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Modifying the Time-Convolutionless Master Equation via the Moore-Penrose Pseudoinverse

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Abstract

The Time Convolutionless (TCL) Master Equation is an exact, non-Markovian master equation for open quantum systems. Its derivation utilizes one essential assumption: that the operator $(\mathrm{I} - \Sigma)$ is invertible. For short times, or in the *weak* coupling case, this assumption holds true. However, there exist examples for which the operator is not invertible, such as the *strong* coupling case of the Jaynes-Cummings model. In this paper, we rederive the TCL without making this assumption, by making use of the Moore-Penrose pseudoinverse. We then rederive the perturbative expansion that makes the TCL analytically solvable to form a new master equation we call the TCL^{+}.

1 Utilizing the Moore-Penrose Pseudoinverse

The Moore-Penrose Pseudoinverse A^+ of a linear operator A is a generalized inverse of A which exists whether or not A is invertible. It is subject to the 4 Moore-Penrose conditions:

$AA^+A = A$
$A^+AA^+ = A^+$
$(AA^+)^\dagger = AA^+$
$(A^+A)^\dagger = A^+A$

$A+$ has a universal definition in the singular value decomposition:

$A = UDV^\dagger \implies A^+ = VD^+U^\dagger$

Additionally, if the system $Ax = b$ has any solutions, the lowest of them is given by $x = A^+b$.

2 Derivation of the Time Convolutionless Master Equation

For the reader's convenience, we give a brief overview of the standard derivation for the TCL-ME, stopping at the step at which the TCL+-ME diverges from it.

2.1 Feshbach Partitioning

The TCL-ME attempts to solve for $Tr_B[\rho] \otimes \rho_B = \mathcal{P}\rho$, where ρ_B is a time-independent "reference state" of the bath. The projection operator $\mathcal{P}$ and its orthogonal projection $\mathcal{Q} = \mathcal{I} - \mathcal{P}$, whose actions on an operator $X \in \mathcal{H}_S \otimes \mathcal{H}_B$ we denote $\hat{X}$ and $\bar{X}$ respectively, form a method of "splitting up" X we call "Feshbach partitioning". This technique may be familiar from the derivation of the Nakajima-Zwanzig master equation (NZ-ME).

Starting from the Liouville von Neumann equation in the interaction picture:

$$\partial\rho = -i\lambda[H(t), \rho(t)] = \lambda\mathcal{L}\rho(t)$$

Where $H(t) = \lambda H_{SB}(t)$ is the total Hamiltonian in the interaction picture. Taking $\partial\hat{\rho}$ and $\partial\bar{\rho}$:

$$\partial\hat{\rho} = \lambda\hat{\mathcal{L}}\hat{\rho} + \lambda\hat{\mathcal{L}}\bar{\rho}$$

Where we used $\mathcal{P} + \mathcal{Q} = \mathcal{I}$

2.2 Solving for $\bar{\rho}(t)$

The formal solution to the partial differential equation for $\bar{\rho}$ above is:

$$\bar{\rho}(t) = \mathcal{G}(t, t_0)\bar{\rho}(t_0) + \lambda \int_{t_0}^{t} \mathcal{G}(t, t')\bar{\mathcal{L}}(t')\hat{\rho}(t')dt'$$
$$\mathcal{G}(t, t') = T_+ e^{\lambda \int_{t'}^{t} \bar{\mathcal{L}}(t'')dt''}$$

Where T_+ denotes a forward time-ordering superoperator. We may also consider the formal solution to the Liouville von Neumann equation:

$$\rho(t) = \mathcal{U}(t, t')\rho(t')$$
$$\mathcal{U}(t, t') \equiv T_+ e^{\lambda \int_{t}^{t'} \mathcal{L}(t'')dt''}$$

We can then invert $\mathcal{U}(t, t')$ and apply $\mathcal{P}$ to both sides to obtain:

$$\hat{\rho}(t') = \hat{\mathcal{U}}(t', t)\rho(t)$$
$$\hat{\mathcal{U}}(t', t) \equiv T_- e^{\lambda \int_{t'}^{t} \mathcal{L}(t'')dt''}$$

