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
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- Fermionic Reservoirs
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- Strongly Interaction

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

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 ?

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- representation of the system
- quantum modelling

Context and Motivations

Problem and problematic

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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

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

Contents

Complex representation

Quantum modelling

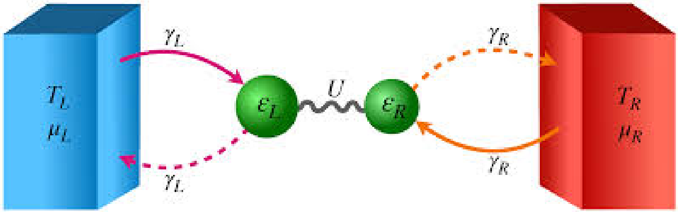

Figure – *sytem representation for two fermionics baths*

Complex representation

Quantum modelling

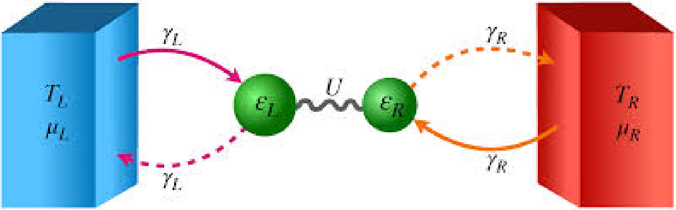

Figure – *sytem representation for two fermionics baths*

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

Complex representation

Quantum modelling

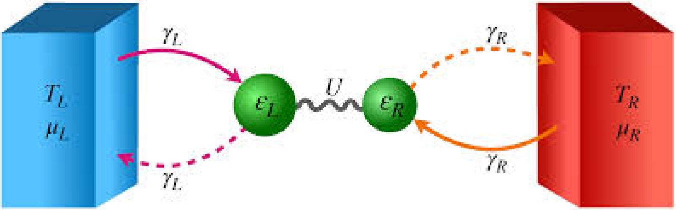

Figure – *sytem representation for two fermionics baths*

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

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

Interacting Picture

Quantum Modelling

$$H_{SF} = \sum_{\alpha=L,R} \sum_{\sigma_f=\uparrow,\downarrow} \sum_k g_{\alpha,k} c^\dagger_{\alpha,\sigma_f,k} d_{\sigma_f} + g^*_{\alpha,k} d^\dagger_{\sigma_f} c_{\alpha,\sigma_f,k}$$

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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

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

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

$$\left. + C_\alpha^\nu(t_2, t_1)\left[.d_s^{\overline{\nu}}(t_2), d_s^\nu(t_1)\right]_{-p}\right.$$

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$$+\, C_\alpha^\nu(t_2,t_1)\left[.d_s^{\overline{\nu}}(t_2), d_s^\nu(t_1)\right]_{-p}$$

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

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

Correlation functions

Correlation function

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

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

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

HEOM equation form

Auxilliary Statistical Operators (ASO)

$$\partial_t \rho^{(n,p)}_{j|q}(t) \equiv \hat{M}^{(n,p)} \rho^{(n,p)}_{j|q}(t)$$

$$= \text{-} \left(i\tilde{\mathcal{L}}_s + \textstyle\sum_{w=1}^{n} \gamma_{q_w} \right) \rho^{(n,p)}_{j|q}(t)$$

$$-i \sum_{q' \notin q} \hat{A}_{q'} \rho^{(n+1,p)}_{j|q^+}(t) - i \sum_{w=1}^{n} (-1)^{(n-w)} \hat{C}_{q_w} \rho^{(n-1,p)}_{j|q_w^-}(t)$$

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

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

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

HEOM Liouvillian Superoperator (HEOMLS)

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

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

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

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

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

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

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

Julia implementation

Julia Implementation

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

HierarchicalEOM.jl Package

Figure – *HierarchicalEOM.jl*

Heom Workflow

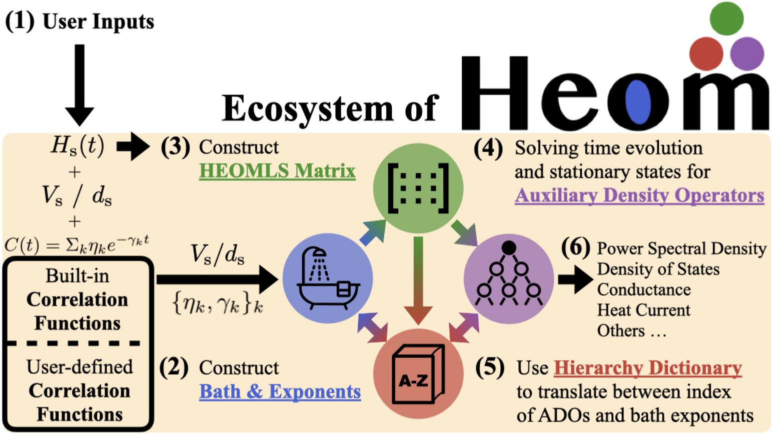

Figure – *HierarchicalEOM.jl*

Jupyter implementation

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see jupyter code