August 16, 2024

Contents

0.1 Bloch-Redfield and Redfield Failing for degenerate Hamiltonians

In The SYK model:

In this section we consider the SYK model whose Hamiltonian is given by (Ryu paper, introduction)

$$H = \sum_{i<j<k<l=1}^{N} J_{i,j,k,l}\psi_i\psi_j\psi_k\psi_l \tag{1}$$

Where $J_{i,j,k,l}$ is drawn randomly from a Gaussian ensemble with mean $\mu = 0$ and variance $\sigma = \sqrt{3!}\frac{J}{N^{3/2}}$ where J is a constant with dimension of mass. And the ψ_i denote the operators of the majorana fermions which are representations of the clifford algebra. They satisfy

$$\{\psi_i, \psi_j\} = \delta_{i,j} \tag{2}$$

For convenience people usually just consider the even case and one dimensional majorana fermions (appendix A). We introduce the new basis

$$c_i = \frac{1}{\sqrt{2}}(\psi_{2i} - i\psi_{2i+1}) \tag{3}$$

$$c_i^\dagger = \frac{1}{\sqrt{2}}(\psi_{2i} + i\psi_{2i+1}) \tag{4}$$

These satisfy

$$\{C_i, C_j^\dagger\} = \delta_{i,j} \tag{5}$$

$$\{C_i^\dagger, C_j^\dagger\} = 0 \tag{6}$$

To construct this basis we consider picking a vacuum annhilated by all modes such that

$$(C_1^\dagger)^{n_1} \dots (C_k^\dagger)^{n_k} 0 \dots 0 = 0 \tag{7}$$

There are $2^{N/2} = 2^K$ such states. This is the only irreducible representation of (2) , upn top unitary equailvalence, the representation is given by 2^k matriceswhich can be found by the recursion relaton

$$\psi_i^K = \psi_i^{k-1} \otimes \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{for} \quad i = 1, 2, \dots, N-2 \tag{8}$$

$$\psi_{N-1}^K = \frac{1}{\sqrt{2}} 1_{2^{K-1}} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{9}$$

$$\psi_N^K = \frac{1}{\sqrt{2}} 1_{2^{K-1}} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{10}$$

The superscript K is omitted in the Hamiltonian for convenience. Though not a great example, Let us use $N = 2$. To illustrate how solving by Bloch-Redfield may fail

```
import matplotlib.pyplot as plt
import numpy as np
from qutip import ( basis, expect, mesolve, qeye, sigmax, sigmay, sigmaz,destroy,
                   tensor,fidelity,tracedist,brmesolve,Qobj)
from qutip.solver import heom
from scipy.integrate import quad
from pseudomode import pseudomode,zero_temp_bath,rotation
from hamiltonians import syk_full,plot_ground,plot_fidelities,plot_trd,plot_positivity,plot_po
from nmm import csolve,redfield
```

```
N=2
seeds=list(range(42,52))
k=7
H,psis=syk_full(N,seed=seeds[k])
```

The Hamiltonian in this example is then given by

```
H=20*H
H
```

```
Quantum object: dims=[[2, 2], [2, 2]], shape=(4, 4), type='oper', isherm=True
Qobj data =
[[ -2.18176916  0.          0.          0.        ]
 [ 0.          2.18176916  0.          0.        ]
 [ 0.          0.          2.18176916  0.        ]
 [ 0.          0.          0.         -2.18176916]]
```

While the coupling operator to the bath is simply
$Q = \sum_i a_i \psi_i$
Where each a_i is a real number

```
Q=sum([(1/2 +1/(2*i+2))*psis[i] for i in range(len(psis))])
Q
```

```
Quantum object: dims=[[2, 2], [2, 2]], shape=(4, 4), type='oper', isherm=True
Qobj data =
[[ 0.        +0.j          0.53033009 -0.70710678j  0.44194174 -0.47140452j
   0.        +0.j        ]
 [ 0.53033009+0.70710678j  0.        +0.j          0.        +0.j
  -0.44194174+0.47140452j]
 [ 0.44194174+0.47140452j  0.        +0.j          0.        +0.j
   0.53033009 -0.70710678j]
 [ 0.        +0.j         -0.44194174 -0.47140452j  0.53033009+0.70710678j
   0.        +0.j        ]]
```

We consider the initial state to be

```
N=2
state_list = [basis(2, 1)] + [ -1j*basis(2, 0)] * (N - 1) # change the initial state to be awa
state_list2 = [basis(2, 1)] + [basis(2, 0)] * (N - 1) # change the initial state to be away fr
state_list.reverse()
psi0 = (tensor(state_list)+tensor(state_list2))/np.sqrt(2)
rho0=psi0*psi0.dag()
H.dims=rho0.dims
Q.dims=rho0.dims
times=np.linspace(0,50,100)
tfit=np.linspace(0, 80, 1000)
rho0
```