Substituting the above into the equation with $\mathcal{G}(t, t')$:

$\bar{\rho}(t) = \mathcal{G}(t,t_0)\bar{\rho}(t_0) + \Sigma(t)\rho(t)$
$\Sigma(t) \equiv \lambda \int_{t_0}^{t} \mathcal{G}(t,t')\bar{\mathcal{L}}(t')\hat{\mathcal{U}}(t',t)dt'$

Once again using $\mathcal{I} = \mathcal{P} + \mathcal{Q}$, we find:

$[\mathcal{I} - \Sigma]\bar{\rho}(t) = \mathcal{G}(t,t_0)\bar{\rho}(t_0) + \Sigma(t)\hat{\rho}(t)$

At this point in the derivation, $[\mathcal{I} - \Sigma]$ is assumed invertible and moved to the other side, where it can be easily perturbed with the geometric series. The subsequent *different* steps required to reach the TCL+-ME are covered in detail within the next section.

3 Derivation of the TCL+-ME

We begin our divergence from the standard TCL by taking pseudoinverse of $[\mathcal{I} - \Sigma]$ rather than the inverse. This eliminates the assumption that $[\mathcal{I} - \Sigma]$ is invertible, as the pseudoinverse is defined for all linear operators. Naturally, we assume via a qualitative argument that a solution for the system exists, as the system continues to evolve whether or not $[\mathcal{I} - \Sigma]$ is invertible. Now:
$\bar{\rho}(t) = [\mathcal{I} - \Sigma]^{+}\mathcal{G}(t,t_0)\bar{\rho}(t_0) + [\mathcal{I} - \Sigma]^{+}\Sigma(t)\hat{\rho}(t)$

Substituting this into our equation for $\partial\hat{\rho(t)}$ from 4.1:

$\partial\hat{\rho} = \lambda\hat{\mathcal{L}}[\mathcal{I} - \Sigma]^{+}\mathcal{G}(t,t_0)\bar{\rho}(t_0) + \lambda\hat{\mathcal{L}}[\mathcal{I} - \Sigma]^{+}\Sigma(t)\hat{\rho}(t)$

$= \mathcal{J}_{+}(t)\rho(t_0) + \mathcal{K}_{+}(t)\rho(t)$
$\mathcal{J}_{+}(t) \equiv \lambda\hat{\mathcal{L}}[\mathcal{I} - \Sigma]^{+}\mathcal{G}(t,t_0)\mathcal{Q}$
$\mathcal{K}_{+}(t) \equiv \lambda\hat{\mathcal{L}}[\mathcal{I} - \Sigma]^{+}\Sigma(t)\mathcal{P}$

Where we may set $\mathcal{PLP} = 0$ by choosing a modified bath operator: $B' = B - \langle B \rangle I_B$. This is the explicit form of the TCL+-ME. For the rest of this paper, we will assume factorized initial conditions, i.e. $\rho(t_0) = \rho_S(t_0) \otimes \rho_B(t_0)$, so that the $\mathcal{J}$ term vanishes and we are simply left with:

$\partial\hat{\rho} = \mathcal{K}_{+}(t)\rho(t)$

For analytical solvability, it is now necessary to do perturbation on the time-local generator $\mathcal{K}_{+}(t)$. This is trivial in the invertible case, as the geometric series representation is well known, but the method is slightly more complex for the pseudoinverse.

