

Electronic System Strongly Interacting With Fermionic Reservoirs

Théodore GOUMAI VEDEKOI
19E2617

PhD candidate in physics

Under the direction of :

NANA ENGO S. G., Professor-UY1
TCHAPET NJAFA J-P., Lecturer-UY1

University of Yaoundé 1
Laboratory of Nuclear, Atomic, Molecular and Biophysical Physics
Year 2025

April 2025

Context and motivations

Key words definitions / Reformulation

- Fermionic Reservoirs
- Electronic system
- Strongly Interaction

Context and motivations

Key words definitions / Reformulation

- Fermionic Reservoirs
- Electronic system
- Strongly Interaction

Set of electrons in a material that strongly exchanges energy or particles with fermionic baths

Context and motivations

Key words definitions / Reformulation

- Fermionic Reservoirs
- Electronic system
- Strongly Interaction

Set of electrons in a material that strongly exchanges energy or particles with fermionic baths

- Quantum transport
- Dissipation and decoherence
- Out-of-equilibrium phenomena
- Kondo effect

Context and Motivations

Problem and problematic

Problematic

How do strong interactions between an electronic system and one or more fermionic reservoirs influence the dynamic and out-of-equilibrium properties of the system?

Context and Motivations

Problem and problematic

Problematic

How do strong interactions between an electronic system and one or more fermionic reservoirs influence the dynamic and out-of-equilibrium properties of the system ?

- representation of the system

Context and Motivations

Problem and problematic

Problematic

How do strong interactions between an electronic system and one or more fermionic reservoirs influence the dynamic and out-of-equilibrium properties of the system ?

- representation of the system
- quantum modelling

Context and Motivations

Problem and problematic

Problematic

How do strong interactions between an electronic system and one or more fermionic reservoirs influence the dynamic and out-of-equilibrium properties of the system ?

- representation of the system
- quantum modelling
- correlation functions

Context and Motivations

Problem and problematic

Problematic

How do strong interactions between an electronic system and one or more fermionic reservoirs influence the dynamic and out-of-equilibrium properties of the system ?

- representation of the system
- quantum modelling
- correlation functions
- Compute statistical state with Julia using HierarchicalEOM

Contents

- 1 Complex representation
- 2 Correlation functions
- 3 Julia implementation
- 4 Jupyter implementation

Complex representation

Quantum modelling

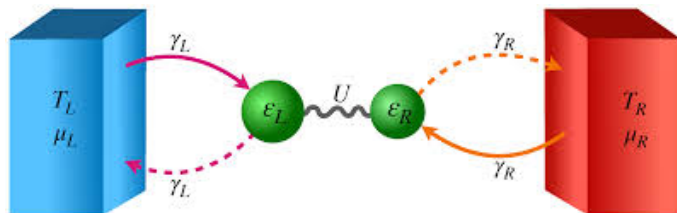


Figure – system representation for two fermionic baths

Complex representation

Quantum modelling

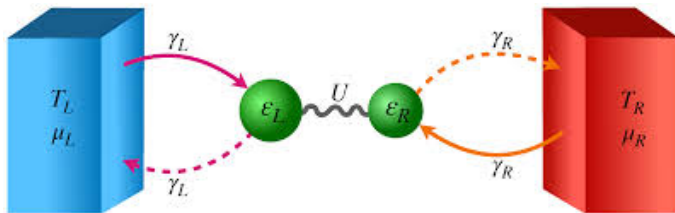


Figure – system representation for two fermionic baths

$$H_s = \varepsilon \left(d_{\uparrow}^{\dagger} d_{\uparrow} + d_{\downarrow}^{\dagger} d_{\downarrow} \right) + U \left(d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow} \right)$$

Complex representation

Quantum modelling

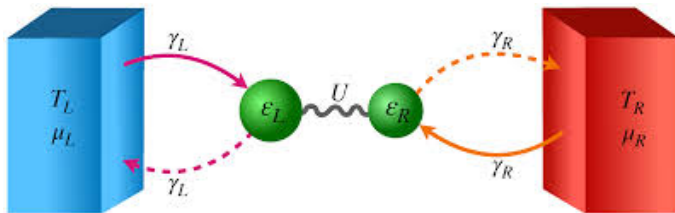


Figure – system representation for two fermionic baths

$$H_s = \varepsilon \left(d_{\uparrow}^{\dagger} d_{\uparrow} + d_{\downarrow}^{\dagger} d_{\downarrow} \right) + U \left(d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow} \right)$$

$$H_f = \sum_{\alpha=L,R} \sum_{\sigma_f=\uparrow,\downarrow} \sum_k \varepsilon_{\alpha,\sigma_f,k} c_{\alpha,\sigma_f,k}^{\dagger} c_{\alpha,\sigma_f,k},$$