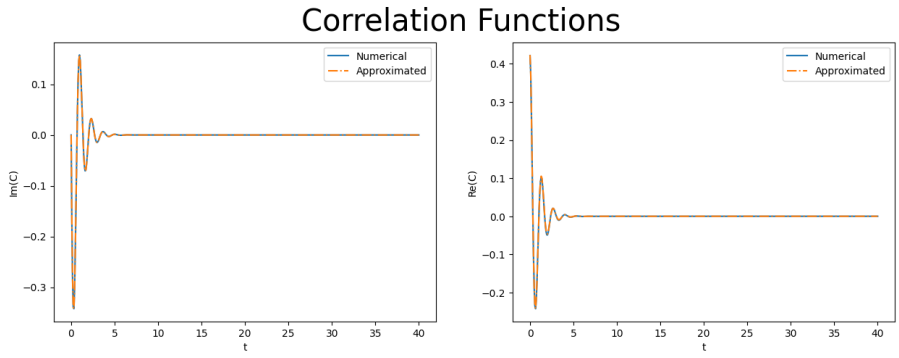
```
Quantum object: dims=[[2, 2], [2, 2]], shape=(4, 4), type='oper', isherm=True
Qobj data =
[[0. +0.j  0. +0.j  0. +0.j  0. +0.j ]
 [0. +0.j  0.5+0.j  0. -0.5j 0. +0.j ]
 [0. +0.j  0. +0.5j 0.5+0.j  0. +0.j ]
 [0. +0.j  0. +0.j  0. +0.j  0. +0.j ]]
```

```
E01=H.eigenenergies()[2] -H.eigenenergies()[0]#it is mostly degenerate, this does not help muc
w0=1.1 *E01#since I have no g parameter then It doesn't scale uniformingly as ising
gamma=w0/2.05
Gamma=gamma/2
Omega=np.sqrt(w0**2 -Gamma**2)
lam=np.sqrt(Omega)
```

And consider an underdamped spectral density at zero temperature with γ =2.3414108070880553 , λ =2.157529680721121 ,ω_0 =4.799892154530513. After fitting the correlation function one obtains

```
bath = heom.UnderDampedBath(
        Q=Q,
        lam=lam, gamma=gamma, w0=w0, T=0, Nk=5) # fix runtime warning
cfiitter2 = heom.CorrelationFitter(
    Q, 0, tfit, bath.correlation_function)
bath1, fit2info = cfiitter2.get_fit(Ni=1, Nr=2)
# notice one mode is also a pretty good approximation
print(fit2info['summary'])
```

```
/home/mcditoos/github/qutip_gsoc_app/qutip/solver/heom/bofin_baths.py:925: RuntimeWarning: inv
  * (1 / np.tanh(beta * (Om + 1.0j * Gamma) / 2)),
/home/mcditoos/github/qutip_gsoc_app/qutip/solver/heom/bofin_baths.py:927: RuntimeWarning: inv
  * (1 / np.tanh(beta * (Om - 1.0j * Gamma) / 2)),

Fit correlation class instance:

Result of fitting The Real Part Of                                          |Result of fitting The
 the Correlation Function with 2 terms:                                     | Of the Correlation F
                                                                            |
 Parameters|    a     |    b     |    c                                     | Parameters|    a
 1         | -9.49e -02 | -4.50e+00 |5.87e -10                              |    1         | -5.0
 2         | 5.18e -01 | -1.20e+00 |4.64e+00                                 |
                                                                            |A  normalized RMSE of
A  normalized RMSE of  1.74e -05 was obtained for the The Real Part Of      | Of the Correlation
 the Correlation Function                                                   |
 The current fit took  0.121521 seconds                                     | The current fit took

times2 = np.linspace(0,40,500)
cvis = bath.correlation_function(times2)

# using the variable axs for multiple Axes
fig, axs = plt.subplots(1, 2,figsize=(15,5))
axs[0].plot(times2, np.imag(cvis),label="Numerical")
axs[0].plot(times2, np.imag(bath1.correlation_function_approx(times2)), " -.",label="Approxima
axs[0].set_xlabel("t")
axs[0].set_ylabel("Im(C)")
axs[0].legend()
axs[1].plot(times2, np.real(cvis),label="Numerical")
axs[1].plot(times2, np.real(bath1.correlation_function_approx(times2)), " -.",label="Approxima
axs[1].set_xlabel("t")
axs[1].set_ylabel("Re(C)")
axs[1].legend()
fig.suptitle('Correlation Functions', fontsize=30)
plt.show()
```




```
solver = heom.HEOMSolver(H,
                         [bath1], max_depth=7, options={"atol": 1e -14})
result = solver.run(rho0, times)
```

```
10.1%. Run time:   5.34s. Est. time left: 00:00:00:47
20.2%. Run time:  11.43s. Est. time left: 00:00:00:45
30.3%. Run time:  16.77s. Est. time left: 00:00:00:38
40.4%. Run time:  22.14s. Est. time left: 00:00:00:32
50.5%. Run time:  27.47s. Est. time left: 00:00:00:26
60.6%. Run time:  32.79s. Est. time left: 00:00:00:21
70.7%. Run time:  38.16s. Est. time left: 00:00:00:15
80.8%. Run time:  43.50s. Est. time left: 00:00:00:10
90.9%. Run time:  48.83s. Est. time left: 00:00:00:04
100.0%. Run time:  53.67s. Est. time left: 00:00:00:00
Total run time:  53.67s
```

```
bath.bose=None
cum = csolve(
    Hsys=H, t=times, baths=[bath],
    Qs=[Q],
    eps=1e -6, cython=False)

result_cum = cum.evolution(rho0)

result_cum = rotation(result_cum, H, times)
```

```
bath.bose=None
```

