Unitary Integration of Open Atomic Systems

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M.Sc. Project stage-I Presentation

Under the Supervision of
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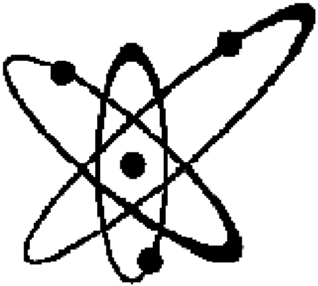
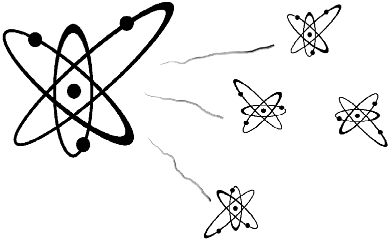
Towards Open Quantum Systems

Main idea we want to incorporate in our framework

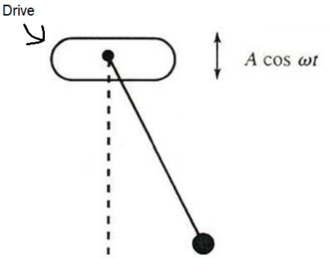




Environment can be contextually modelled for different atoms or photons!

Two ways of Implementation

Time Dependent Hamiltonians:



Density Operator Formalism:

$$\langle\psi|\, M_A \otimes \mathbb{I}\,|\psi\rangle = \Big(\sum_{i'j'} \psi^*_{i'j'} \langle A_{i'}| \otimes \langle B_{j'}|\Big)$$

$$(M_A \otimes \mathbb{I})\ \Big(\sum_{ij} \psi_{ij}\,|A_i\rangle \otimes |B_j\rangle\Big)$$

$$\rho_A = \sum_i p_i\,|i\rangle\langle i|$$

$$\rho_A = Tr_B\{|\psi\rangle\langle\psi|\}$$

$$\langle M_A\rangle = Tr\{\rho_A M_A\}$$

$$\varepsilon(\rho) = \sum_a M_a \rho M_a^\dagger$$

$$\partial_t \rho = -\frac{i}{\hbar}[H,\rho] = \mathcal{L}\rho$$

von-Neumann Liouville Equation

$$i\dot{U}(t) = H(t)U(t) \qquad \text{with} \qquad U(0) = \mathcal{I}$$

where U is unitary, following $UU^\dagger = U^\dagger U = \mathcal{I}$.

Non-exhaustive List of Features:

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1. Equivalent to Schrodinger Equation with definition $|\Psi(t)\rangle = U(t, t_0)\,|\Psi(t_0)\rangle$

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5. Approximated Analytical Solutions (for example: Time Dependent Perturbation Theory)

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5. Approximated Analytical Solutions (for example: Time Dependent Perturbation Theory)
6. Numerical Integration (for example: Runge Kutta-4*)

Baker–Campbell–Hausdorff formula

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, [X, Y]] + [Y, [Y, X]]) + \dots$$

where

$$e^Z = e^X e^Y$$

Remark

This expression highlights the non-commutativity of the SU(N) operations

Density operators

Open system is a sub-part of a larger closed system.

The density operator needs to be a

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1. Hermitian matrix: $\rho^\dagger = \rho$
2. Positive matrix (all non-negative eigenvalues): $\rho \geq 0 \equiv \langle \Psi | \, \rho \, | \Psi \rangle \geq 0$
3. and with unit trace: $\textbf{Tr}\{\rho\} = 1$

Lindblad Master Equation

$$\dot{\rho} = i[\rho, H] + \sum_i \Gamma_i (L_i \rho L_i^\dagger - \frac{1}{2}\{L_i L_i^\dagger, \rho\}) = \mathcal{L}\rho$$

Features:

1. Markovian Interaction

$$\dot{\rho} = i[\rho, H] + \sum_i \Gamma_i (L_i \rho L_i^\dagger - \frac{1}{2}\{L_i L_i^\dagger, \rho\}) = \mathcal{L}\rho$$

Features:

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7. Vectorisation in Liouville Space: Liouvillian Super-operator

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7. Vectorisation in Liouville Space: Liouvillian Super-operator
8. Exponentiation
9. Blows up in the number of variables