3.1 Power Series Representation of the Pseudoinverse

Israel and Charnes [1] expand the pseudoinverse of an arbitrary square matrix as follows setting the constant α to 1:

$A^{+} = \sum_{k=0}^{\infty}(\mathrm{I} - A^{\dagger}A)A^{\dagger}$

Because this representation is not well-known, we give a brief proof below:

By the singular value decomposition $A = VDU^\dagger$:
$A^k = \sum_{k=0}^{\infty}(\mathrm{I} - VD^\dagger U^\dagger UDV^\dagger)^{\mathrm{k}} VD^\dagger U^\dagger$

By unitarity of U and V:

$A^k = \sum_{k=0}^{\infty}(VV^\dagger - V|D|^2V^\dagger)^{\mathrm{k}} VD^\dagger U^\dagger$

Then, we can pull out V on each term:

$A^k = \sum_{k=0}^{\infty}(V(I - |D|^2)V^\dagger)^{\mathrm{k}} VD^\dagger U^\dagger$

By unitarity:

$A^k = \sum_{k=0}^{\infty} V(I - |D|^2)^{\mathrm{k}} D^\dagger U^\dagger$

Now,

$\sum_{k=0}^{\infty}(\mathrm{I} - D^\dagger D)^{\mathrm{k}} D^\dagger$

$= \mathrm{diag}\sum_{k=0}^{\infty}(1 - |d_i|^2)^k d_i^*$

For $|d_i|^2 \leq 2$, this converges and is

$\mathrm{diag}(\frac{1}{|d_i|^2} d_i^*) = \mathrm{diag}\begin{cases} \frac{1}{d_i} \; d_i \neq 0 \\ 0 \; d_i = 0 \end{cases} = \mathrm{diag}(d_i^+)$

Which is D^+. Adding back V and $U^\dagger$:

$VD^+U^\dagger = A^+$

So, $A^+ = \sum_{k=0}^{\infty}(I - A^\dagger A)A^\dagger$

The $|d_i| \leq \sqrt{2}$ condition we take as valid, as the geometric series expansion used in the derivation of the standard TCL holds a tighter bound, $|d_i| \leq 1$ for the series to converge.

For a brief check, assuming the matrix A is invertible means A^TA is also invertible; in this special case, the expansion converges to $(A^TA)^{-1} = A^{-1}A^{T^{-1}}A^T = A^{-1}$

This is consistent with the pseudoinverse being a generalization of the regular inverse and ensures the extra terms present in the following expansion vanish in the invertible case.

3.2 Sorting by Powers of λ

We can now expand the operator $(\mathcal{I} - \Sigma)^+$ into a power series in λ, finding:

$\mathcal{K}(t) = \lambda\hat{\mathcal{L}}(t)(\sum_{k=0}^{\infty}(\mathcal{I} - (\mathcal{I} - \Sigma)^{\dagger}(\mathcal{I} - \Sigma))^{\mathrm{k}}(\mathcal{I} - \Sigma)^{\dagger}(\Sigma)$

$= \lambda\hat{\mathcal{L}}(t)(\sum_{k=0}^{\infty}(\sum^{\dagger} + \sum + \sum^{\dagger}\sum)^{k}(\mathcal{I} - \Sigma)^{\dagger})\Sigma$

$\Sigma(t) = \sum_{m=0}^{\infty}\lambda^{m}\Sigma_{m}$

$\implies \lambda\hat{\mathcal{L}}(t)(\sum_{k=0}^{\infty}\sum_{m=1}^{\infty}\lambda^{m}\Sigma_{m}(t) + \lambda^{m}\Sigma_{m}(t) - |\lambda|^{2}\Sigma_{m}^{\dagger})(t)\Sigma_{m}(t))(\mathcal{I} - \hat{\lambda^{m}\Sigma_{m}^{\dagger}}) \cdot \Sigma_{m=0}^{\infty}\lambda^{m}\Sigma_{m}$

Matching powers of lambda gives, for the first 4 terms, in analogy to the common TCL 4th-order expansion:

$\lambda_1 : \mathrm{O}$
$\lambda_2 : \Sigma_1$
$\lambda_3 : \Sigma_1^2 + \Sigma_2$
$\lambda_4 : \Sigma_1^3 + \Sigma_1\Sigma_2 + \Sigma_2\Sigma_1 + \Sigma_3 + 2\Sigma_1^{\dagger}\Sigma_2$

This may be easily recognized as the TCL-4 master equation, with an extra term:

$2\Sigma_1^{\dagger}\Sigma_1^2$

We note that all "extra" terms would include these new "adjoint Σs", as the power series expansion without the adjoint terms is simply the regular TCL.

