

PHI User's Guide

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1 Introduction and theory

PHI is a multi-threaded software implementation of a hierarchy equation of motion (HEOM) integrator to run on shared memory parallel computers. The HEOM is a method to calculate the noise-averaged time evolution of density matrix that describes a quantum system in contact with a thermal environment. The dynamics of quantum systems in a thermal environment, sometimes called dissipative quantum dynamics or open quantum dynamics, is of interest in many areas of research and has been studied for many decades with various methods. This User's Guide gives a brief introduction of the specify a quantum system in the input parameter file, and then run PHI to calculate the density matrix evolution. For a thorough treatment of open quantum systems please read:

- H.P Breuer and F. Petruccione. "The theory of open quantum systems." Oxford University Press. 2002
- U. Weiss. "Dissipative quantum systems." World Scientific. 2008

1.1 Modeling the quantum system

To describe the input parameters for PHI, first the model of the quantum system has to be specified. The quantum system is described by a total Hamiltonian

$$H_T = H_S + H_B + H_{SB} + H_{ren}, \quad (1)$$

where H_S describes the system of interest, H_B the thermal environment, H_{SB} the system-environment coupling, and H_{ren} is a renormalization term (specified below) dependent on the system-environment coupling. The system Hamiltonian describes states $|i\rangle$, $i = 1, \dots, N$ with energies E_i and interaction V_{ij} as

$$H_S = \sum_{i=1}^N |i\rangle\langle i| E_i + \sum_{i \neq j=1}^N V_{ij} |i\rangle\langle j|, \quad (2)$$

The environment is modeled as an infinite set of harmonic oscillators with

$$H_B = \sum_{\xi} \frac{p_{\xi}^2}{2m_{\xi}} + \frac{m_{\xi} \omega_{\xi}^2 q_{\xi}^2}{2} \quad (3)$$

The system-environment coupling is assumed to be linear given by

$$H_{SB} = \sum_{a=1}^M F_a \sum_{\xi} c_{a\xi} q_{\xi} = \sum_{a=1}^M F_a u_a, \quad (4)$$

where $F_a = \sum_{i,j=1}^N f_{aij} |i\rangle\langle j|$ specifies the exact form of the coupling. At present only diagonal forms of F_a are implemented in PHI, such that $f_{aij} = \delta_{ij} f_{ai}$. In the present implementation only three types of F_a are allowed:

1. diagonal, independent coupling: $M = N$, $F_a = |a\rangle\langle a|$
2. diagonal, independent coupling: $M \neq N$, $F_a = |i_a\rangle\langle i_a|$ for $i_a \in \{1, \dots, N\}$.
3. diagonal, correlated coupling: $M = N$, $F_a = \sum_{i=1}^N f_{ai} |i\rangle\langle i|$

The coupling introduces a shift in the bath coordinates q_ξ that needs to be countered with the renormalization term

$$H_{ren} = \sum_{a,b=1}^M F_a F_b \sum_{\xi} \frac{c_{a\xi} c_{b\xi}}{2m_\xi \omega_\xi^2}. \quad (5)$$

Note that the renormalization term is NOT added to the system Hamiltonian in PHI – this is left up to the user to include in the Hamiltonian section of the input parameters. PHI implements the HEOM to calculate the system density matrix $\rho(t)$ averaged over environmental fluctuations

$$\rho(t) = \langle W(t) \rangle_B, \quad (6)$$

where $W(t)$ is the density matrix of the complete system + environment. The time evolution of $W(t)$ is formally calculated as

$$W(t) = e^{-iH_T/\hbar} W(0) e^{iH_T/\hbar}, \quad (7)$$

Where $W(0)$ specifies the density matrix of the complete system at $t = 0$. Assuming that the environment is in thermal equilibrium and that initially the system and environment are uncorrelated, the initial density matrix is given by

$$W(0) = \rho(0) \otimes R, \quad (8)$$

where $R = \exp(-\beta H_B) / \text{tr}_B \{ \exp(-\beta H_B) \}$, tr_B is the partial trace over bath coordinates and $\beta = 1/T$ is the inverse temperature. The system density matrix evolution can be written as

$$\rho(t) = \left\langle e^{-iH_T/\hbar} \rho(0) e^{iH_T/\hbar} \right\rangle_B = \text{tr}_B \left\{ e^{-iH_T/\hbar} \rho(0) \otimes R e^{iH_T/\hbar} \right\} \quad (9)$$

