ACE Documentation

Moritz Cygorek

1 Introduction

This document is intended to describe how to use the C++ code ACE for the solution of open quantum systems using the *automated compression of environments* (ACE) method. The article explaining the method can be found here.

Generally, ACE provides numerically exact simulation of the dynamics of an open quantum systems described by the microscopic Hamiltonian

$$H = H_S + H_E = H_S + \sum_{k=1}^{N_E} H_E^k, \tag{1}$$

where H_S is the system Hamiltonian and the environment Hamiltonian H_E, which also includes the system-environment coupling, is assumed to be separable into N_E independent modes k. Throughout this document we will denote the dimension of the system Hilbert space by N while the dimension of the k-th environment mode is M^k (or simply M if all M^k are identical).

The goal is to obtain the reduced system density matrix discretized on a time grid $t_l = t_a + l\Delta t$ up to a given final time $t_n = t_a + n\Delta t = t_e$. This can be done using the path integral expression

$$\rho_{\alpha_n} = \sum_{\substack{\alpha_{n-1}\dots\alpha_0 \\ \tilde{\alpha}_n\dots\tilde{\alpha}_1}} \mathcal{I}^{(\alpha_n\tilde{\alpha}_n)\dots(\alpha_1\tilde{\alpha}_1)} \bigg(\prod_{l=1}^{n} \mathcal{M}^{\tilde{\alpha}_l\alpha_{l-1}}\bigg)\rho_{\alpha_0}, \tag{2}$$

where $\rho_{\alpha_l} = \rho_{\nu_l\mu_l}$ is the reduced system density matrix at time step l, $\mathcal{M}$ describes the free time evolution of the system, and $\mathcal{I}$ is the *process tensor* (PT) accounting for the effects of the environment. To keep the notation compact, we combine two Hilbert space indices on the system density matrix ν_l and μ_l into a single Liouville space index $\alpha_l = (\nu_l, \mu_l)$. The GIF can always expressed in the form of a matrix product operator (MPO)

$$\mathcal{I}^{(\alpha_n,\tilde{\alpha}_n)(\alpha_{n-1},\tilde{\alpha}_{n-1})\dots(\alpha_1,\tilde{\alpha}_1)} = \sum_{d_{n-1}\dots d_1} \mathcal{Q}^{(\alpha_n,\tilde{\alpha}_n)}_{1d_{n-1}} \mathcal{Q}^{(\alpha_{n-1},\tilde{\alpha}_{n-1})}_{d_{n-1}d_{n-2}} \dots \mathcal{Q}^{(\alpha_1,\tilde{\alpha}_1)}_{d_1 1}. \tag{3}$$

In the explicit derivation of the matrices $\mathcal{Q}$, the inner indices d_l correspond to a complete basis of the Liouville space of the full environment, which can be extremely large. However, the inner dimensions of MPOs can be systemaically reduced using established compression techniques. Here, we use a compression method based on singular value decomposition (SVD), where singular values below a predefined threshold ϵ are disregarded. The time discretization Δt and the compression threshold ϵ are the main convergence parameters of ACE.

The working principle of ACE is to construct the PT in compressed MPO form by calculating the PTs for the individual environment modes k and then combining them one by one. After each combination step, the GIF MPO is compressed using SVDs to reduce the inner dimensions to a manageable size at all times. Once the compressed PT is calculated, the reduced system density matrix for a given system Hamiltonian and system initial state can be obtained by contracting a simple tensor network.

2 Code, Compilation, Dependencies, and Design Choices

The code has been written in C++ to combine low-level optimization (memory storage, access to LAPACK routines) with high-level abstraction for better usability. Although nothing in the code depends explicitly on the operating system, the code has been tested only on Linux.

We have tried to keep the dependencies on other codes minimal. However, the Eigen library is very handy and provides useful and efficient routines, e.g., for matrix exponentials. We use it in particular to specify Hamiltonians and density matrices. The numerically most demanding part of ACE is the calculation of SVDs. Here, we make use of the corresponding LAPACK routines. In my experience, the Intel MKL implementation of the SVD LAPACK routines can be significantly faster than other implementations, sometimes by orders of magnitudes. Therefore, we assume that Eigen as well as the Intel MKL is installed on the computer.