Interacting Picture

Quantum Modelling

$$H_{SF} = \sum_{\alpha=L,R} \sum_{\sigma_f=\uparrow,\downarrow} \sum_k g_{\alpha,k} c_{\alpha,\sigma_f,k}^\dagger d_{\sigma_f} + g_{\alpha,k}^* d_{\sigma_f}^\dagger c_{\alpha,\sigma_f,k}$$

Interacting Picture

Quantum Modelling

$$H_{SF} = \sum_{\alpha=L,R} \sum_{\sigma_f=\uparrow,\downarrow} \sum_k g_{\alpha,k} c_{\alpha,\sigma_f,k}^\dagger d_{\sigma_f} + g_{\alpha,k}^* d_{\sigma_f}^\dagger c_{\alpha,\sigma_f,k}$$

Conditions assume

- System and environments (baths) are initialized in a separable state
- Each of the fermionic baths is initially in thermal equilibrium characterized by a Fermi Dirac distribution
- The bath operator within the system-bath interaction Hamiltonian should be linear in the bath annihilation and creation operators

Reduce Statistical Matrix

Dyson series

$$\rho_s^{p=+}(t) = \hat{G}(t) \left[\rho_s^{p=+}(0) \right]$$

Reduce Statistical Matrix

Dyson series

$$\rho_s^{p=+}(t) = \hat{G}(t) [\rho_s^{p=+}(0)]$$

$$\hat{G}(t)[.] = \hat{\mathcal{T}} \exp \left\{ - \int_0^t dt_1 \int_0^t dt_2 [\hat{W}_f(t_1, t_2)[.]] \right\}$$

Reduce Statistical Matrix

Dyson series

$$\rho_s^{p=+}(t) = \hat{G}(t) [\rho_s^{p=+}(0)]$$

$$\hat{G}(t)[.] = \hat{\mathcal{T}} \exp \left\{ - \int_0^t dt_1 \int_0^{t_1} dt_2 [\hat{W}_f(t_1, t_2)[.]] \right\}$$

$$\begin{aligned} \hat{W}(t_1, t_2)[.] = \sum_{\alpha} \sum_{p=\pm} \sum_{\nu=\pm}^1 \left\{ C_{\alpha}^{\nu}(t_1, t_2) [d_s^{\bar{\nu}}(t_2), d_s^{\nu}(t_1).]_{-p} \right. \\ \left. + C_{\alpha}^{\nu}(t_2, t_1) [.d_s^{\bar{\nu}}(t_2), d_s^{\nu}(t_1)]_{-p} \right\} \end{aligned}$$

Reduce Statistical Matrix

Dyson series

$$\rho_s^{p=+}(t) = \hat{G}(t) [\rho_s^{p=+}(0)]$$

$$\hat{G}(t)[.] = \hat{\mathcal{T}} \exp \left\{ - \int_0^t dt_1 \int_0^{t_1} dt_2 [\hat{W}_f(t_1, t_2)[.]] \right\}$$

$$\begin{aligned} \hat{W}(t_1, t_2)[.] = \sum_{\alpha} \sum_{p=\pm} \sum_{\nu=\pm}^1 & \left\{ C_{\alpha}^{\nu}(t_1, t_2) [d_s^{\bar{\nu}}(t_2), d_s^{\nu}(t_1).]_{-p} \right. \\ & \left. + C_{\alpha}^{\nu}(t_2, t_1) [.d_s^{\bar{\nu}}(t_2), d_s^{\nu}(t_1)]_{-p} \right\} \end{aligned}$$

For the basis $\{|i\rangle, |j\rangle\}$

$$\langle i | \rho_S^p | j \rangle \longrightarrow \langle i | (c \tilde{\rho}_e \tilde{\rho}_s^p c^{\dagger} + \tilde{\rho}_e \tilde{\rho}_s^p) | j \rangle$$

Correlation functions

- 1 Complex representation
- 2 Correlation functions**
- 3 Julia implementation
- 4 Jupyter implementation