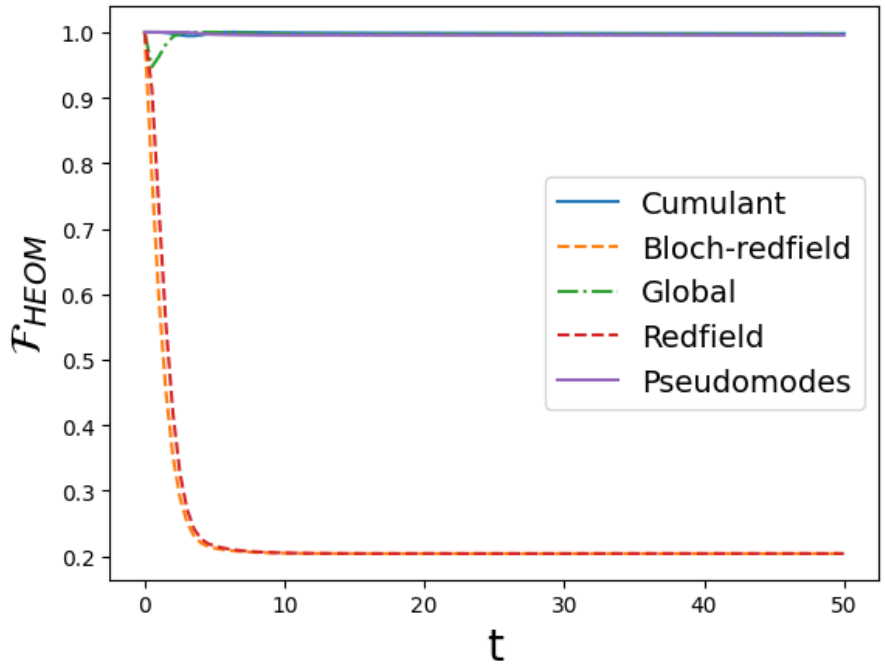
```
Calculating Integrals ...: 100%|| 4/4 [00:02<00:00,  1.96it/s]
Calculating time independent matrices...: 100%|| 4/4 [00:00<00:00, 1233.07it/s]
Calculating time dependent generators: 100%|| 4/4 [00:00<00:00, 848.71it/s]
Computing Exponential of Generators . . . .: 100%|| 100/100 [00:00<00:00, 870.67it/s]
```

```
red=redfield.redfield(Hsys=H, t=times, baths=[bath],
    Qs=[Q],
    eps=1e -12,matsubara=False)

result_red = red.evolution(rho0)
```

```
Started interpolation
```

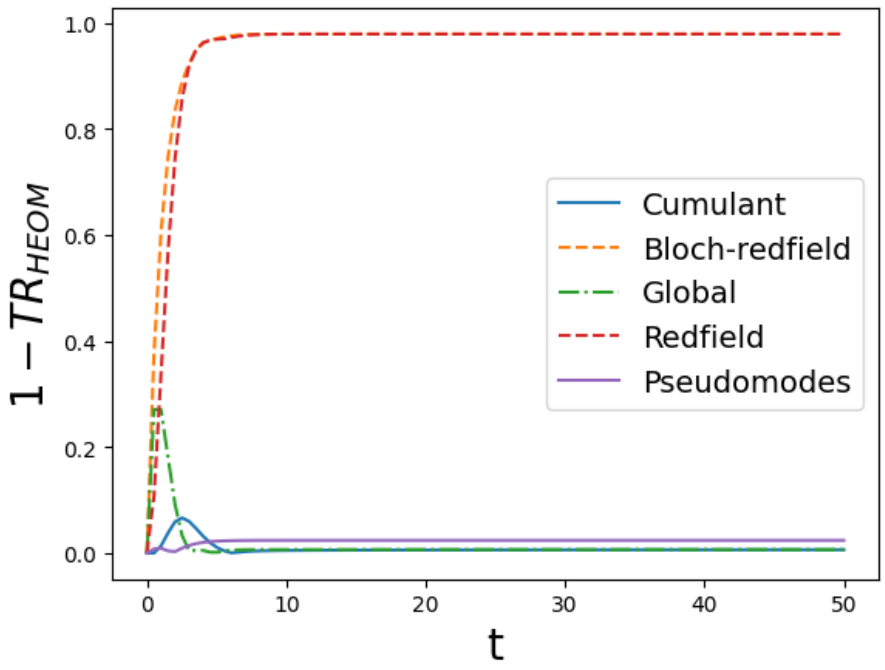
```
result_red = [Qobj(i) for i in result_red]
for i in result_red:
    i.dims=H.dims
```

```
result_red = rotation(result_red, H, times)

a_ops = [[Q, bath.power_spectrum]]
resultBR = brmesolve(H, rho0, times, a_ops=a_ops, options={
    "rtol": 1e -14}, sec_cutoff= -1)

a_ops = [[Q, bath.power_spectrum]]
resultBR2 = brmesolve(H, rho0, times, a_ops=a_ops, options={
    "rtol": 1e -14},sec_cutoff=.00000000001)

global_one=cum.jump_operators(Q) # Global Jump Operators for Bath 1 2 ->4

c_ops2=[Qobj((np.sqrt(bath.power_spectrum(k))*v).data) for k, v in global_one.items()]
for i in range(len(c_ops2)):
    c_ops2[i].dims=H.dims
result_lindblad_global2 = mesolve(H, rho0, times, c_ops2)

Ncutoff=3
modes=2
bathu = zero_temp_bath(Q, tfit, lam, gamma, w0, N=modes)
example = pseudomode(Hsys=H, Q=Q, bath=bathu)

ans = example.evolution(rho0, Ncutoff, times, options={
                        "atol": 1e -14, "normalize_output": False, "store_states": True})
ans = [i.ptrace(range(N))for i in ans.states]

results=[result,result_cum,resultBR,result_lindblad_global2,result_red,ans]

def plot_fidelities(states,H,times):
    labels=["HEOM","Cumulant","Bloch -redfield","Global","Redfield","Pseudomodes"]
    style=["solid","solid","dashed","dashdot",'dashed',"solid"]
    for k,i in enumerate(states[1:],1):
        try:
            sdd=np.array([fidelity(i.states[j],states[0].states[j]) for j in range(len(times))
        except:
            sdd=np.array([fidelity(i[j],states[0].states[j]) for j in range(len(times))])
        plt.plot(times,sdd,label=labels[k],linestyle=style[k])
    plt.legend(fontsize=14)
    plt.ylabel(r"$\mathcal{F}_{HEOM}$",fontsize=20)
    plt.xlabel(r"t",fontsize=20)
    plt.show()

plot_fidelities(results,H,times)
```




```
def trd(states,H,times):
    labels=["HEOM","Cumulant","Bloch -redfield","Global","Redfield","Pseudomodes"]
    style=["solid","solid","dashed","dashdot",'dashed',"solid"]
    for k,i in enumerate(states[1:],1):
        try:
            sdd=np.array([tracedist(i.states[j],states[0].states[j]) for j in range(len(times)
        except:
            sdd=np.array([tracedist(i[j],states[0].states[j]) for j in range(len(times))])
        plt.plot(times,sdd,label=labels[k],linestyle=style[k])
    plt.legend(fontsize=14)
    plt.ylabel(r"$1 -TR_{HEOM}$",fontsize=20)
    plt.xlabel(r"t",fontsize=20)
    plt.show()
```

```
trd(results,H,times)
```