Unitary Integration

Summarizing Problems in both regimes

- Dimensionality
- Non-commutativity of operators
- Constraint equations

Unitary Integration Tackles Last Two in its Construction

Unitary Integration Scheme

As an example, we take

$$\begin{aligned} i\dot{U}(t) &= [a(t)A + b(t)B]U(t) \\ &= [(X_-(t)J_- + X_+(t)J_+)/2 + X_z(t)J_z]U(t) \quad \text{where } [A, B] \neq 0 \end{aligned}$$

Ansatz:

$$U(t) = e^{-i\mu_+(t)J_+} e^{-i\mu_-(t)J_-} e^{-i\mu_z(t)J_z}$$

Evaluating $i\dot{U}(t)$:

$$\begin{aligned} i\dot{U}(t) =& \dot{\mu_+}(t)J_+ \; e^{-i\mu_+(t)J_+} e^{-i\mu_-(t)J_-} e^{-i\mu_z(t)J_z} + \dot{\mu_-}(t) \; e^{-i\mu_+(t)J_+} \; J_- \; e^{-i\mu_-(t)J_-} e^{-i\mu_z(t)J_z} \\ &+ \dot{\mu_z}(t) \; e^{-i\mu_+(t)J_+} e^{-i\mu_-(t)J_-} \; J_z \; e^{-i\mu_z(t)J_z} \end{aligned}$$

Comparing to $H(t)U(t)$:

$$
\begin{aligned}
\dot{\mu_+} + i\mu_+ X_z - \frac{1}{2}\mu_+^2 X_+ =& \frac{1}{2}X_-,\\
\dot{\mu_-} - i\mu_-\mu_z =& \frac{1}{2}X_+,\\
\dot{\mu_z} - i\mu_+ X_+ =& X_z
\end{aligned}
$$

Comparing to $H(t)U(t)$:

$$
\begin{aligned}
\dot{\mu}_+ + i\mu_+ X_z - \frac{1}{2}\mu_+^2 X_+ &= \frac{1}{2}X_-, \\
\dot{\mu}_- - i\mu_- \dot{\mu}_z &= \frac{1}{2}X_+, \\
\dot{\mu}_z - i\mu_+ X_+ &= X_z
\end{aligned}
$$

Features

- Choice of Hamiltonian
- Closed Algebra
- Time Dependent Scalar Coefficients
- Non-Commuting Operators
- Reduction to solving Coupled Non-linear Differential Equations!

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Implementation I: Landau Zener Stuckleberg Majorana (LZSM) Transition

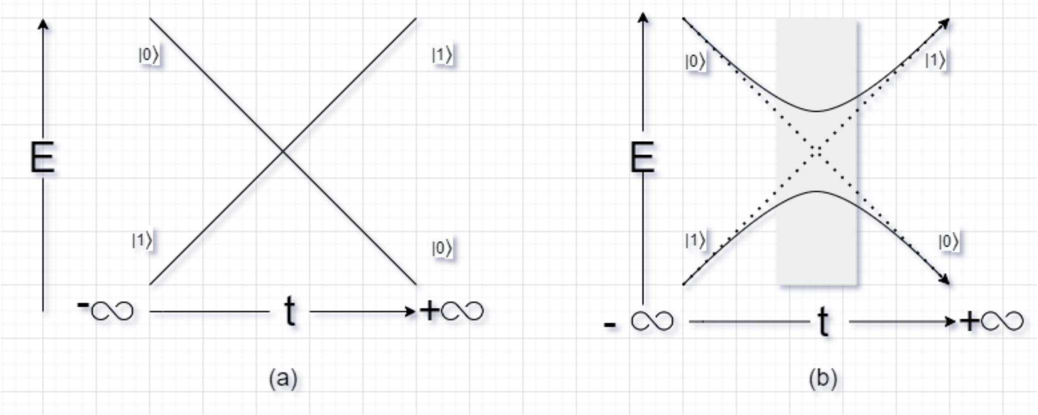


Figure 2: **(a)** No coupling between the states **(b)** Coupling produce **avoided energy level crossing**

Hamiltonian

The Hamiltonian is $H = -\frac{1}{2}\left(\Delta\sigma_x + vt\sigma_z\right)$
In our closed-algebra basis $H = -\frac{\Delta}{2}J_+ - \frac{\Delta}{2}J_- - vtJ_z$.

