SSE

Consider a small time interval Δt, the Lindblad equation is equivalent to the quantum channel $\rho(t+\Delta t) = M_0\rho(t)M_0^\dagger + \sum_m M_m\rho M_m^\dagger$, where

$$M_0 = 1 - i\left(H - i\frac{\gamma}{2}\sum_m L_m^\dagger L_m\right)\Delta t, \quad M_m = \sqrt{\gamma\Delta t}L_m.$$

A quantum channel can be simulated by a stochastic evolution of pure states:

$$|\psi(t+\Delta t)\rangle \propto \begin{cases} L_m|\psi(t)\rangle & p = p_m(t)\gamma\Delta t \\ \exp(-iH_{\text{eff}}\Delta t)|\psi(t)\rangle & p = 1 - \sum_m p_m(t) \end{cases}, \quad \text{where } p_m(t) = \langle\psi(t)|L_m^\dagger L_m|\psi(t)\rangle. \tag{7}$$

Here the effective (non-Hermitian) Hamiltonian is

$$H_{\text{eff}} = H - i\frac{\gamma}{2}\sum_m L_m^\dagger L_m. \tag{8}$$

We can introduce a Poisson variable dW_m satisfying

$$dW_m dW_n = \delta_{mn}dW_m, \quad \overline{dW_m} = \langle L_m^\dagger L_m\rangle\gamma dt,$$

and the evolution can be cast into the stochastic differential equation

$$d|\psi\rangle = -iHdt|\psi\rangle + \sum_m\left[\left(\frac{L_m}{\langle L_m^\dagger L_m\rangle^{\frac{1}{2}}} - 1\right)dW_m - \frac{\gamma}{2}\left(L_m^\dagger L_m - \langle L_m^\dagger L_m\rangle\right)dt\right]|\psi\rangle. \tag{9}$$

Note that the $-\langle L_m^\dagger L_m\rangle dt|\psi\rangle$ comes from the renormalization. For numerical simulation, we can ignore it.

2. Gaussian SSE

We can also use the Wiener processes dW_m satisfying

$$\overline{dW_m} = 0, \quad \overline{dW_m dW_n} = \delta_{mn}\gamma dt.$$

The Gaussian SSE is

$$d|\psi\rangle = -iHdt|\psi\rangle + \sum_m\left[\left(L_m - \langle L_m\rangle\right)\mathrm{d}W_m - \frac{\gamma}{2}\left(L_m^\dagger - \langle L_m\rangle\right)\left(L_m - \langle L_m\rangle\right)dt\right]|\psi\rangle. \tag{10}$$

To retain the Lindblad, note that $d\rho = \overline{|d\psi\rangle\langle\psi|} + \overline{|\psi\rangle\langle d\psi|} + \overline{|d\psi\rangle\langle d\psi|}$. Without going into the detail, we note that $L_m dW_m$ term in $\overline{|d\psi\rangle\langle d\psi|}$ will contribute a term $\gamma L_m\rho L_m^\dagger dt$; $-\frac{\gamma}{2}L_m^\dagger L_m dt$ term in $\overline{|d\psi\rangle\langle\psi|} + \overline{|\psi\rangle\langle d\psi|}$ contribute a tern $-\frac{\gamma}{2}\{L_m^\dagger L_m, \rho\}$ term. All terms involving expectation value can be regarded as coming from the renormalization.

II. QUADRATIC LINDBLADIAN

Consider the Lindblad in the Heisenberg picture:

$$\frac{d}{dt}\hat{O} = i[\hat{H}, \hat{O}] + \sum_{\mu} \hat{L}_{\mu}^{\dagger} \hat{O} \hat{L}_{\mu} - \frac{1}{2} \sum_{\mu} \{\hat{L}_{\mu}^{\dagger} \hat{L}_{\mu}, \hat{O}\}, \tag{11}$$

where we choose $\hat{O}_{ij} = \omega_i \omega_j$ satisfying the relation $\hat{O}^T = 2\mathbb{I} - \hat{O}$. The covariance matrix is then $\Gamma_{ij} = i\langle \hat{O} \rangle - i\delta_{ij}$.