Via a slight modification to the multinomial expansion theorem that arises due to the noncommuting nature of the sigma operators, we find that, in general, for a term lam**n:

$\mathcal{K}_{+n}(t) =$
$\lambda\hat{\mathcal{L}}(t)\sum_{p=0}^{n-2}\sum_{\sigma\in Sn}\sum_{a,b,c,o=0}\sum_{a+b+c=p}\sum_{i,j,k,l,m,n,p=1}\sum_{ia+bj+(k+l)c+o+p=n-1}$
$(\lambda^{ia}\Sigma_i^a)_{\sigma_1}(\lambda^{jb}\Sigma_j^{\dagger b})_{\sigma_2}(\lambda^{(k+l)c}\sum_{m+n=c}\Sigma_k^{\dagger m}\Sigma_l^{n})_{\sigma_3}(-\lambda^{o}(1-\delta_{o,0})\Sigma_o + \delta_{o,0})\lambda^{p}\Sigma_p\mathcal{P}$

**A note: the above is why the standard choice of Σ for the expansion operators is enormously asinine*

Where the sum $\sum_p$ is over powers, as in the multinomial theorem, and the sum $\sum_{\sigma\in Sn}$ is over permutations of the σ_n terms.

Upon inspection of the power series, it is apparent that all these extra terms will have $\Sigma^{\dagger}$ terms. This simplifies the generalization of the TCL+:
TCL+ = TCL + $\sum_{a\in A} a$, where A is the set of terms including one or more $\Sigma^{\dagger}$s.

3.3 Proving the Adjoint Operators

These unique adjoint operators of the TCL+ expansion may be proven to be the following:

By linearity of the inner product, we may take the adjoints of the P and L operators inside the integrals as:

$\mathcal{L}^\dagger = i[H(t), \cdot] = \mathcal{L}^*$

$\mathcal{P}^\dagger = Tr_B[\cdot(I_s \otimes \rho_b)] \otimes I_b$

Proof for $\mathcal{L}^\dagger$:

$\langle \mathcal{L}v, w \rangle = \langle v, \mathcal{L}^\dagger w \rangle$

$-i\langle Hv - vH, w \rangle$

By linearity of the inner product, we have:

$-i\langle Hv, w \rangle + i\langle vH, w \rangle$

Now, since H is Hermitian:

$-i\langle v, Hw \rangle + i\langle v, Hw \rangle$

$i\langle v, [H, w] \rangle$

QED

Thus, $\mathcal{L}^\dagger = i[H, \cdot] = \mathcal{L}^*$

Proof for $\mathcal{P}^\dagger$

$\langle \mathcal{P}v, w \rangle = \langle v, \mathcal{P}^\dagger w \rangle$

Using the Hilbert-Schmidt definition for the inner product of superoperators:

$\langle X, Y \rangle = Tr[X^\dagger Y]$

$\implies Tr[(\mathcal{P}v)^\dagger w] = Tr[v^\dagger (\mathcal{P}^\dagger w)]$

For the left hand side, we have:

$Tr[Tr_B[v^\dagger] \otimes \rho_B w]$

We can represent $v^\dagger$ and w as the kronecker product of their respective system-bath basis vectors:

$v^\dagger = \sum_i A_i^\dagger \otimes B_i^\dagger$

$w = \sum_j C_j \otimes D_j$

Where $A_i, C_j \in \mathcal{H}_S$ and $B_i, D_j \in \mathcal{H}_B$

Then, the inner product simplifies to:

$\sum_{i,j} Tr[Tr[B_i^\dagger](A_i^\dagger \otimes \rho_B)(C_j \otimes D_j)$

$\sum_{i,j} Tr[B_i]^* Tr[A_i^\dagger C_j] Tr[D_j \rho_B]$

For the right hand side, we have:

$\langle v, Tr_B[w(I_S \otimes \rho_B)] \otimes I_B \rangle = Tr[v^\dagger Tr_B[w(I_S \otimes \rho_B)] \otimes I_B]$

Using the same representations of $v^\dagger$ and w that we did for the left hand side:

$\sum_{i,j} Tr[(A_i^\dagger \otimes B_i^\dagger) Tr_B[(C_j \otimes D_j)(I_S \otimes \ \rho_B)] \otimes I_B]$

$\sum_{i,j} Tr[(A_i^\dagger \otimes B_i^\dagger) Tr_B[(C_j \otimes D_j \rho_B] \otimes I_B]$

$\sum_{i,j} Tr[D_j \rho_B] Tr[A_i^\dagger C_j \otimes B_i^\dagger]$

$\sum_{i,j} Tr[B_i]^* Tr[A_i^\dagger C_j] Tr[D_j \rho_B]$

QED

3.4 $\mathcal{PLP} = 0$ Relations for Adjoints

For the purpose of simplification, it is also necessary to derive certain relations for these adjoint operators which are analogous to $\mathcal{PLP} = 0$ for the regular TCL expansion. We find that:

$\mathcal{P}^\dagger \mathcal{L}^\dagger \mathcal{P}^\dagger X = \mathcal{P}^\dagger \mathcal{L} \mathcal{P}^\dagger X = 0$ for all $X \in \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_B)$.

Proof:

Similar to before, we represent $\mathcal{H}_{SB}$ as $\sum_\alpha A_\alpha \otimes B_\alpha$. Then:

$\mathcal{P}^\dagger \mathcal{L}^\dagger \mathcal{P}^\dagger X = \sum_\alpha i Tr_B[[A_\alpha \otimes B_\alpha, Tr_B[X(I_S \otimes \rho_B)] \otimes I_B](I_S \otimes \rho_B)] \otimes I_B$

$\sum_\alpha i Tr_B[([A_\alpha, Tr_B[X(I_S \otimes \rho_B)]] \otimes B_\alpha)(I_S \otimes \rho_B)] \otimes I_B$

$\sum_\alpha i Tr_B[[A_\alpha, Tr_B[X(I_S \otimes \rho_B)]] \otimes B_\alpha \rho_B)] \otimes I_B$

$\sum_\alpha i[A_\alpha, Tr_B[X(I_S \otimes \rho_B)]] Tr[B_\alpha \rho_B] \otimes I_B$

Now, we can show that the term $Tr[B_\alpha \rho_B] = 0$ by choosing a modified bath operator. Say:

$B' = B - \langle B \rangle I_B$

Where $\langle B \rangle = Tr[\rho_B B]$ is the expectation value of B. Now:

$\langle B' \rangle = Tr[\rho_B B'] = Tr[\rho_B (B - \langle B \rangle I_B)]$

By linearity of the trace, this is:

$Tr[\rho_B B] - Tr[\rho_B \langle B \rangle I_B] = Tr[\rho_B B] - Tr[\rho_B Tr[\rho_B B] I_B] = Tr[\rho_B B] - Tr[\rho_B B] = 0$

Since $Tr[\rho_B] = 1$. Thus, rechoosing $B'(t)$ for our bath operators:

$\langle B' \rangle = Tr[B_\alpha \rho_B] = 0 \implies \mathcal{P}^\dagger \mathcal{L}^\dagger \mathcal{P}^\dagger X = 0$

This also holds for $\mathcal{L}$ instead of $\mathcal{L}^\dagger$, as the only difference is a factor of -1.

However, importantly, when we do similar calculations for $\mathcal{P}^\dagger \mathcal{L} \mathcal{P}$ and $\mathcal{P} \mathcal{L}^\dagger \mathcal{P}^\dagger$, we find that they do not, in general, equal 0; if this were the case, then all our $\Sigma^\dagger$s would vanish (due to there being no terms with exclusively $\Sigma^\dagger$s), and A would be 0, leaving us with no more than the standard TCL-ME.