Riccati Equation and Two Others

$$\dot{\mu_+} - iv\,t\,X_z + \frac{\Delta}{2}\mu_+^2 + \frac{\Delta}{2} = 0,$$
$$\dot{\mu_-} - i\mu_-\dot{\mu_z} + \frac{\Delta}{2} = 0,$$
$$\dot{\mu_z} + i\Delta\mu_+ + v\,t = 0$$

with $\mu_-(0) = \mu_+(0) = \mu_z(0) = 0$.

Dealing with Stiffness

Problem:

Solving equations using RK-4 turns out to be numerically difficult due to their stiffness

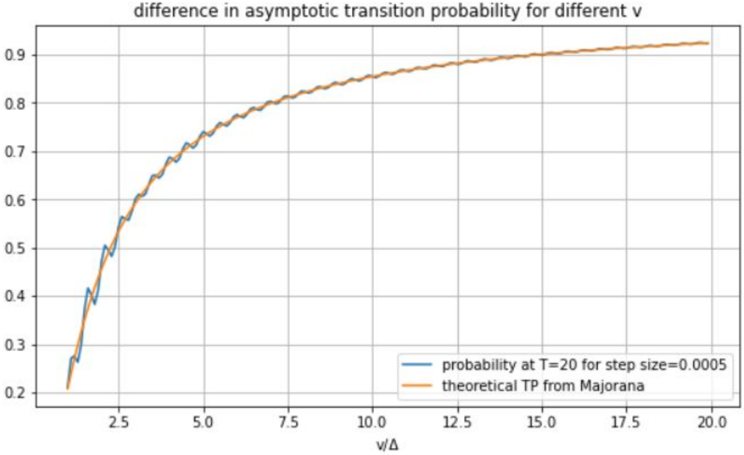
Solution:

apply the Unitarity constraint explicitly, $U^\dagger U = \mathcal{I}$

$$\mu_- = \mu_+^*/(1+|\mu_+|^2)$$
$$e^{\mathbb{I}(\mu_z)} = 1+|\mu_+|^2$$

Results Comparison: Majorana's Solution and Unitary Integration's

Ettore Majorana's asymptotic solution: $\mathcal{P} = |\beta(t \to \infty)|^2 = \exp(-2\pi\delta)$[1].

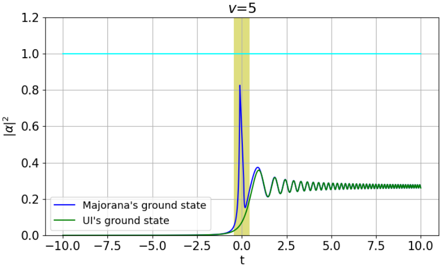


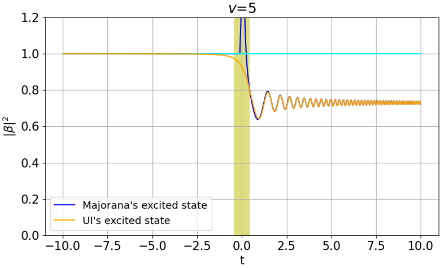
[1] Kofman, P., Ivakhnenko, O., Shevchenko, S., & Nori, F.(2022)

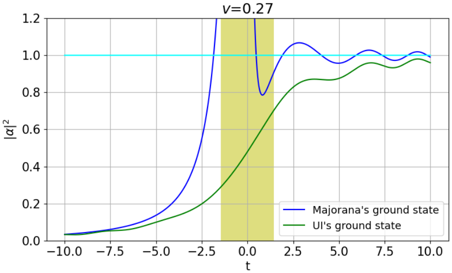
Occupation probabilities

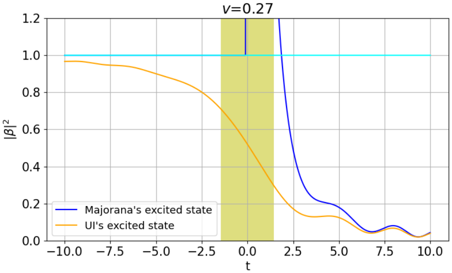
Correct dynamics far from avoided level crossing

But only in the vicinity of t=0 (transition region), the solution diverges






v=0.27
1.2
1.0
0.8
0.6
0.4
0.2
0.0
|α|²
−10.0 −7.5 −5.0 −2.5 0.0 2.5 5.0 7.5 10.0
t
Majorana's ground state
UI's ground state


v=0.27
1.2
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0.4
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0.0
|β|²
−10.0 −7.5 −5.0 −2.5 0.0 2.5 5.0 7.5 10.0
t
Majorana's excited state
UI's excited state

Implementation II: Periodically Driven Two-Level System

Generalising the previous Hamiltonian and Unitary Integration

$$H = \frac{\epsilon(t)}{2}\sigma_z + J\sigma_x, \qquad L_k = \sqrt{\frac{\Gamma}{2}}\sigma_k$$

where L_k are the Lindblad Operators and $\epsilon(t) = a\cos\omega t$. Using the same anstaz for Lindblad equation in Liouville Space !!