We assume that the jump operator has up to quadratic Majorana terms. In particular, we denote the linear terms and the Hermitian quadratic terms as

$$\hat{L}_r = \sum_{j=1}^{2N} L_j^r \omega_j, \quad \hat{L}_s = \sum_{j,k=1}^{2N} M_{jk}^s \omega_j \omega_k.$$

When the **jump operator** $\hat{L}_{\mu}$ contains only the linear Majorana operator, the Lindblad equation preserves Gaussianity. For jump operators containing up to quadratic Majorana terms, the evolution will break the Gaussian form, however, the $2n$-point correlation is still solvable for free fermion systems.

A. Third Quantization

Assume only linear terms in jump operators,

$$\partial_t \hat{O} = \left[i\hat{H}, \hat{O}\right] + \mathcal{D}_r[\hat{O}] = \left[i\hat{H} - \frac{1}{2}\sum_r \hat{L}_r^{\dagger} L_r, \hat{O}\right] + \sum_r \left[\hat{L}_r^{\dagger}, \hat{O}\right] \hat{L}_r.$$

Define $B \equiv \sum_r L_i^r L_j^{r*}$, the first term of EOM is:[2]

$$\begin{aligned}
\left[i\hat{H} - \frac{1}{2}\sum_r \hat{L}_r^{\dagger} L_r, \hat{O}_{ij}\right] &= \sum_{kl} \left(\frac{1}{4}H - \frac{1}{2}B\right)_{kl} [\omega_k \omega_l, \omega_i \omega_j] \\
&= \sum_{kl} \left(\frac{1}{2}H - B\right)_{kl} (\delta_{ki}\omega_j\omega_l - \delta_{kj}\omega_i\omega_l + \delta_{li}\omega_k\omega_j - \delta_{lj}\omega_k\omega_i) \\
&= \left[\left(\frac{1}{2}H - B\right) \cdot \hat{O}^T + \left(\frac{1}{2}H - B\right)^T \cdot \hat{O} - \hat{O} \cdot \left(\frac{1}{2}H - B\right)^T - \hat{O}^T \cdot \left(\frac{1}{2}H - B\right)\right]_{ij} \\
&= \left[(-H + 2B^I) \cdot \hat{O} + \hat{O} \cdot (H - 2B^I)\right]_{ij}
\end{aligned}$$

The second term is

$$\begin{aligned}
\sum_r \left[L_r^{\dagger}, \hat{O}_{ij}\right] \hat{L}_r &= \sum_{kl} B_{kl} [\omega_k, \omega_i \omega_j] \omega_l = 2\sum_{kl} B_{kl} \left(\delta_{ki}\omega_j\omega_l - \delta_{kj}\omega_i\omega_l\right) \\
&= \left[2B \cdot \hat{O}^T - 2\hat{O} \cdot B^T\right]_{ij} = \left[-2B \cdot \hat{O} - 2\hat{O} \cdot B^* + 4B\right]_{ij}
\end{aligned}$$

Therefore

$$\partial_t \hat{O}_{ij} = \left[(-H - 2B^R) \cdot \hat{O} + \hat{O} \cdot (H - 2B^R) + 4B\right]_{ij}$$

The EOM of the covariance matrix is then

$$\partial_t \Gamma = X^T \cdot \Gamma + \Gamma \cdot X + Y, \tag{12}$$

[2] Use the commutation relation $\{\omega_i, \omega_j\} = 2\delta_{ij}$, we have the relation $[\omega_k, \omega_i\omega_j] = 2(\delta_{ki}\omega_j - \delta_{kj}\omega_i)$ and $[\omega_k\omega_l, \omega_i\omega_j] = 2(\delta_{ki}\omega_j\omega_l - \delta_{kj}\omega_i\omega_l + \delta_{li}\omega_k\omega_j - \delta_{lj}\omega_k\omega_i)$.

where $X = H - 2B^R$, $Y = 4B^I$. Note that the constant part is replaced by its anti-symmetric part.