The installation of ACE via Makefiles needs to be able to find these libraries. To this end, the corresponding Linux environment variables have to be set. A successful installation of MKL should automatically set the `MKLROOT` environment variable to the correct directory. We assume that the Eigen library is installed in the directory `/usr/include/eigen3/`. If not, please set the variable `EIGEN_HOME` manually in such a way that the file `$EIGEN_HOME/Eigen/Eigen` exists.

To compile the code, go into the main directory of ACE and type in the console

```
> make
```

This should compile the code and copy the binaries into the `bin/` subdirectory. For easy access later on, we suggest to add this directory to your Linux environment via the `PATH` variable. For example, add the follwing line to your `~/.bashrc` file

```
PATH=/.../ACE/bin/:$PATH
```

where the ... are to be replaced to point to the correct absolute directory. Log out and log in again to activate the changes. Then, go to a temporary directory and run

```
> ACE
```

This should generate a file `ACE.out` whose first lines are

```
0 0 0 1 0 0 0 inf inf
0.01 0 0 1 0 0 0 1 0
```

```
0.02 0 0 1 0 0 0 1 0
0.03 0 0 1 0 0 0 1 0
0.04 0 0 1 0 0 0 1 0
...
```

Congratulations! You have just executed your first (rather boring) simulation using ACE.

3 System dynamics

ACE can be controlled by command line parameters. Alternatively, the command line parameters can be written into a driver file and the driver file can be specified via the `-driver` command line option. The ACE method can deal with arbitrary system-environment couplings, but it is difficult to provide hard-coded support for the specification of arbitrary time-dependent and mode-dependent Hamiltonians. So far, only a few specific environments are implemented. For others, there is no way around adding more C++-code. However, time-independent system Hamiltonians or Lindblad operators as well as a few predefine time-dependent Hamiltonians (e.g., Gaussian pulses) can be specified by command line options using a bra-ket notation.

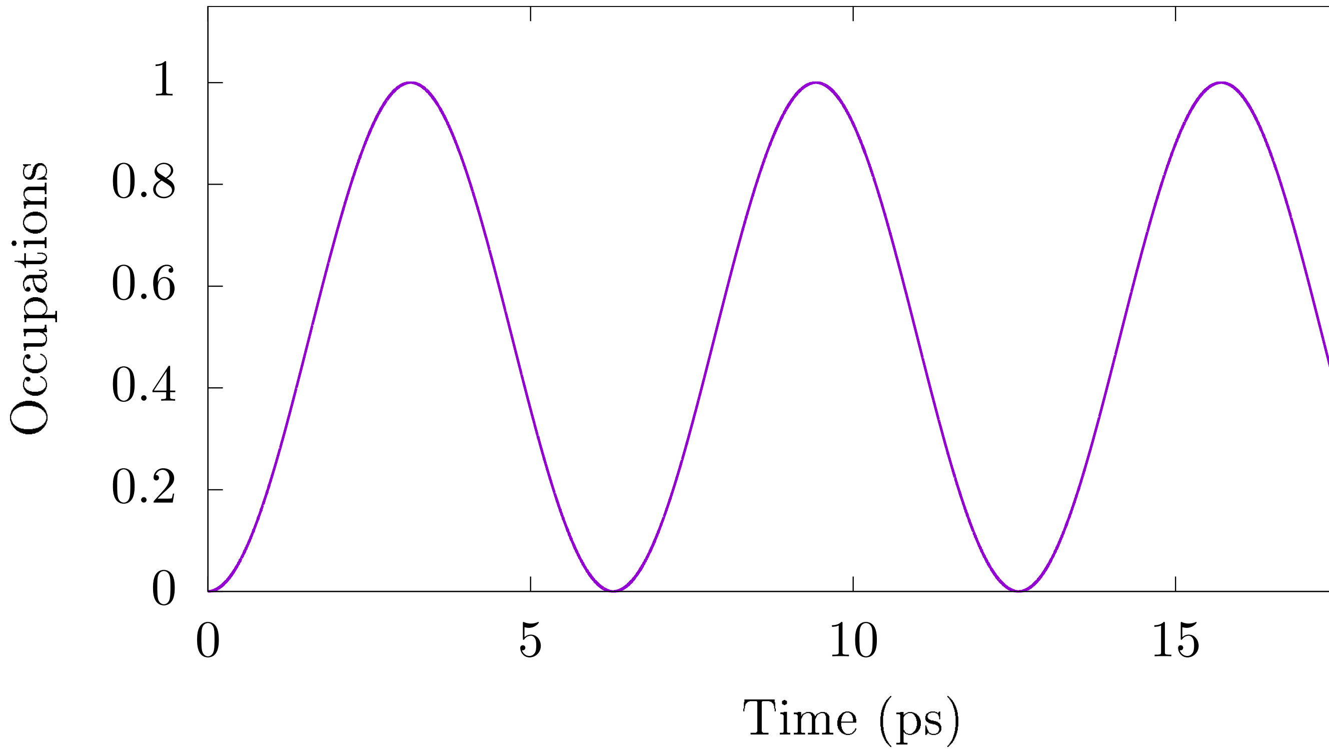
First, let us discuss some of the most important parameters: The starting time, the final time, and the time step width can be specified by the command line options `-ta`, `-te`, and `-dt`, respectively, which have the default values 0, 10, and 0.01 (times are assumed to be measured in picoseconds if not otherwise specified). You will find the corresponding time grid in the first column of output file `ACE.out`, whose name may be changed via the option `-outfile`. By default, there will be no environment, the system is a two-level system (TLS) initially in its ground state, and the system Hamiltonian is $H_S = 0$. For TLSs, if not specified otherwise, the second and third columns in the output file will be the real and imaginary part of the diagonal element of the system density matrix corresponding to the exited state. If no parameters are specified explicitly, these columns should remain 0.