From what we see in both the trace distance and fidelity plots, the Bloch-Redfield approach does terribly when we consider this scenario (multiple implementations where checked). Notice that this issue seems to be about the coupling operator, rather than the Hamiltonian. Consider a different coupling operator just the majorana fermion denoted by the index 0 coupled to the environment

```
Q=psis[0]
Q
```

```
Quantum object: dims=[[2, 2], [2, 2]], shape=(4, 4), type='oper', isherm=True
Qobj data =
[[0.+0.j         0. -0.70710678j 0.+0.j         0.+0.j        ]
 [0.+0.70710678j 0.+0.j         0.+0.j         0.+0.j        ]
 [0.+0.j         0.+0.j         0.+0.j         0. -0.70710678j]
 [0.+0.j         0.+0.j         0.+0.70710678j 0.+0.j        ]]
```

```
bath = heom.UnderDampedBath(
        Q=Q2,
        lam=lam, gamma=gamma, w0=w0, T=0, Nk=5) # fix runtime warning
cfiitter2 = heom.CorrelationFitter(
    Q, 0, tfit, bath.correlation_function)
bath1, fit2info = cfiitter2.get_fit(Ni=1, Nr=2)
# notice one mode is also a pretty good approximation
print(fit2info['summary'])
```

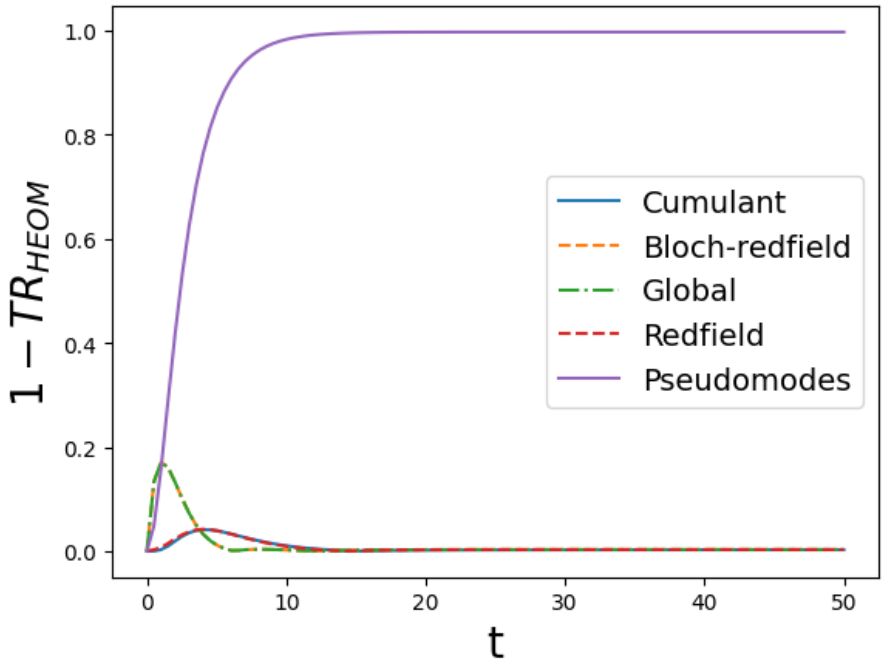
```
Fit correlation class instance:

Result of fitting The Real Part Of                                          |Result of fitting The
 the Correlation Function with 2 terms:                                     | Of the Correlation F
                                                                            |
 Parameters|    a     |    b     |    c                                     | Parameters|    a
 1         | -9.49e -02 | -4.50e+00 |5.87e -10                               |  1         | -5.0
 2         | 5.18e -01 | -1.20e+00 |4.64e+00                                 |
                                                                            |A  normalized RMSE of
A  normalized RMSE of  1.74e -05 was obtained for the The Real Part Of      | Of the Correlation
 the Correlation Function                                                   |
 The current fit took  0.100556 seconds                                     | The current fit took
```

```
solver = heom.HEOMSolver(H,
                         [bath1], max_depth=7, options={"atol": 1e -14})
result = solver.run(rho0, times)
```