The steady state of the system is solved by the Lyapunov equation

$$X^T \cdot \Gamma + \Gamma \cdot X = -Y. \tag{13}$$

B. Quadratic Jump Operators

Now include the Hermitian quadratic quantum jumps:

$$\begin{aligned}\partial_t \hat{O} &= i[\hat{H}, \hat{O}] + \mathcal{D}_r[\hat{O}] + \mathcal{D}_s[\hat{O}],\\ \mathcal{D}_s[\hat{O}] &= \sum_s \hat{L}_s \hat{O} \hat{L}_s - \frac{1}{2}\sum_r \{\hat{L}_s^2, \hat{O}\} = -\frac{1}{2}\sum_s [\hat{L}_s, [\hat{L}_s, \hat{O}]].\end{aligned} \tag{14}$$

1. Majorana Case

A direct calculation gives

$$\begin{aligned}D_s[\hat{O}] &= -\frac{1}{2}\sum_s \sum_{kl} M^s_{kl} \langle [\hat{L}_s, [\omega_k\omega_l, \omega_i\omega_j]]\\ &= 2\sum_s \sum_k \left\{ M^s_{ik}[\hat{L}_s, \omega_k\omega_j] - [\hat{L}_s, \omega_i\omega_k] M^s_{kj} \right\}\\ &= 8\sum_{s,kl} \left[M^s_{ik}(-M^s_{kl}\omega_l\omega_j + \omega_k\omega_l M^s_{lj}) + (M^s_{il}\omega_l\omega_k - \omega_i\omega_l M^s_{lk}) M^s_{kj} \right]\\ &= 8\sum_s \left[2M^s \cdot \hat{O} \cdot M^s - (M^s)^2 \cdot \hat{O} - \hat{O} \cdot (M^s)^2 \right]_{ij}.\end{aligned}$$

Together, we get the EOM of the variance matrix Γ_{ij}:

$$\partial_t \Gamma = X^T \cdot \Gamma + \Gamma \cdot X + \sum_s (Z^s)^T \cdot \Gamma \cdot Z^s + Y, \tag{15}$$

where

$$X = H - 2B^R + 8\sum_s (\mathrm{Im} M^s)^2, \quad Y = 4B^I, \quad Z = 4M^s. \tag{16}$$

2. Dirac Fermion Case

In this section, we consider the free fermion system preserving the U(1) charge. The jump operators are assumed to be quadratic: $\hat{L}_s = \sum_{jk} M^s_{jk} c_j^\dagger c_k$ where $\{M^s\}$ are Hermitian matrices.

For the fermion case, we choose $\hat{O}_{ij} = c_i^\dagger c_j$, and consider the Lindbladian

$$\partial_t \hat{O} = i[\hat{H}, \hat{O}] + \mathcal{D}_s[\hat{O}] = i[\hat{H}, \hat{O}] - \frac{1}{2}\sum_s [\hat{L}_s, [\hat{L}_s, \hat{O}]],$$

where each $\hat{L}_s = M^s_{ij} c_i^\dagger c_j$ is a Hermitian fermion bilinear.

The Hamiltonian part is:[3]

$$i\sum_{kl} H_{kl}[c_k^\dagger c_l, c_i^\dagger c_j] = i\sum_{kl} H_{kl}(\delta_{il} c_k^\dagger c_j - \delta_{jk} c_i^\dagger c_l) = i[H^T \cdot \hat{O} - \hat{O} \cdot H^T]_{ij}.$$

[3] Using the fact $[c_k^\dagger c_l, c_i^\dagger c_j] = c_k^\dagger [c_l, c_i^\dagger c_j] + [c_k^\dagger, c_i^\dagger c_j] c_l = \delta_{il} c_k^\dagger c_j - \delta_{jk} c_i^\dagger c_l$, we know that for a quadratic form $\hat{A} = \sum_{ij} A_{ij} c_i^\dagger c_j$, $[\hat{A}, \hat{O}_{ij}] = [A^T, \hat{O}]_{ij}$.