1.2 Correlation functions

The bath correlation functions $C_{ab}(t)$ determines how the environment fluctuations affect the system through the couplings F_a . The bath correlation functions are given as

$$C_{ab}(t) = \langle u_a(t) u_b(0) \rangle_B = \text{tr}_B \left\{ u_a(t) u_b(0) \frac{\exp(-\beta H_B)}{\text{tr}_B \{ \exp(-\beta H_B) \}} \right\}. \quad (10)$$

Here $u_a(t)$ evolve according to the interaction representation with respect to H_{SB} and $\beta = 1/T$ is the inverse temperature. The correlation function tells us how a perturbation of the environment caused by the coupling F_a affects the system at a later time through the coupling F_b . The correlation functions are usually specified through the Fourier-Laplace transform of the spectral density $J_a(\omega)$ as

$$C_{ab}(t) = \frac{1}{\pi} \int_0^\infty d\omega J_{ab}(\omega) \frac{e^{-i\omega t}}{1 - e^{-\beta\hbar\omega}}, \quad (11)$$

where,

$$J_{ab}(\omega) = \sum_\xi \frac{\pi}{2} \sum_\xi \frac{c_{a\xi} c_{b\xi}}{m_\xi \omega_\xi} \delta(\omega - \omega_\xi). \quad (12)$$

The HEOM arise by assuming a form of bath correlation functions given by

$$C_{ab}(t) = \sum_{k=0}^K c_{abk} e^{-(\nu_{abk} + i\Omega_{abk})t}. \quad (13)$$

The huge computational expense of such arbitrary correlation functions (especially with large M and K) restricts us to forms with $C_{ab}(t) = \delta_{ab} C_a(t)$ and $\Omega_{abk} = 0$. This gives the bath correlation functions as

$$C_a(t) = \sum_{k=0}^\infty c_{ak} e^{-\nu_{ak}t}, \quad (14)$$

which corresponds to spectral densities of the Drude form given by

$$J_a(\omega) = 2\lambda_a \frac{\omega\gamma_a}{\omega^2 + \gamma_a^2}. \quad (15)$$

The Drude spectral density, and employing a Matsubara expansion of $1/(1 - \exp(-\beta\hbar\omega))$ is Eq. 11, results in correlation function coefficients

$$c_{a0} = \gamma_a \lambda_a [\cot(\beta\hbar\gamma_a/2) - i] \quad (16)$$

$$c_{ak \geq 1} = \frac{4\lambda_a \gamma_a}{\beta\hbar} \frac{\nu_{ak}}{\nu_{ak}^2 - \gamma_a^2}. \quad (17)$$

and damping constants $\nu_{a0} = \gamma_a$, $\nu_{ak \geq 1} = 2\pi k/\beta\hbar$. The infinite number of Matsubara terms ν_{ak} in Eq. 14 is truncated to a finite K where for all $k > K$, $\nu_{ak} \exp(-\nu_{ak}t) \approx \delta(t)$.

The parameters needed to model the system are summarized in Table 1.