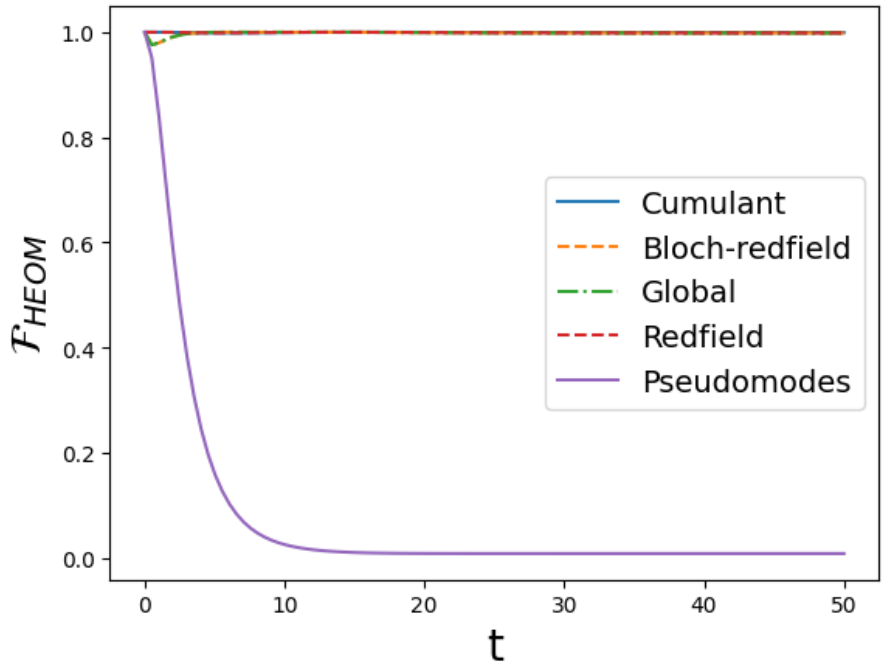
```
10.1%. Run time:   3.36s. Est. time left: 00:00:00:29
20.2%. Run time:   6.46s. Est. time left: 00:00:00:25
30.3%. Run time:   9.86s. Est. time left: 00:00:00:22
40.4%. Run time:  13.39s. Est. time left: 00:00:00:19
50.5%. Run time:  17.11s. Est. time left: 00:00:00:16
60.6%. Run time:  20.53s. Est. time left: 00:00:00:13
70.7%. Run time:  24.39s. Est. time left: 00:00:00:10
80.8%. Run time:  27.98s. Est. time left: 00:00:00:06
90.9%. Run time:  31.43s. Est. time left: 00:00:00:03
100.0%. Run time:  34.49s. Est. time left: 00:00:00:00
Total run time:  34.49s
```

```
bath.bose=None
cum = csolve(
```

```
    Hsys=H, t=times, baths=[bath],
    Qs=[Q],
    eps=1e -6, cython=False)

result_cum = cum.evolution(rho0)

result_cum = rotation(result_cum, H, times)

bath.bose=None

Calculating Integrals ...: 100%|| 4/4 [00:01<00:00,  2.39it/s]
Calculating time independent matrices...: 100%|| 4/4 [00:00<00:00, 1079.20it/s]
Calculating time dependent generators: 100%|| 4/4 [00:00<00:00, 1071.62it/s]
Computing Exponential of Generators . . . .: 100%|| 100/100 [00:00<00:00, 477.69it/s]

red=redfield.redfield(Hsys=H, t=times, baths=[bath],
    Qs=[Q],
    eps=1e -12,matsubara=False)

result_red = red.evolution(rho0)
result_red = [Qobj(i) for i in result_red]
for i in result_red:
    i.dims=H.dims
result_red = rotation(result_red, H, times)

Started interpolation

a_ops = [[Q, bath.power_spectrum]]
resultBR = brmesolve(H, rho0, times, a_ops=a_ops, options={
    "rtol": 1e -14}, sec_cutoff= -1)

a_ops = [[Q, bath.power_spectrum]]
resultBR2 = brmesolve(H, rho0, times, a_ops=a_ops, options={
    "rtol": 1e -14})

global_one=cum.jump_operators(Q) # Global Jump Operators for Bath 1 2 ->4
c_ops2=[Qobj((np.sqrt(bath.power_spectrum(k))*v).data) for k, v in global_one.items()]
for i in range(len(c_ops2)):
    c_ops2[i].dims=H.dims
result_lindblad_global2 = mesolve(H, rho0, times, c_ops2)

Ncutoff=3
modes=2
bathu = zero_temp_bath(Q2, tfit, lam, gamma, w0, N=modes)
example = pseudomode(Hsys=H, Q=Q2, bath=bathu)

Q2.dims=Q.dims

ans = example.evolution(rho0, Ncutoff, times, options={
                        "atol": 1e -14, "normalize_output": False, "store_states": True})
ans = [i.ptrace(range(N))for i in ans.states]

results=[result,result_cum,resultBR,result_lindblad_global2,result_red,ans]

trd(results,H,times)
```




```
plot_fidelities(results,H,times)
```