Similarly, the double commutation in the second term is:

$$\mathcal{D}_s[\hat{O}] = -\frac{1}{2}\sum_s [(M^{s*})^2 \cdot \hat{O} + \hat{O} \cdot (M^{s*})^2 - 2M^{s*} \cdot \hat{O} \cdot M^{s*}].$$

Together, the EOM of correlation $G_{ij} = \langle c_i^\dagger c_j \rangle$ is

$$\partial_t G = X^\dagger \cdot G + G \cdot X + \sum_s M^{s*} \cdot G \cdot M^{s*}, \tag{17}$$

where $X = -iH^* - \frac{1}{2}\sum_s (M^{s*})^2$.

III. FERMIONIC GAUSSIAN STATES

In this section, we discuss the general fermionic Gaussian state, in the framework of the Grassmann representation. We will closely follow Ref. [1].

A. Grassmann Representation

The Majorana operators are defined as $\hat{\omega}_j^a = \hat{c}_i + \hat{c}_i^\dagger$, $\hat{\omega}_j^b = i(\hat{c}_i - \hat{c}_i^\dagger)$. A general operator in Fermionic Fock space can be expanded on the Majorana basis:

$$\hat{X} = \alpha \hat{I} + \sum_{p=1}^{2n} \sum_{1 \le a_1 < \cdots < a_p \le 2n} \alpha_{a_1 \cdots a_p} \hat{\omega}_{a_1} \cdots \hat{\omega}_{a_p}. \tag{18}$$

Define a linear map from Fermionic operator space to Grassmann algebra:

$$\hat{X} \mapsto X(\theta) = \alpha + \sum_{1 \le a_1 < \cdots < a_p \le 2n} \alpha_{a_1 \cdots a_p} \theta_{a_1} \cdots \theta_{a_p}. \tag{19}$$

This mapping is called the Grassmann representation of $\hat{X}$.

One can formally define calculus on Grassmann algebra:

$$\frac{\partial}{\partial \theta_i}\theta_j = \int d\theta_i \theta_j = \delta_{ij}, \quad \frac{\partial}{\partial \theta_i} 1 = \int d\theta_i 1 = 0. \tag{20}$$

The Gaussian integral of Grassmann algebra is

$$\int D\theta \exp\left(\eta^T\theta + \frac{i}{2}\theta^T M \theta\right) = i^n \operatorname{Pf}(M) \exp\left(-\frac{i}{2}\eta^T M^{-1} \eta\right). \tag{21}$$

One useful result concerning the expectation value is

Theorem 1. *For two operator $\hat{X}$ and $\hat{Y}$, we have the following identity*

$$\operatorname{Tr}\left(\hat{X}\hat{Y}\right) = (-2)^n \int D[\theta,\mu] e^{\theta^T \cdot \mu} X(\theta) Y(\mu).$$

where $\int D\theta = \int d\theta_{2n} \cdots \int d\theta_1$, $\int D\mu = \int d\mu_{2n} \cdots \int d\mu_1$.

Proof. We prove the statement by considering only m-th order monomial. On the one hand

$$\text{LHS} = \operatorname{Tr}[\hat{\omega}_1 \cdots \hat{\omega}_m \hat{\omega}_1 \cdots \hat{\omega}_m] = 2^n (-1)^{m(m-1)/2}.$$

On the other hand,

$$\begin{aligned} \text{RHS} &= (-2)^n \int D[\theta,\mu]\ \theta_1 \cdots \theta_m (\theta_{m+1}\mu_{m+1} \cdots \theta_{2n}\mu_{2n}) \mu_1 \cdots \mu_m \\ &= (-2)^n\,(-1)^{(4n-m)m + (m+1+2n)(2n-m)/2} \\ &= 2^n (-1)^{-m(m+3)/2} = 2^n (-1)^{m(m-1)/2}. \end{aligned}$$