Correlation function

$$C_{\alpha}^{\nu}(t_1, t_2) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega J_{\alpha}(\omega) \left[\frac{1-\nu}{2} + \nu n_{\alpha}^{\text{eq}}(\omega) \right] e^{\nu i\omega(t_1-t_2)}$$

Correlation function

$$C_{\alpha}^{\nu}(t_1, t_2) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega J_{\alpha}(\omega) \left[\frac{1-\nu}{2} + \nu n_{\alpha}^{\text{eq}}(\omega) \right] e^{\nu i\omega(t_1-t_2)}$$

$$J_{\alpha}(\omega) = 2\pi \sum_k |g_{\alpha,k}|^2 \delta(\omega - \omega_k)$$

$$n_{\alpha}^{\text{eq}}(\omega) = \frac{1}{e^{\frac{\omega - \nu\alpha}{k_B T_{\alpha}}} + 1}$$

Correlation function

$$C_{\alpha}^{\nu}(t_1, t_2) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega J_{\alpha}(\omega) \left[\frac{1-\nu}{2} + \nu n_{\alpha}^{\text{eq}}(\omega) \right] e^{\nu i\omega(t_1-t_2)}$$

$$J_{\alpha}(\omega) = 2\pi \sum_k |g_{\alpha,k}|^2 \delta(\omega - \omega_k)$$

$$n_{\alpha}^{\text{eq}}(\omega) = \frac{1}{e^{\frac{\omega - \nu\omega_{\alpha}}{k_B T_{\alpha}}} + 1}$$

$$C_{\alpha}^{\nu}(\tau) = \sum_{h=1}^{N_{\alpha}} \eta_{\alpha,h}^{\nu} \exp(-\gamma_{\alpha,h}^{\nu} \tau)$$

HEOM equation form

Auxilliary Statistical Operators (ASO)

$$\begin{aligned}\partial_t \rho_{j|q}^{(n,p)}(t) &\equiv \hat{M}^{(n,p)} \rho_{j|q}^{(n,p)}(t) \\ &= - \left(i \tilde{\mathcal{L}}_s + \sum_{w=1}^n \gamma_{q_w} \right) \rho_{j|q}^{(n,p)}(t) \\ &\quad - i \sum_{q' \notin q} \hat{A}_{q'} \rho_{j|q^+}^{(n+1,p)}(t) - i \sum_{w=1}^n (-1)^{(n-w)} \hat{C}_{q_w} \rho_{j|q_w^-}^{(n-1,p)}(t)\end{aligned}$$

$$\hat{\mathcal{L}}_s[.] = [H_S(t), .]_-$$

$$q^+ = [q', q_n, \dots, q_1],$$

$$q_w^- = [q_n, \dots, q_{w+1}, q_{w-1}, \dots, q_1]$$

HEOM Liouvillian Superoperator (HEOMLS)

$$\hat{A}_q[.] = (-1)^{\delta_{p,-}} \{d_{\sigma_f}^\nu[.] - \hat{P}_s[.]d_{\sigma_f}^{\bar{\nu}}\}$$

$$\hat{C}_q[.] = (-1)^{\delta_{p,-}} \left\{ \eta_{\alpha,h}^\nu d_{\sigma_f}^\nu[.] + \left(\eta_{\alpha,h}^\nu \right)^* \hat{P}_s \left[[.] d_{\sigma_f}^\nu \right] \right\}$$

HEOM Liouvillian Superoperator (HEOMLS)

$$\hat{A}_q[.] = (-1)^{\delta_{p,-}} \{ d_{\sigma_f}^\nu[.] - \hat{P}_s[.] d_{\sigma_f}^{\bar{\nu}} \}$$

$$\hat{C}_q[.] = (-1)^{\delta_{p,-}} \left\{ \eta_{\alpha,h}^\nu d_{\sigma_f}^\nu[.] + \left(\eta_{\alpha,h}^\nu \right)^* \hat{P}_s \left[[.] d_{\sigma_f}^\nu \right] \right\}$$

$$\hat{\mathcal{P}}_s \left[\rho_{j|q}^{(m,n,\pm)}(t) d_{\sigma_f}^\nu \right] = \mp (-1)^n \rho_{j|q}^{(m,n,\pm)}(t) d_{\sigma_f}^\nu$$

$$\hat{\mathcal{P}}_s[.] = \left(\prod_{\sigma_f} \exp \left[i\pi d_{\sigma_f}^\dagger d_{\sigma_f} \right] \right) [.] \left(\prod_{\sigma_f} \exp \left[i\pi d_{\sigma_f}^\dagger d_{\sigma_f} \right] \right)$$