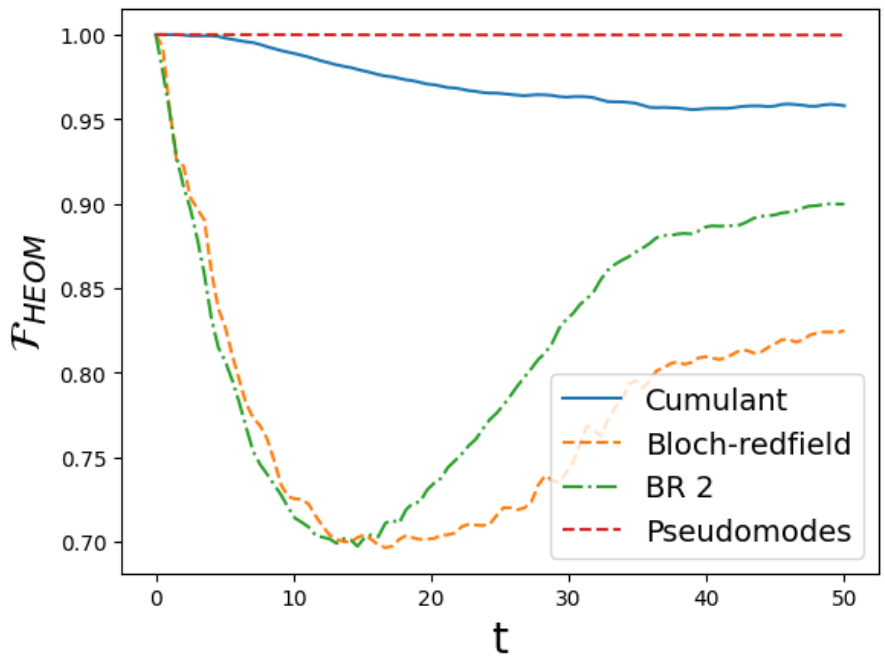



```
from qutip import qsave,qload

#qsave(results,f"N={N}_syk_{lam}_nocheating_seed_{seeds[k]}")
```

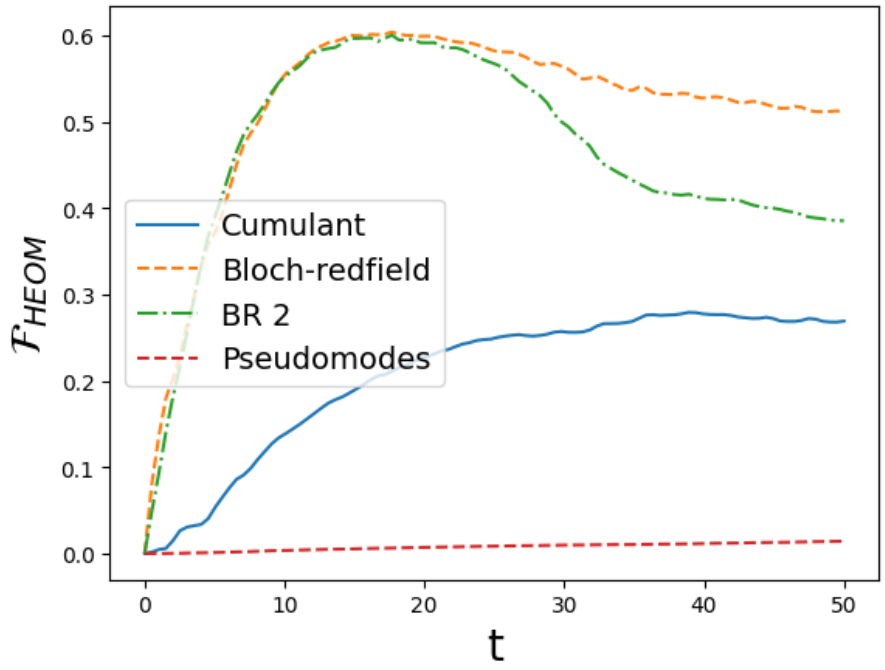
We can observe the same behaviour in the ising model when the N is large I should run this example for longer times, so that I can make sure is analogous to the previous case and not just being better in the transient regime (which would still be good) but along the lines of what was claimed in This paper. Than when the cutoff frequency is large bloch redfield does not capture time dependent redfield (I should Also add redfield here and see if the cumulant can do better)

```
example_ising= qload("results_cluster/N=6_ising_3.9585112530093003_nocheating_goodq")
```