We therefore proved the statement. □

1. Gaussian States

Definition 1. *A quantum state $\hat{\rho}$ is Gaussian if it has Gaussian Grassmann representation:*

$$\rho(\theta) = \frac{1}{2^n} \exp\left(\frac{i}{2}\theta^T M \theta\right),$$

where the antisymmetric matrix $M_{ab} = \frac{i}{2}\operatorname{Tr}(\hat{\rho}[\hat{\omega}_a, \hat{\omega}_b])$ is the ***covariance matrix****.*

All higher correlations of a Gaussian state are determined by the Wick theorem, namely

$$\operatorname{Tr}(i^p \hat{\rho}\hat{\omega}_{a_1} \cdots \hat{\omega}_{a_p}) = \operatorname{Pf}(M|_{a_1,\ldots,a_p}).$$

The canonical form of antisymmetric matrix M is:

$$M = R \begin{bmatrix} 0 & \operatorname{diag}(\lambda_1, \cdots, \lambda_n) \\ -\operatorname{diag}(\lambda_1, \cdots, \lambda_n) & 0 \end{bmatrix} R^T, \quad R \in \mathrm{SO}(2n).$$

Under the new Grassmann variance $\mu = R\theta$, ρ has the form

$$\rho(\mu) = \frac{1}{2^n} \prod_j \exp\left(i\lambda_j \mu_j \mu_{j+n}\right) = \frac{1}{2^n} \prod_j \left(1 + i\lambda_j \mu_j \mu_{j+n}\right). \tag{22}$$

We can then obtain the operator form:

$$\hat{\rho} = 2^{-n} \prod_{j=1}^{n} (1 + i\lambda_j \hat{\gamma}_j \hat{\gamma}_{j+n}) \tag{23}$$

where $\hat{\gamma}$'s are a new set of Majorana operators. In the fermion basis

$$\hat{d}_j = \frac{\hat{\gamma}_j - i\hat{\gamma}_{j+n}}{2}, \quad \hat{d}_j^\dagger = \frac{\hat{\gamma}_j + i\hat{\gamma}_{j+n}}{2}, \tag{24}$$

the density matrix has the form

$$\hat{\rho} = \prod_j \left(\frac{1+\lambda_j}{2} - \lambda_j d_j^\dagger d_j\right) = \bigotimes_j \begin{bmatrix} \frac{1+\lambda_j}{2} & 0 \\ 0 & \frac{1-\lambda_j}{2} \end{bmatrix}_j. \tag{25}$$

Without loss of generality, we assume $\lambda_i \geq 0$. For pure state, $\lambda_i = 1$, $\forall i$. For mixed state, the entropy of ρ is just

$$S(\hat{\rho}) = \sum_j H\left(\frac{1+\lambda_j}{2}\right) = -\sum_j \left[\left(\frac{1+\lambda_j}{2}\right)\log\left(\frac{1+\lambda_j}{2}\right) + \left(\frac{1-\lambda_j}{2}\right)\log\left(\frac{1-\lambda_j}{2}\right)\right]. \tag{26}$$

2. Gaussian Operators

Definition 2. *An operator $\hat{X}$ (with nonzero trace) is Gaussian if*

$$X(\theta) = C \exp\left(\frac{i}{2}\theta^T M \theta\right)$$

for some complex number C and some ***complex antisymmetric*** *matrix M. M is called a correlation matrix of $\hat{X}$. If $\hat{X}$ is traceless, it should be thought of as a limit $\hat{X} = \lim_{m\to\infty} \hat{X}_m$ for some converging sequence of Gaussian operators with nonzero trace.*