As a first example, run

```
> ACE -dt 0.001 -te 20 -add_Hamiltonian "{hbar/2*(|1><0|_2+|0><1|_2)}" -outfile ACE1.out
```

This will generate an output file `ACE1.out`, which contains the dynamics of a constantly driven TLS from 0 to 20 ps with time steps of 0.001 ps. The driving is described by the Hamiltonian $H_S = (\hbar/2)(|X\rangle\langle G| + |G\rangle\langle X|)$ (note: hbar is given in units of meV/ps). Here, the bra-ket notation for Hamiltonians has the form `|i><j|_d`, where d is the dimension of the Hilbert space. The curly braces are used to indicate the beginning and end of matrix-valued expressions. On the command line, quotes are required to avoid the removal of curly braces by the `bash` shell.

Plotting the second column of `ACE1.out` (in gnuplot: `plot "ACE1.out" using 1:2 with lines`) reveals clear Rabi oscillations of the excited state occupations:



The same result can be obtained creating and editing the file `driver1.param`:

```
dt                    0.001
te                   20

add_Hamiltonian       {hbar/2*(|1><0|_2+|0><1|_2)}


outfile               ACE1.out
```

and running

```
> ACE -driver driver1.param
```

or simply

```
> ACE driver1.param
```

I.e., the first parameter is interpreted as a driver file.

A more complicated scenario can be described by the following driver file (`driver2.param`), where an initially excited TLS, optionally subject to radiative decay described by a Lindblad term, is driven by a Gaussian laser pulse:

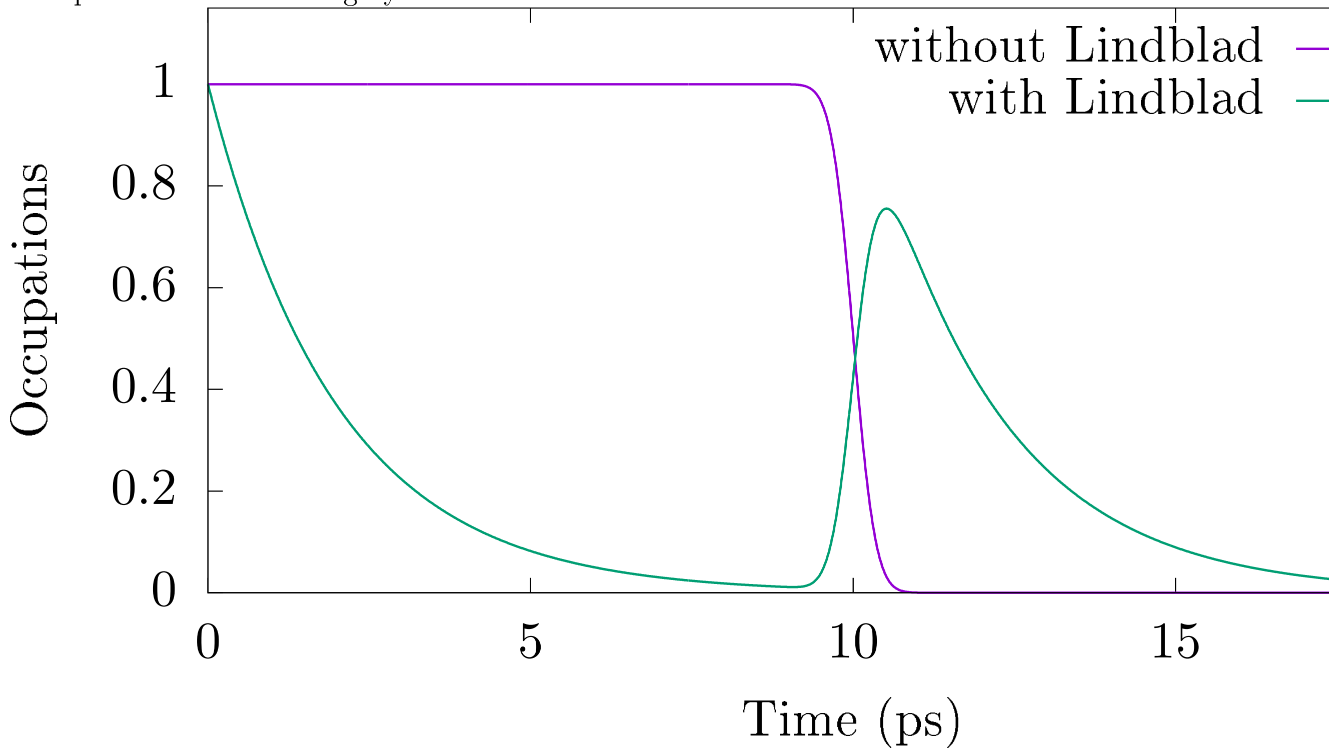
```
dt                    0.01
te                   20

initial              {|1><1|_2}

#add_Lindblad          0.5  {|0><1|_2}
add_Pulse             Gauss  10 1 1 0  {(|1><0|_2+|0><1|_2)}

outfile               ACE2.out
```

This produces the following dynamics:



where the two curves are results of calculation where the Lindblad term is either turned off or on. The # symbol in a driver file indicates a comment, i.e. anything after it is ignored. The parameters of `add_Lindblad` are the rate γ and the operator A for the Lindblad term

$$\gamma\mathcal{L}[A](\rho) = \gamma\Big[A\rho A^\dagger - \tfrac{1}{2}\big(A^\dagger A\rho + \rho A^\dagger A\big)\Big]. \tag{4}$$

The parameters of `add_Pulse Gauss` are the pulse center (here: 10 ps), the pulse duration ($\tau_{FWHM} = 1$ ps), the pulse area (1π), the detuning (0 meV), and the operator describing the light-matter coupling.

Finally, we mention that one can also explicitly specify which operator average are to be printed into the output file by the parameter `add_Output`, which takes as an argument an expression (in curly braces) describing the respective operator. When it is first specified, the default output operators are overridden and replaced by the specified operator average. Specifying `add_Output` multiple times adds more columns to the output file.

4 Environments

In the following subsections, the usage of some of the predefined environments is demonstrated. The driver files for the examples presented in the published article are contained in the first 4 subdirectories in the `examples` directory provided with the code.

4.1 Fermionic environment

One of the predefined environments is defined by the hopping Hamiltonian

$$H_E^k = \hbar g\big(c_k^\dagger c_S + c_S^\dagger c_k\big) + \hbar\omega_k c_k^\dagger c_k \tag{5}$$

Here, the system is meant to be a Fermionic state that may be occupied or not. The occupation is created by $c_S^\dagger$ or destroyed by c_S. Similarly, the environment consists of several Fermionic states, whose occupations are created and destroyed by $c_k^\dagger$ and c_k, respectively. In the limit $N_E \to \infty$, the environment consists of a continuum of state, which can be used to model the electronic states in metallic leads in proximity to a quantum dot. Consider the driver file:

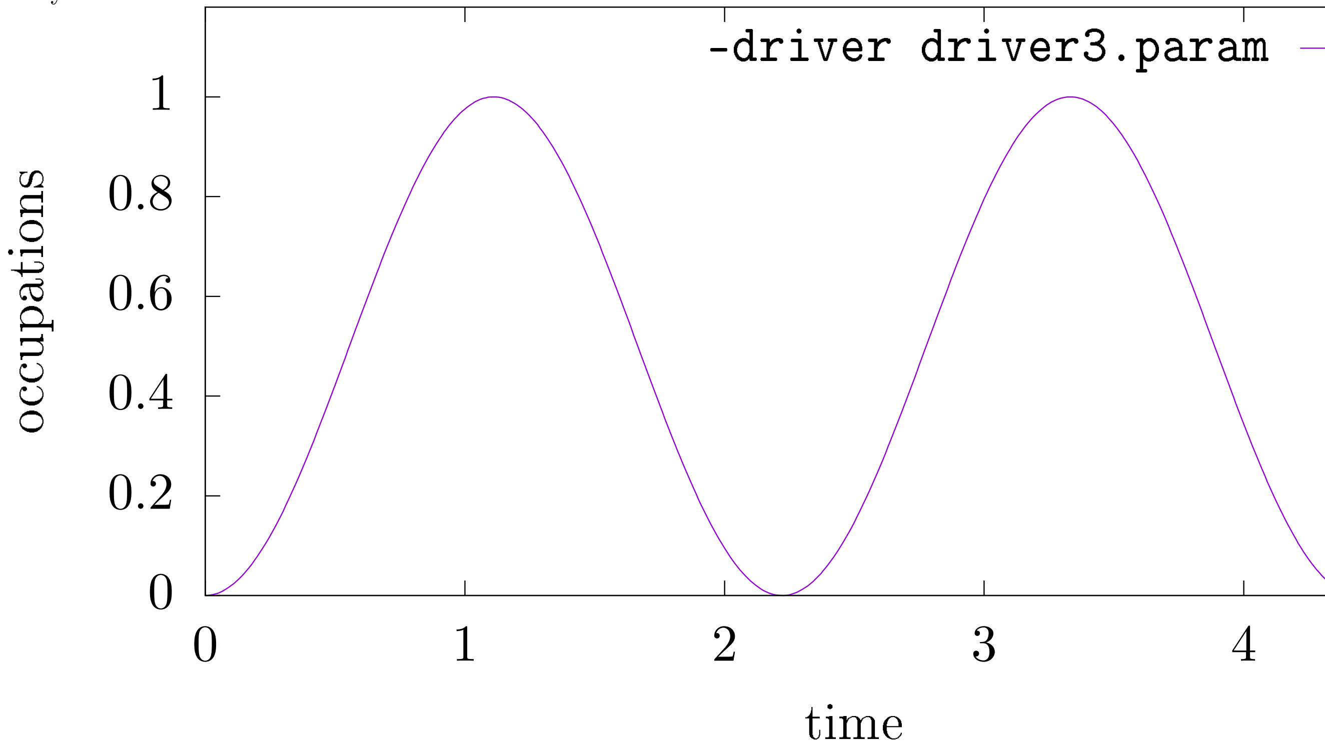
```
te                  5
dt                  1e-2
threshold           1e-7

Leads_N_modes       2
Leads_g             1
Leads_omega_min     0
Leads_omega_max     0
Leads_EFermi        1e4

outfile             ACE3.out
```

Whenever we add an environment, we should specify a compression `threshold` (denoted ϵ in the paper). The smaller the threshold, the more accurate the simulation. However, for very smaller thresholds also the calculation times as well as the memory demands increase.

`Leads_*` indicates that what comes after is a parameter for the leads-type environment specified by the above Hamiltonian. `Leads_N_modes` tells the code to use 2 Fermionic states as environment. The coupling strength is determined by `Leads_g` and the energies are equidistantly sampled from `Leads_omega_min` to `Leads_omega_max` (in picoseconds; there also exist `Leads_E_min` and `Leads_E_max` if we want to specify the band width in units of meV). Here, both limits are set to zero, so that both environment modes are resonant to the TLS transition. By setting `Leads_EFermi 1e4` (note that 1e4 is the C++ notation for 1×10^4) the Fermi level is set to such a high value that all environment states are initially occupied. There is also the parameter `Leads_temperature` to specify the temperature (in units of Kelvin) of the Fermi distribution. If not specified, the global `temperature` parameter will be used, whose default is 4 K. The initial state of the system is empty. Therefore, electrons will start to move from the leads to the system. The dynamics is show below and it is discussed further in the article.