Liouville Fock Space

$$\frac{d}{dt}\begin{bmatrix}\rho_{11}\\ \rho_{12}\\ \rho_{21}\\ \rho_{22}\end{bmatrix} = \begin{bmatrix} i\Gamma & -J & J & i\Gamma \\ -J & (\epsilon - 2i\Gamma) & 0 & J \\ J & 0 & -(\epsilon + 2i\Gamma) & -J \\ i\Gamma & J & -J & -i\Gamma \end{bmatrix}\begin{bmatrix}\rho_{11}\\ \rho_{12}\\ \rho_{21}\\ \rho_{22}\end{bmatrix}$$

Remark

One needs **fifteen** 4X4 matrices to model the dynamics completely !!

Fortunately

Conversion to Liouville-Bloch:

$$i\frac{d}{dt}\begin{bmatrix}\rho_{12}+\rho_{21}\\ \rho_{21}-\rho_{12}\\ \rho_{11}-\rho_{22}\end{bmatrix} = \begin{bmatrix}-i\Gamma & -\epsilon(t) & 0\\ -\epsilon(t) & -i\Gamma & 2J\\ 0 & 2J & -i\Gamma\end{bmatrix}\begin{bmatrix}\rho_{12}+\rho_{21}\\ \rho_{21}-\rho_{12}\\ \rho_{11}-\rho_{22}\end{bmatrix}$$

Effective Hamiltonian Becomes

$$i\dot{\eta} = \mathcal{L}(t)\eta(t) = \big(-i\Gamma\mathbb{I} - a\epsilon(t)A_z + 2JA_x\big)\eta(t); \qquad \eta(0) = (0,0,1)$$

Features

- Non-Hermitian $\mathcal{L}$
- Complex and linearly independent coefficients $\mu_-,\ \mu_+,\ \mu_z$
- Decomposed as a sub algebra of Gell-Mann set $\{A_x,\ A_y,\ A_z\}$

Unitary Integration for Open Quantum System: Scheme

Ansatz

$$\eta(t) = \exp\left(-\Gamma t\right)\exp\left(-i\mu_+(t)A_+\right)\exp\left(-i\mu_-(t)A_-\right)\exp\left(-i\mu(t)A_z\right)\eta(0)$$

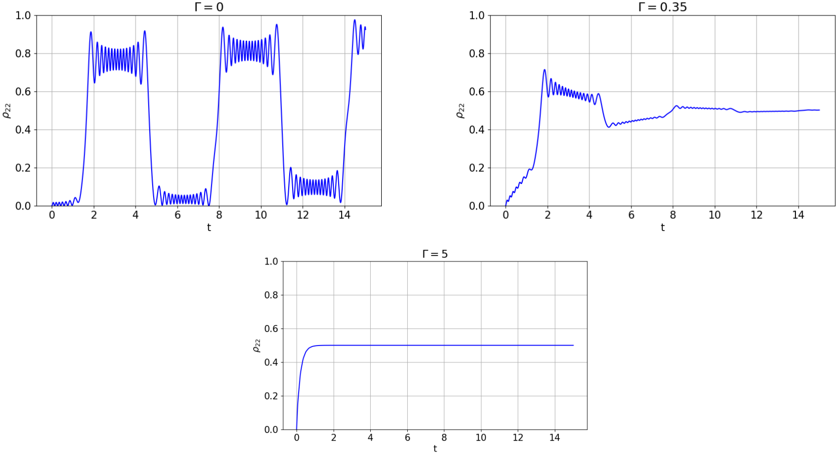
Obtained a Set of Differential Equations

$$\begin{aligned}
0 =& \dot{\mu}_+ - i\epsilon(t)\mu_+ - J(1+\mu_+^2) \\
0 =& \dot{\mu}_- - i\mu_-\dot{\mu} - J \\
0 =& \dot{\mu} - 2iJ\mu_+ + \epsilon(t), \qquad \mu_i(0) = 0
\end{aligned}$$

Remark

No Constraint Equation !!