Note that for traceless $\hat{X}$, the explicit form of $X(\theta)$ is

$$X(\theta) = C\left(\prod_{a=1}^{2k} \mu_a\right) \exp\left(\frac{i}{2} \sum_{a,b=2k+1}^{2n} M_{ab}\mu_a\mu_b\right), \tag{27}$$

where $\mu_a = \sum_b T_{ab}\theta_b$ for some invertible complex matrix T. The factor is a limiting point of the sequence:

$$\prod_{a=1}^{2k} \mu_a = \lim_{t\to\infty} \prod_{a=1}^{k} \left(\mu_{2a-1}\mu_{2a} + \frac{1}{t}\right) = \lim_{t\to\infty} \frac{1}{t^k} \exp\left(t \sum_{a=1}^{k} \mu_{2a-1}\mu_{2a}\right).$$

Introducing the operator $\hat{\Lambda} \equiv \sum_{a=1}^{2n} \hat{\omega}_a \otimes \hat{\omega}_a$, we have the following theorem:

Theorem 2. *An operator $\hat{X}$ is Gaussian iff $\hat{X}$ is even and satisfies*

$$[\hat{\Lambda}, \hat{X} \otimes \hat{X}] = 0.$$

Proof. The adjoint action of $\hat{\Lambda}$ in the Grassmann representation has the form:

$$\Lambda_{\text{ad}} = 2 \sum_a \left(\theta_a \otimes \frac{\partial}{\partial\theta_a} + \frac{\partial}{\partial\theta_a} \otimes \theta_a\right) \equiv \sum_a \Delta_a. \tag{28}$$

That is, $[\hat{\omega}_a \otimes \hat{\omega}_a, Y \otimes Z](\theta) = \Delta_a \cdot Y(\theta) \otimes Z(\theta)$ for any operators Y, Z having the same parity. Without loss of generality, both Y and Z are monomials in $\hat{\omega}$'s. In this case each of them either commutes or anticommutes with $\hat{\omega}_a$. Consider two cases:

1. Both Y and Z contain $\hat{\omega}_a$, or both Y and Z do not contain $\hat{\omega}_a$. Then the commutator $[\hat{\omega}_a \otimes \hat{\omega}_a, Y \otimes Z]$ is zero since both factors yield the same sign. The right-hand side is also zero, since either θ_a or $\partial/\partial\theta_a$ annihilates both Y and Z.

2. Y contains $\hat{\omega}_a$ while Z does not contain $\hat{\omega}_a$ (or vice verse). In this case $\hat{\omega}_a \otimes \hat{\omega}_a$ anticommutes with $Y \otimes Z$. Let us write $Y = \hat{\omega}_a \tilde{Y}$, where $\tilde{Y}$ is a monomial which does not contain $\hat{\omega}_a$. We have:

$$[\hat{\omega}_a \otimes \hat{\omega}_a, Y \otimes Z] = 2(\hat{\omega}_a \otimes \hat{\omega}_a)(Y \otimes Z) = 2\tilde{Y} \otimes (\hat{\omega}_a Z).$$

   On the other hand,

$$\theta_a \otimes \frac{\partial}{\partial\theta_a} \cdot Y \otimes Z = 0, \quad \frac{\partial}{\partial\theta_a} \otimes \theta_a \cdot Y \otimes Z = \tilde{Y} \otimes \theta_a Z.$$

   We again get equality.

Necessity: Note that Λ_{ad} is invariant under change of variables since

$$\mu_a = \sum_b T_{ab}\theta_b, \quad \frac{\partial}{\partial\mu_a} = \sum_b (T^{-1})_{ab} \frac{\partial}{\partial\theta_b} \implies \sum_a \theta_a \otimes \frac{\partial}{\partial\theta_a} = \sum_a \mu_a \otimes \frac{\partial}{\partial\mu_a}.$$

Direct application of the operator to the general Gaussian form will prove the necessity.
Sufficiency: Denote $C = 2^{-n}\operatorname{tr}(X) \equiv X(0)$ and represent $X(\theta)$ as

$$X(\theta) = C \cdot 1 + \frac{iC}{2} \sum_{a,b=1}^{2n} M_{ab}\,\theta_a\theta_b + \text{higher order terms}.$$