3.5 Finding $\Sigma^\dagger$s

By expanding $\mathcal{G}(t,t') = T_+ e^{\lambda \int_{t'}^{t} \bar{\mathcal{L}}(t'')dt''}$ and $\hat{\mathcal{U}(t'}, t) = T_- e^{\lambda \int_{t'}^{t} \mathcal{L}(t'')dt''}$ into powers of λ themselves, it can be found that for the first 2 terms:

$\Sigma_1(t) = \int_{t_0}^{t} \mathcal{L}(t')\mathcal{P} dt'$
$\Sigma_2(t) = \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt' [\mathcal{L}(t'')\mathcal{L}(t')\mathcal{P} - \mathcal{P}\mathcal{L}(t'')\mathcal{L}(t')\mathcal{P} - \mathcal{L}(t')\mathcal{P}\mathcal{L}(t'')]$

We can then naturally find the adjoints of these operators by reordering the operators inside the integrals (via linearity):

$\Sigma_1^\dagger(t) = \int_{t_0}^{t} \mathcal{P}^\dagger \mathcal{L}^\dagger(t') dt'$
$\Sigma_2^\dagger(t) = \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt' [\mathcal{P}^\dagger \mathcal{L}^\dagger(t')\mathcal{L}^\dagger(t'') - \mathcal{P}^\dagger \mathcal{L}^\dagger(t')\mathcal{L}^\dagger(t'')\mathcal{P}^\dagger - \mathcal{L}^\dagger(t'')\mathcal{P}^\dagger \mathcal{L}^\dagger(t')]$

3.6 Going to Higher Order

As mentioned, to 4th order, the TCL+-ME contains a singular additional term, compared with the standard TCL: $2\Sigma_1^\dagger \Sigma_1^2$. However, when expanded using the Σ operators found in the previous section, we find that this term contains $\mathcal{P}\mathcal{L}\mathcal{P} = 0$ for our chosen interaction picture; in order to find relevant terms, it is necessary to go to fifth order.

After cancellation via the aforementioned $\mathcal{P}\mathcal{L}\mathcal{P} = 0$ identities, the TCL+-5 yields another term in A, this one non-vanishing: $\Sigma_1^\dagger \Sigma_2 \Sigma_1$. An important consequence of this is that unlike the regular TCL, the terms with odd powers of lambda in the TCL+ do not necessarily vanish for a Gaussian bath.

3.7 Full TCL+-5 Equation

For the convenience of the reader, we have written out the full form of the TCL+ to 5th order below:

$\partial\rho_S = \lambda^2 \int_{t_0}^{t} dt' Tr_B[\mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathcal{P}\rho]$
$+\lambda^4 \int_{t0}^{t} dt' \int_{t0}^{t'} dt'' \int_{t0}^{t''} dt''' Tr_B[(\mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathcal{L}(t'')\mathcal{L}(t''')\mathcal{P} - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathcal{P}\mathcal{L}(t'')\mathcal{L}(t''')\mathcal{P} - \mathcal{P}\mathcal{L}(t)\mathcal{L}(t'')\mathcal{P}\mathcal{L}(t')\mathcal{L}($
$\mathcal{P}\mathcal{L}(t)\mathcal{L}(t''')\mathcal{P}\mathcal{L}(t')\mathcal{L}(t'')\mathcal{P})\rho]$
$+\ \lambda^5 \int_{t0}^{t} dt' \int_{t0}^{t} dt'' \int_{t0}^{t''} dt''' \int_{t0}^{t} dt'''' Tr_B[\mathcal{P}\mathcal{L}(t)\mathcal{P}^\dagger\mathcal{L}^\dagger(t')\mathcal{L}(t''')\mathcal{P}\mathcal{L}(t'')\mathcal{L}(t'''')\mathcal{P}\rho]$

References

[1] A. Ben-Israel and A. Charnes. Contributions to the theory of generalized inverses. *Journal of the Society for Industrial and Applied Mathematics*, 11(3):667–699, 1963.