HEOM Liouvillian Superoperator (HEOMLS)

$$\hat{A}_q[.] = (-1)^{\delta_{p,-}} \{ d_{\sigma_f}^\nu[.] - \hat{P}_s[.] d_{\sigma_f}^{\bar{\nu}} \}$$

$$\hat{C}_q[.] = (-1)^{\delta_{p,-}} \left\{ \eta_{\alpha,h}^\nu d_{\sigma_f}^\nu[.] + \left(\eta_{\alpha,h}^\nu \right)^* \hat{P}_s \left[[.] d_{\sigma_f}^\nu \right] \right\}$$

$$\hat{\mathcal{P}}_s \left[\rho_{j|q}^{(m,n,\pm)}(t) d_{\sigma_f}^\nu \right] = \mp (-1)^n \rho_{j|q}^{(m,n,\pm)}(t) d_{\sigma_f}^\nu$$

$$\hat{\mathcal{P}}_s[.] = \left(\prod_{\sigma_f} \exp \left[i\pi d_{\sigma_f}^\dagger d_{\sigma_f} \right] \right) [.] \left(\prod_{\sigma_f} \exp \left[i\pi d_{\sigma_f}^\dagger d_{\sigma_f} \right] \right)$$

$$\pi A(\omega) = \text{Re} \left\{ \int_0^\infty dt \left[\langle d(t) d^\dagger(0) \rangle^* + \langle d^\dagger(t) d(0) \rangle \right] e^{-i\omega t} \right\} \quad (1)$$

$$\pi S(\omega) = \text{Re} \left\{ \int_0^\infty dt \langle P(t) Q(0) \rangle e^{-i\omega t} \right\}$$

Julia implementation

- 1 Complex representation
- 2 Correlation functions
- 3 Julia implementation**
- 4 Jupyter implementation

Julia Implementation



- *Performance*
- *Ease of Use*
- *Support for Numerical Computations*
- *Programming Paradigms*
- *Rich Ecosystem*
- *Ease of Parallelism*
- *Visualization*

```
Hierarchical Equations of Motion
```

Julia framework for Hierarchical Equations of Motion

Copyright © QuTiP team 2023 and later.
Lead developer : Yi-Te Huang
Other developers:
Simon Cross, Neill Lambert, Po-Chen Kuo and Shen-Liang Yang

Package information:

```
=====
 Julia                Ver. 1.11.4
 HierarchicalEOM      Ver. 2.5.1
 QuantumToolbox       Ver. 0.30.0
 SciMLOperators       Ver. 0.3.13
 LinearSolve          Ver. 3.7.2
 OrdinaryDiffEqCore   Ver. 1.22.0
```

System information:

```
=====
 OS           : Linux (x86_64-linux-gnu)
 CPU          : 4 × Intel(R) Pentium(R) CPU N4200 @ 1.10GHz
 Memory       : 3.632 GB
 WORD_SIZE    : 64
 LIBM         : libopenlibm
```

Navigation icons: back, forward, search, etc.

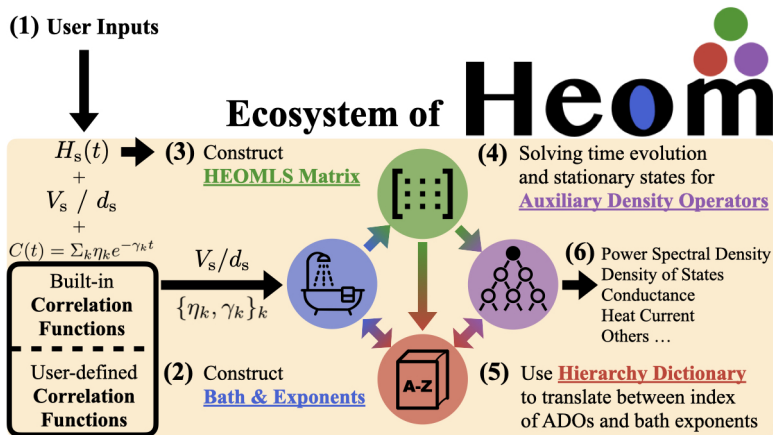


Figure – HierarchicalEOM.jl

Jupyter implementation

- 1 Complex representation
- 2 Correlation functions
- 3 Julia implementation
- 4 Jupyter implementation

Jupyter Implementation

see jupyter code