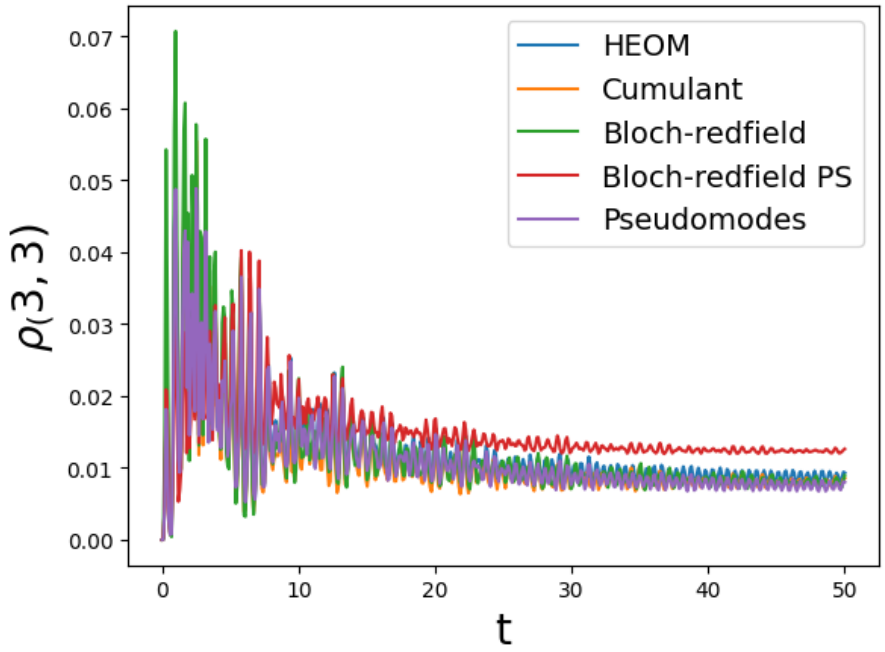
```
def plot_fidelities2(states):
    times=states[0].times
    labels=["HEOM","Cumulant","Bloch -redfield","BR 2","Pseudomodes"]
    style=["solid","solid","dashed","dashdot",'dashed',"solid"]
    for k,i in enumerate(states[1:],1):
        try:
            sdd=np.array([fidelity(i.states[j],states[0].states[j]) for j in range(len(times))
        except:
            sdd=np.array([fidelity(i[j],states[0].states[j]) for j in range(len(times))])
        plt.plot(times,sdd,label=labels[k],linestyle=style[k])
    plt.legend(fontsize=14)
    plt.ylabel(r"$\mathcal{F}_{HEOM}$",fontsize=20)
    plt.xlabel(r"t",fontsize=20)
    plt.show()

def trd2(states):
    times=states[0].times
    labels=["HEOM","Cumulant","Bloch -redfield","BR 2","Pseudomodes"]
    style=["solid","solid","dashed","dashdot",'dashed',"solid"]
    for k,i in enumerate(states[1:],1):
        try:
            sdd=np.array([tracedist(i.states[j],states[0].states[j]) for j in range(len(times)
        except:
            sdd=np.array([tracedist(i[j],states[0].states[j]) for j in range(len(times))])
        plt.plot(times,sdd,label=labels[k],linestyle=style[k])
    plt.legend(fontsize=14)
    plt.ylabel(r"$\mathcal{F}_{HEOM}$",fontsize=20)
    plt.xlabel(r"t",fontsize=20)
    plt.show()

plot_fidelities2(example_ising)
```




```
trd2(example_ising)
```




```
def plot_populations(states,l=3,m=3):
    times=states[0].times
    labels=["HEOM","Cumulant","Bloch -redfield","Bloch -redfield PS","Pseudomodes"]
    for k,i in enumerate(states):
        try:
            sdd=np.array([j[l,m] for j in i.states])
        except:
            sdd=np.array([j[l,m] for j in i])

        plt.plot(times,sdd,label=labels[k])
    plt.legend(fontsize=14)
    plt.ylabel(rf"$\rho_{l,m}$",fontsize=20)
    plt.xlabel(r"t",fontsize=20)
    plt.show()

plot_populations(example_ising)
```



0.1.1 The schwinger model

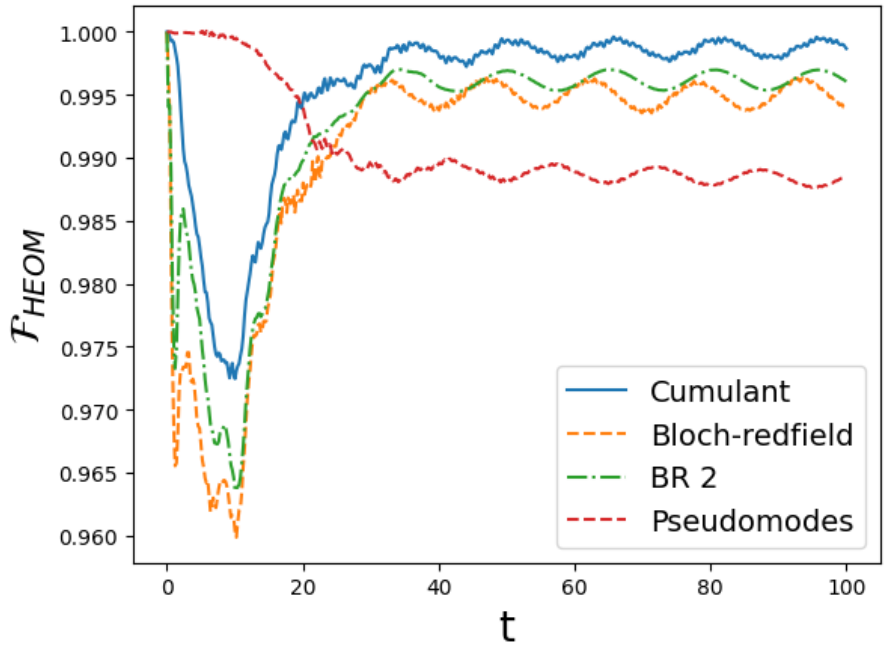
Same thing happening here, where I expected Bloch redfield to be better

But Again I should run this example to longer times to make sure is not a terribly innacurate transient effect but rather the equation breaking down. Also should add redfield to the mix