Typically, the environments of open quantum system are assumed to form a continuum. In ACE, we simply discretize the continuum. For the case of metallic leads, it turns out that using $N_E = 10$ modes is already not too bad. Consider the driver file `driver4.param`:

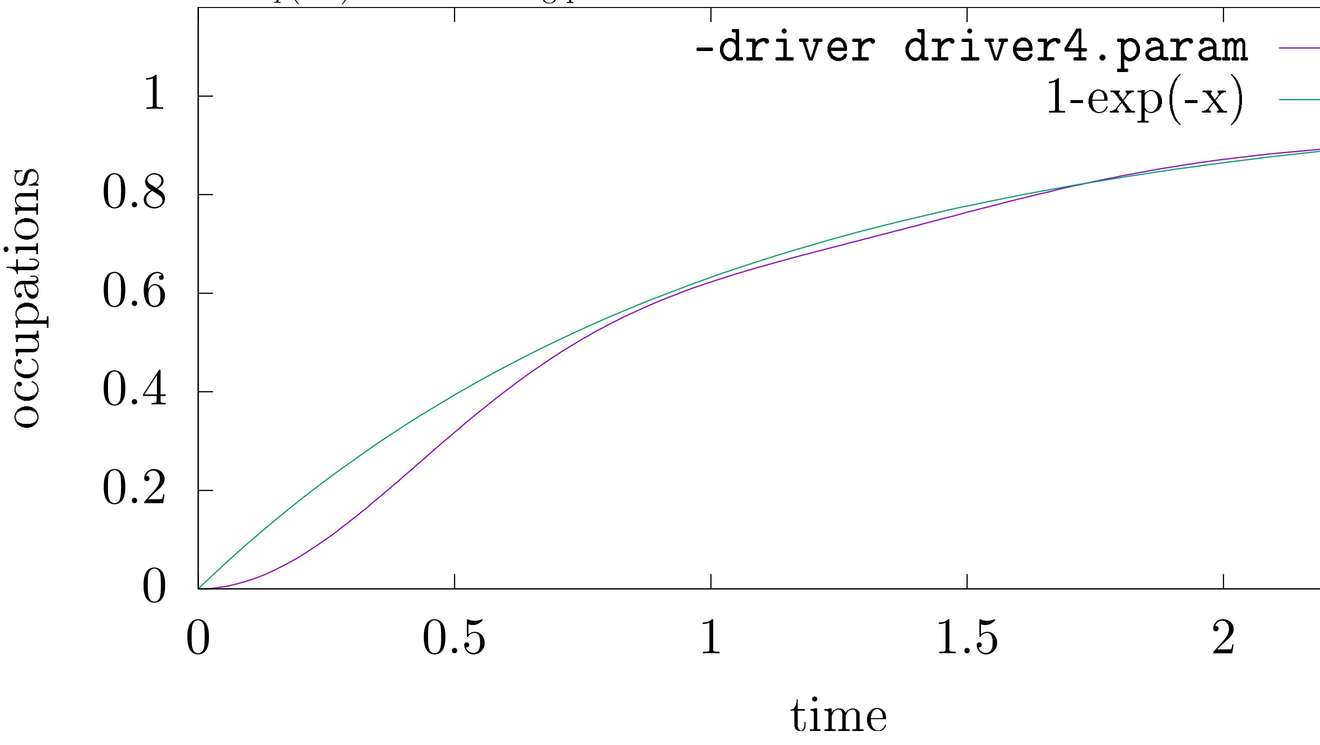
```
te                    2.5
dt                    1e-2
threshold             1e-7

Leads_N_modes        10
Leads_rate            1
Leads_omega_min      -5
Leads_omega_max       5
```

```
Leads_EFermi        1e4

outfile             ACE4.out
```

Here, instead of `Leads_g`, we use `Leads_rate` to specify the rate that we would expect in the Markov limit. Then, the coupling constant is calculated internally by solving the Fermi's golden rule expression for g. The respective dynamics is compared with the Markovian result $1 - \exp(-x)$ in the following plot:



Increasing N_E even further to about 100 while keeping the same density of states (i.e. increasing the band width simultaneously) will produce a behaviour very close to the Markovian results.