1.3 Hierarchy equations of motion

The exponential terms in Eq. 14 lead to a hierarchy of matrices $\rho_n(t)$, called auxiliary density matrices (ADMs), to take into account the non-Markovian evolution of $\rho(t)$. The

Table 1: Parameters defining model of quantum system

Parameter	Meaning	Units
N	Number of states $ i\rangle$	
E_i	Energy level of state $ i\rangle$	[Energy]
V_{ij}	Interaction between states $ i\rangle$ and $ j\rangle$	[Energy]
M	Number of system-environment coupling terms	
f_{ai}	Elements of F_a specifying system-environment coupling	
λ_a	Strength of coupling F_a	[Energy]
γ_a	Response frequency of environment from F_a coupling	[time] ⁻¹
K	Number of Matsubara terms to include	
L_T	Hierarchy truncation level	

ADMs are indexed by a vector $\mathbf{n} = (n_{10}, \dots, n_{1K}, \dots, n_{M0}, \dots, n_{MK})$ and coupled through the index operators $\mathbf{n}_{ak}^\pm = (n_{10}, \dots, n_{ak} \pm 1, \dots, n_{MK})$. The hierarchy equations of motion are

$$\dot{\rho}_{\mathbf{n}} = -\frac{i}{\hbar} [H_S, \rho_{\mathbf{n}}] - \sum_{a=1}^M \sum_{k=0}^K n_{ak} \nu_{ak} \rho_{\mathbf{n}} \quad (18)$$

$$- \sum_{a=1}^M \left(\frac{2\lambda_a}{\beta \hbar^2 \gamma_a} - \sum_{k=0}^K \frac{c_{ak}}{\hbar \nu_{ak}} \right) [F_a, [F_a, \rho_{\mathbf{n}}]] \quad (19)$$

$$-i \sum_{a=1}^M \left[F_a, \sum_{k=0}^K \rho_{\mathbf{n}_{ak}^+} \right] - \frac{i}{\hbar} \sum_{a=1}^M \sum_{k=0}^K n_{ak} \left(c_{ak} F_a \rho_{\mathbf{n}_{ak}^-} - \rho_{\mathbf{n}_{ak}^-} F_a c_{ak}^* \right). \quad (20)$$

More simply written as

$$\dot{\rho}_{\mathbf{n}} = \mathcal{L}_{eff} \rho_{\mathbf{n}} + \sum_a \sum_k \mathcal{P}_{ak} \rho_{\mathbf{n}_{ak}^+} + \sum_a \sum_k \mathcal{N}_{ak} \rho_{\mathbf{n}_{ak}^-}, \quad (21)$$

where \mathcal{L}_{eff} , \mathcal{P}_{ak} and \mathcal{N}_{ak} are Liouville space operators \mathcal{X} , such that $\mathcal{X}\bullet = X\bullet - \bullet X^\dagger$ for the corresponding Hilbert space operator X . Any ADM with a negative in the index vector \mathbf{n} is set to 0.

The ADMs need to be truncated to a finite number. Each ADM can be assign to a level $L = \sum_{a=1}^M \sum_{k=0}^K n_{ak}$. There are two ways to truncate the hierarchy of ADMs to some level L_T : time non-local (TNL) truncation and time local (TL) truncation. In case of TNL truncation, all ADMs with $L \geq L_T$ is set to zero. In case of TL truncation, all ADMs with $L = L_T - 1$ the Markovian approximation is assumed, such that

$$\sum_{k=0}^K \hat{\rho}_{\mathbf{n}_{ak}^+} \approx -i \left(\hat{Q}_a^K(t) \rho_{\mathbf{n}} - \rho_{\mathbf{n}} \hat{Q}_a^K(t)^\dagger \right), \quad (22)$$

where

$$\hat{Q}_a^K(t) = \int_0^t \left(\sum_{k=0}^K c_{ak} \exp(-\nu_{ak}\tau) \right) \exp\left(-\frac{i}{\hbar} H_S \tau\right) \hat{F}_a \exp\left(\frac{i}{\hbar} H_S \tau\right) d\tau. \quad (23)$$

1.4 Integrating the HEOM

PHI implements two methods to integrate the HEOM: Runge-Kutta 4'th (RK4) order integration and Runge-Kutta-Fehlberg 4/5 (RKF45) adaptive integration. In case of RK4 integration, only a fixed timestep dt needs to be chosen. In case of RKF45 integration, a minimum timestep dt_{min} and integration tolerance δ_I needs to be chosen.

2 Input Parameters

PHI parses an input file specified at the command line to specify the quantum system, construct the hierarchy and choose integration parameters.