Applying a differential operator $1 \otimes \frac{\partial}{\partial\theta_b}$ to both sides:

$$\sum_{a=1}^{2n} \left(\theta_a X \otimes \frac{\partial^2}{\partial\theta_b\partial\theta_a} X - \frac{\partial}{\partial\theta_a} X \otimes \theta_a \frac{\partial}{\partial\theta_b} X\right) + \frac{\partial}{\partial\theta_b} X \otimes X = 0.$$

Now let us put $\theta \equiv 0$ in the second factor:

$$\frac{\partial}{\partial\theta_b} X = i \sum_{a=1}^{2n} M_{ba}\theta_a X.$$

This differential equation can be easily solved by $X(\theta) = C \exp\left(\frac{i}{2}\,\theta^T M \theta\right)$.

For general cases, we denote $\mathcal{K} \subseteq \mathcal{M}_1$ a subspace spanned by linear functions which annihilate $\hat{X}$, i.e.

$$\mathcal{K} = \{f \in \mathcal{M}_1 \ : \ f(\theta)X(\theta) = 0\}.$$

Let us perform a linear change of variables $\mu_a = \sum_b T_{ab}\theta_b$, with T being an invertible complex matrix chosen such that the first k variables μ span the subspace $\mathcal{K}$, i.e. $\mathcal{K} = \mathrm{span}\,[\mu_1, \dots, \mu_{2k}]$. From equalities $\mu_j X = 0$, $j \in [1, 2k]$ it follows that

$$X(\theta(\mu)) = \left(\prod_a \mu_a\right) \tilde{X}(\mu),$$

where $\tilde{X}(\mu)$ depends only upon $\mu_{2k+1}, \dots, \mu_{2n}$. The function $\tilde{X}(\mu)$ satisfies the equation

$$\sum_{a=2k+1}^{2n} \left(\mu_a \otimes \frac{\partial}{\partial \mu_a} + \frac{\partial}{\partial \mu_a} \otimes \mu_a\right) \tilde{X} \otimes \tilde{X} = 0.$$

Therefore we get the general Gaussian form. □

3. Gaussian Linear Maps

We define linear maps that preserve Gaussian states as the following:

Definition 3. *A linear map $\mathcal{E}$ is Gaussian iff it admits an integral representation*

$$\mathcal{E}(X)(\theta) = C \int D[\eta, \mu] \exp\left[S(\theta, \eta) + i\eta^T \mu\right] X(\mu), \tag{29}$$

where

$$S(\theta, \eta) = \frac{i}{2}(\theta^T, \eta^T) \begin{pmatrix} A & B \\ -B^T & D \end{pmatrix} \begin{pmatrix} \theta \\ \eta \end{pmatrix} \tag{30}$$

for some complex $2n \times 2n$ matrices A, B, D, and some complex number C.

Consider a Gaussian operator $\hat{X}$ which can be described by a correlation matrix M and a Gaussian map $\mathcal{E}$. Applying the Gaussian integration, one can show that $\mathcal{E}(X)$ has a correlation matrix

$$\mathcal{E}(M) = A + B\left(M^{-1} + D\right)^{-1} B^T = A + B\left(I + MD\right)^{-1} MB^T,$$

while a pre-exponential factor of the operator $\mathcal{E}(X)$ can be found from an identity

$$\mathrm{tr}\left(\mathcal{E}(X)\right) = C(-1)^n \,\mathrm{Pf}(M)\,\mathrm{Pf}(M^{-1} + D)\,\mathrm{tr}\,(X).$$

The value of $\mathrm{tr}\left(\mathcal{E}(X)\right)$ can be found up to a factor ± 1 using a regularized version:

$$\mathrm{tr}\left(\mathcal{E}(X)\right)^2 = C^2 \det\left(I + MD\right) \mathrm{tr}\,(X)^2.$$

B. Operator Form

1. Dirac Fermion Case

For particle number conserving systems, the Gaussian state can be represented as a matrix:

$$|B\rangle \equiv \prod_{j=1}^{N} \sum_i B_{ij} c_i^\dagger |0\rangle \equiv \bigotimes_{j=1}^{N} |B_j\rangle. \tag{31}$$