4.2 Radiative decay

The coupling of a quantum emitter to the electromagnetic field modes of free space gives rise to radative decay and can be described by the Hamiltonian

$$H = \sum_{\mathbf{k}} \left[\hbar\omega_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \hbar g_{\mathbf{k}} \big(a^\dagger_{\mathbf{k}} |G\rangle\langle X| + a_{\mathbf{k}} |X\rangle\langle G| \big) \right], \tag{6}$$

where $a^\dagger_{\mathbf{k}}$ and $a_{\mathbf{k}}$ are Bosonic creation and annihilation operators. In practice, $\mathbf{k}$ is a three-dimensional vector and the photon bands $\mathbf{k}$ may be modified by structuring the photon environment, e.g. by embedding the emitter in a microcavity.

Here, we assume isotropy (i.e., we work exclusively with the modulus $k = |\mathbf{k}|$) and a flat spectral density of state (as a function of the modulus $|\mathbf{k}|$), and discretize the light field continuum equidistantly. The only difference between this situation and the coupling to Fermionic leads is that the mode operators are Bosonic, i.e., they can in principle contain an arbitarily large number of excitations and the initial state is given by a Bose distribution instead of a Fermi distribution. Therefore, we use the same set of parameters, just replacing `Leads_*` by `RadiativeDecay_*`. Additionally, we use the parameter `RadiativeDecay_M` to specify the cut-off in the number of excitations (dimension of the respective Hilbert space, i.e., 1+maximal number of photons per mode; default value: 2).

4.3 Phonons/spin-boson model/independent-boson model

A TLS diagonally coupled to a continuum of independent bosons is known as the independent-boson model or spin-boson model. It also describes the coupling between a quantum dot (QD) and longitudinal acoustic phonons. In this example, we take the latter as our use case. The corresponding Hamiltonian is

$$H_E = \sum_{\mathbf{q}} \Big[\hbar\omega_{\mathbf{q}} b^\dagger_{\mathbf{q}} b_{\mathbf{q}} + \hbar\gamma_{\mathbf{q}}\big(b^\dagger_{\mathbf{q}} + b_{\mathbf{q}}\big)|X\rangle\langle X|\Big], \tag{7}$$

where $b^\dagger_{\mathbf{q}}$ and $b_{\mathbf{q}}$ are creation and annihilation operators for phonons with wave vector $\mathbf{q}$. It can be shown that the effects of such an environment are fully characterized by the spectral density

$$J(\omega) = \sum_{\mathbf{q}} \gamma^2_{\mathbf{q}} \delta(\omega - \omega_{\mathbf{q}}) \tag{8}$$

Solving the original Hamiltonian is very difficult when the number of phonon modes is large. Thus, we instead solve a replacement Hamiltonian by discretizing the respective spectral density $J(\omega)$. Internally, we can specify arbitrary spectral densities. However, so far only the spectral density for phonons (described in the article) is accessible via command line options. A working driver file may be:

```
QDPhonon_temperature           4         # default: 4

QDPhonon_subtract_polaron_shift  true    # default: true
QDPhonon_N_modes     100
QDPhonon_M_max         3                 # default: 4
QDPhonon_E_max         5                 # default: 4
```

Here, `QDPhonon_N_modes` is the number of modes, i.e. the number of sample points for the discretization. `QDPhonon_E_max` is the cut-off energy determining the maximal value of ω for the discretization of $J(\omega)$. `QDPhonon_M_max` is the dimension of the Hilbert space for a single phonon mode (1+maximal number of phonons per mode). The temperature for the initial state of the bath is given by `QDPhonon_temperature` (if not specified, `temperature` is checked). By setting `QDPhonon_subtract_polaron_shift` to `true` (which is the default behaviour) the polaron shift $-\sum_{\mathbf{q}}(\gamma_{\mathbf{q}}^2)/(\omega_{\mathbf{q}})$ is subtracted from (i.e. the modulus is added to) the Hamiltonian. This is done to eliminate the effects of the polaron shift when comparing calculations with and without phonons, which would otherwise affect resonance conditions.

As an alternative to ACE, the process tensor for Gaussian baths can be calculated using expressions where the bath is already integrated out [cf. Jørgensen and Pollock Phys. Rev. Lett. 123, 240602 (2019)]. This method is usually much more efficient and does not require discretization or truncation of the phonon Hilbert spaces (Recall: The advantage of ACE is its generality, while the latter method only works for Gaussian baths.) To use this method instead for phonon simulations with our standard phonon spectral density, the following can be added to the driver file:

```
use_process_tensor      true
temperature             4
```

5 Concluding remarks

Further developments of ACE as well as the code are ongoing projects. The documentation naturally lags behind.