2.1 Parameter file format

The input file has a few general formatting rules:

1. `#` at the start of a line specifies a comment.
All comments have to be on separate lines.
2. Empty lines are ignored.
3. Scalar parameters are specified using
`Parameter=value`
on one line.
4. Vector and matrix parameters are specified using
`VectorParameter:`
`value1,value2,value3`
and
`MatrixParameter:`
`value11,value12,value13`
`value21,value22,value23`
`value31,value32,value33`

5. Complex numbers $a + ib$ are input using (a,b). E.g.
Parameter=(a,b)
6. NumStates and NumCouplingTerms must be specified before any vector or matrix parameters can be input.

The following parameters MUST be specified in the input file to run PHI:

- NumStates
- HierarchyTruncation

Although, specifying only those parameters will allow you to only check memory requirements or print a hierarchy. The minimum parameters for an integration calculation are

- OutputFile
- NumStates
- HierarchyTruncation
- Hamiltonian
- InitialDensityMatrix
- Lambda
- Gamma
- Timestep
- Runlength

2.2 System parameters

The system parameters specify the N quantum states $|i\rangle$ and matrix elements of the Hamiltonian $H_{i,j}$.

- NumStates < N >
Acceptable Values: positive integers
Default Value: 0
Description: Specifies the number of quantum states [required]
Example line(s):
 NumStates=2

- **Hamiltonian** $\langle H_S + H_{ren} \rangle$
Acceptable Values: $N \times N$ real values
Default Value: None
Description: Specifies the system Hamiltonian. Note that the renormalization term must be included here
Example line(s):
Hamiltonian:
0 ,100.0
100.0,20.00
- **InitialDensityMatrix** $\langle \rho(0) \rangle$
Acceptable Values: $N \times N$ real or complex values
Default Value: None
Description: Specifies the initial values of the density matrix. The initial density matrix must be positive definite.
Example line(s):
InitialDensityMatrix:
(0.5,0.0),(0.2,0.1)
(0.2,-0.1),(0.5,0.0)
- **HamiltonianEigenvalues** $\langle \epsilon_i \rangle$
Acceptable Values: N real values
Default Value: None
Description: Eigenvalues of system Hamiltonian H_S [required for TimeLocal=1].
Example line(s):
HamiltonianEigenvalues:
-90.49875621,110.49875621
- **HamiltonianEigenvectors** $\langle |\tilde{\epsilon}_i\rangle \rangle$
Acceptable Values: $N \times N$ real values
Default Value: None
Description: Orthonormal eigenvectors of system Hamiltonian H_S [required for TimeLocal=1].
Example line(s):
HamiltonianEigenvectors:
-0.74145253,0.67100532
0.67100532,0.74145253

2.3 System-environment coupling parameters

The system-environment coupling is based on the Drude spectral density

$$J_a(\omega) = 2\lambda_a\gamma_a\omega/(\omega^2 + \gamma_a^2). \quad (24)$$

Diagonal (independent) coupling, i.e. $F_a = |a\rangle\langle a|$ and $M = N$, is assumed unless `DiagonalCouplingIndices` or `CorrelatedCouplingTerms` are specified.

- `NumCouplingTerms` $\langle M \rangle$
Acceptable Values: positive integers
Default Value: 0
Description: Specifies the number of system-bath coupling terms.
Example line(s):
`NumCouplingTerms=2`

- `lambda` $\langle \lambda_a \rangle$
Acceptable Values: M real values
Default Value: None
Description: Specifies the reorganization energy λ_a associated with each coupling term F_a . Units are cm^{-1}
Example line(s):
`lambda:`
`100.,50.0`

- `gamma` $\langle \gamma_a \rangle$
Acceptable Values: M real values
Default Value: None
Description: Specifies the response frequency γ_a associated with each coupling term F_a . Units are ps^{-1}
Example line(s):
`gamma:`
`10,10`