Note that the matrix B representing the Gaussian state has the unitary degree of freedom

$$|B\rangle = |B'\rangle, \quad B'_{ij} = \sum_k B_{ik} U_{kj},$$

where U_{kj} is an $N \times N$ unitary matrix. It means that the Gaussian state is determined by the linear subspace that columns of B span. The columns of B need not to orthogonal, while the canonical form can be obtained by the QR decomposition: $B_{L\times N} = Q_{L\times N} \cdot R_{N\times N}$, where the Q matrix is orthonormal and we can set $B' = Q$.

A free fermion state maintains its structure when applied to a quasi-particle creation/annihilation operator. Consider a general quasi-particle $b^\dagger = \sum_i b_i c_i^\dagger$, creating a quasiparticle is simply adding a column to B, since

$$b^\dagger |B\rangle = \sum_k b_k c_k^\dagger \prod_{j=1}^{N} \sum_i c_i^\dagger B_{ij} |0\rangle = \prod_{j=1}^{N+1} \sum_i c_i^\dagger \left[b|B\right]_{ij} |0\rangle \tag{32}$$

In general, the new column b is not orthogonal to linear space B, therefore orthogonalization procedure is needed to obtain canonical form.

Using the Baker-Campbell-Hausdorff formula $e^X Y e^{-X} = \exp(\mathrm{ad}\, X) Y$,

$$e^{-iHt} c_j^\dagger e^{iHt} = c_k^\dagger [e^{-iHt}]_{kj} \implies e^{-iHt}|B\rangle = \prod_{j=1}^{N} \sum_i [e^{-iHt}]_{ki} B_{ij} c_k^\dagger |0\rangle = |e^{-iHt} \cdot B\rangle. \tag{33}$$

For the quasiparticle annihilation operator b,

$$b|B\rangle = \sum_k b_k^* c_k \prod_j \sum_i c_i^\dagger B_{ij} |0\rangle = \sum_j \langle b|B_j\rangle \bigotimes_{l\neq j} |B_l\rangle. \tag{34}$$

We can use the gauge freedom to restrict $\langle b|B'_j\rangle = 0$ for $j > 1$. Such matrix B' always exists since we can always find a column j that $\langle b|B_j\rangle \neq 0$ (otherwise $p_m = 0$ and the jump is impossible). We then move the column to the first and define the column as

$$|B'_j\rangle = |B_j\rangle - \frac{\langle a|B_j\rangle}{\langle a|B_1\rangle} |B_1\rangle, \quad j > 1. \tag{35}$$

Such column transformations do not alter the linear space B spans, while the orthogonality and the normalization might be affected.

2. *Majorana Case*

For the Majorana case, the canonical form (25) for a Gaussian pure state $|\psi$ can be reformulated as

$$|\psi\rangle\langle\psi| = \prod_{j=1}^{n} \hat{d}_j^\dagger \hat{d}_j, \quad \hat{d}_j^\dagger = \frac{\hat{\gamma}_j + i\hat{\gamma}_{j+n}}{2} = \sum_{i=1}^{n} \left(\frac{R_{i,j} + iR_{i,j+n}}{2}\right) \hat{c}_i + \left(\frac{R_{i+n,j} + iR_{i+n,j+n}}{2}\right) \hat{c}_i^\dagger. \tag{36}$$

Note that the state is annihilated by $\{\hat{d}_j^\dagger\}$. We can store the information of $|\psi\rangle$ into a $2n \times n$ complex matrix

$$|\psi\rangle \Longleftrightarrow B = \frac{1}{2} \begin{bmatrix} R_{11} + iR_{12} \\ R_{21} + iR_{22} \end{bmatrix}. \tag{37}$$

The rest of the procedures are parallel to those of the Dirac fermion case.

[1] S. Bravyi, *Lagrangian representation for fermionic linear optics* (2004), quant-ph/0404180.