$\rho_{22}(t)$ for Undamped, Underdamped and Overdamped



where $\omega = 1$, $J = 3$, $A = 45$

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Implementation III: Nuclear Magnetic Resonance Relaxations

- We cheated! Very Special Bath

[2] Phys. Rev. A, 71, 063822. (2005)

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Constructing Spin System Liouville Superoperator

$$H = \frac{\epsilon(t)}{2}\sigma_z + J\sigma_x, \qquad L_\pm = \sqrt{\frac{\Gamma_1}{2}}\sigma_\pm, \qquad L_3 = \sqrt{\frac{\Gamma_2}{2}}\sigma_z$$

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Ansatz for three level η

$$U(t) = e^{-i\delta} e^{-i\mu_8 b_+} e^{-i\mu_7 b_-} e^{-i\mu_6 c_+} e^{-i\mu_5 c_-} e^{-i\mu_4 a_+} e^{-i\mu_3 a_-} e^{-i\mu_2 a_3} e^{-i\mu_1 a_3}$$

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- The solution of this ansatz [2], for our case would give us the following EIGHT equations.

[2] Phys. Rev. A, 71, 063822. (2005)

EIGHT COUPLED Differential Equations for the System

$$\dot{\mu}_8 = -\epsilon(t) - iS\mu_5 - \epsilon\mu_8^2 \tag{1}$$

$$\dot{\mu}_7 = -\epsilon(t) + i\mu_6 R + i\mu_5\mu_7^2 S + 2\epsilon(t)\mu_7\mu_8 \tag{2}$$

$$\dot{\mu}_6 = 2iJ\mu_7 - 2iJ\mu_8\mu_6^2 + \epsilon(t)\mu_6\mu_8 + iS\mu_5\mu_6\mu_7 + \mu_6(\Gamma_2 - \Gamma_1) \tag{3}$$

$$\dot{\mu}_5 = -2iJ\mu_8 - \epsilon(t)\mu_5\mu_8 + 4iJ\mu_5\mu_8\mu_6 - iS\mu_5^2\mu_7 - \mu_5(\Gamma_2 - \Gamma_1) \tag{4}$$

$$\dot{\mu}_4 = i\epsilon(t)\mu_8 + 2J\mu_6\mu_8 - S\mu_5\mu_7 + \frac{i}{3}(\Gamma_2 - \Gamma_1) \tag{5}$$

$$\dot{\mu}_3 = S + R\mu_3^2 - i\mu_3\Big(- i\epsilon(t)\mu_8 + 2J\mu_6\mu_8 + S\mu_5\mu_7 + i(\Gamma_2 - \Gamma_1)\Big) \tag{6}$$

$$\dot{\mu}_2 = 2J(1 - \mu_8\mu_7) + i\mu_2\Big(i\epsilon(t)\mu_8 + 2iR\mu_3 + 2J\mu_6\mu_8 + S\mu_5\mu_7 + i(\Gamma_2 - \Gamma_1)\Big) \tag{7}$$

$$\dot{\mu}_1 = -i\epsilon(t)\mu_8 + S\mu_5\mu_7 + iR\mu_3 + \frac{i}{3}(\Gamma_2 - \Gamma_1) \tag{8}$$

where

$$R = 2J(1 - \mu_7\mu_8)$$

$$S = \frac{2J}{1 - \mu_5\mu_6}$$

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- Unitary integration can solve **many** Small Atomic Systems.
- Not extendable to many-particle systems
- Exact equations up to numerical accuracy.
- **Future Plans:**
    - Deeper Exploration of NMR problem; A subject in itself
    - Collective Atomic Systems with same underlying algebra from the field of quantum optics and molecular physics
- Token of Appreciation to Gourang, Naman and MATHEMATICA

Thank You!

Most Important References I

[1] A. R. P. Rau, Phys. Rev. Lett. 81, 4785 (1998)

[2] S. Vinjanampathy and A R P Rau J. Phys. A: Math. Theor. 42 425303 (2009)

[3] C. Bengs. Journal of Magnetic Resonance, 322, 106868. (2021)

[4] Kofman, P., Ivakhnenko, O., Shevchenko, S., & Nori, F. (2022)