- `DiagonalCouplingIndices` $\langle i_a \rangle$
Acceptable Values: M non-negative integers
Default Value: None
Description: Specifies the state $|i_a\rangle$ to which the term F_a couples. Note: state numbering starts from 0.
Example line(s):

```
#For NumStates=2 and NumCouplingTerms=4
DiagonalCouplingIndices:
0,0,1,1
```

- **CorrelatedCouplingTerms** $\langle f_{ai} \rangle$
Acceptable Values: $M \times N$ real values
Default Value: None
Description: Specifies each system-environment coupling $F_a = \sum_i f_{ai}|i\rangle\langle i|$.
Example line(s):

```
#For NumStates=2 and NumCouplingTerms=3
CorrelatedCouplingTerms:
1,0
0,1
0.7071,-0.7071
```

2.4 Environment parameters

- **Temperature** $\langle T \rangle$
Acceptable Values: positive real value
Default Value: 300 Kelvin
Description: Specifies the temperature of the environment. Units are in Kelvin.
Example line(s):

```
Temperature=300
```
- **MatsubaraTerms** $\langle K \rangle$
Acceptable Values: non-negative integers
Default Value: 0
Description: Specifies the number of terms to include for the Matsubara expansion.
Example line(s):

```
MatsubaraTerms=4
```

2.5 Hierarchy parameters

- **HierarchyTruncation** $\langle L_T \rangle$
Acceptable Values: integer > 1
Default Value: 0
Description: Specifies the level L_T to truncate the hierarchy.

Example line(s):
HierarchyTruncation=5

- TimeLocal < use time local truncation? >
Acceptable Values: 0 or 1
Default Value: 1
Description: Specifies whether to use time local 1 or time non-local 0 truncation.
Example line(s):
TimeLocal=1

2.6 Integration parameters

- Timestep < dt >
Acceptable Values: positive real values
Default Value: 0.001
Description: Specifies the RK4 integration timestep in ps (also used as initial RKF45 timestep).
Example line(s):
Timestep=0.001

- Time < t >
Acceptable Values: positive real values
Default Value: 0
Description: Specifies time in ps to integrate HEOM to.
Example line(s):
Time=1.0

- RKF45mindt < dt_{min} >
Acceptable Values: positive real values
Default Value: 1e-6
Description: Specifies minimum timestep in ps to use in adaptive RKF45 integration.
Example line(s):
RKF45mindt=1e-5

- RKF45tolerance < δ_I >
Acceptable Values: positive real values
Default Value: 1e-6

Description: Specifies integration tolerance for adaptive RKF45 integration.

Example line(s):

```
RKF45tolerance=1e-4
```

- **FilterTolerance** $< \delta_F >$

Acceptable Values: positive real values

Default Value: 1e-6

Description: Specifies filter tolerance for adaptive hierarchy truncation.

Example line(s):

```
FilterTolerance=1e-3
```

3 Running Phi

PHI usage is printed when running

```
$ ./phi
```

3.1 Usage

```
phi paramfile {integrator [threads],print}
  integrator - One of rk4, rkf45, rk4spectrum, rkf45spectrum, steadystate.
  threads    - Number of threads
  memory     - Prints memory requirements
  print      - Prints hierarchy connections
```

The parameter file "paramfile" specifies all system and integration parameters: Hamiltonian, hierarchy truncations, adaptive integration tolerances, integration length, integration step size

3.2 Examples

To print the memory requirements associated with input system.prm

```
$ phi system.prm memory
```

To integrate input system.prm using 4 threads with Runge-Kutta 4:

```
$ phi system.prm rk4 4
```

To calculate the steady state of system.prm using 4 threads:

```
$ phi system.prm steadystate 4
```

An example input for a two-level system can be found in `phi-source/examples/TwoLevelSystem`

4 Compiling Phi

Download the PHI source code from www.ks.uiuc.edu/Research/phi. Then:

1. Unzip and untar.
2. Edit `make.config` in the source root directory to
 - provide paths to CBLAS libraries and headers
 - specify computer architecture (linux, mac, solaris)
 - choose compiler (gcc, icc, sun CC)
3. `./make install` to install the phi binary to `./bin/`