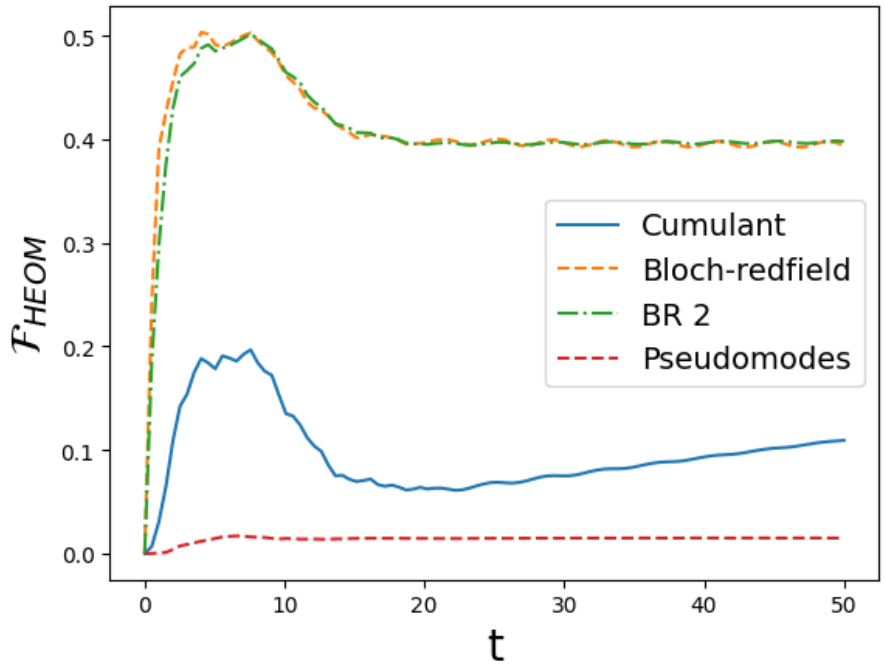
```
example_schwinger= qload("results_cluster/N=4_schwinger_1.9679896712654306_nocheating_m_0.0_th
```

```
import numpy as np
import matplotlib.pyplot as plt
from qutip import fidelity,tracedist
```

```
plot_fidelities2(example_schwinger)
```




```
trd2(example_schwinger)
```


0.5
0.4
0.3
0.2
0.1
0.0
$\mathcal{F}_{HEOM}$
0
10
20
30
40
50
t
Cumulant
Bloch-redfield
BR 2
Pseudomodes

0.2 Redfield Issue check "Analytically"

Since there seems to be an issue with the Bloch-Redfield Solver in qutip and my not so good implementation of the time dependent redfield, here's a quick sympy check to make sure it's not the solvers. By solving the equation for the SYK(2) model symbolically. The Hamiltonian is given by

$$H = \begin{bmatrix} -a & 0 & 0 & 0 \\ 0 & a & 0 & 0 \\ 0 & 0 & a & 0 \\ 0 & 0 & 0 & -a \end{bmatrix}$$

Here I define the coupling operator q that make things break for Bloch-Redfield on the SYK model

$$q = \begin{bmatrix} 0 & b_0 - ib_1 & b_2 - ib_3 & 0 \\ b_0 + ib_1 & 0 & 0 & -b_2 + ib_3 \\ b_2 + ib_3 & 0 & 0 & b_0 - ib_1 \\ 0 & -b_2 - ib_3 & b_0 + ib_1 & 0 \end{bmatrix}$$

I then get the eigenvalues and eigenvectors to obtain the jump operators (this steps are hidden in the pdf)

Jump operator checks

The jump operators must satisfy

$$[H, A(\omega)] = -\omega A(\omega) \tag{11}$$

$$[H, A^\dagger(\omega)A(\omega)] = 0 \tag{12}$$

$$\sum_w A(\omega) = A \tag{13}$$

There's a check below hidden in the pdf

Constucting the Differential equations

We now construct the differential equations from the GKLS form of the bloch Redfield generator

$$\begin{aligned} \dot{\rho_S^I}(t)t = &\sum_{\omega,\omega',\alpha,\beta} \gamma_{\beta,\alpha}(\omega,\omega') \left(S_\alpha(\omega')\rho_S^I(t)S_\beta^\dagger(\omega) - \frac{\{S_\beta^\dagger(\omega)S_\alpha(\omega'), \rho_S^I(t)\}}{2} \right) \\ &+ i \sum_{\omega,\omega',\alpha,\beta} S_{\beta,\alpha}(\omega,\omega') \Big[\rho_S^I(t), S_\beta^\dagger(\omega)S_\alpha(\omega')\Big] \end{aligned}$$

I solve in the interaction picture generally, I did the same in my numerics so it should not be an issue (I rotate in the end). By neglecting Lambshift as in the numerics

$$\dot{\rho_S^I}(t)t = \sum_{\omega,\omega',\alpha,\beta} \gamma_{\beta,\alpha}(\omega,\omega') \left(S_\alpha(\omega')\rho_S^I(t)S_\beta^\dagger(\omega) - \frac{\{S_\beta^\dagger(\omega)S_\alpha(\omega'), \rho_S^I(t)\}}{2} \right) \tag{14}$$

As the sum goes on (ω, ω') pairs I construct all combinations

```
ws = list(jumps.keys())
combinations = list(itertools.product(ws, ws))
combinations
```

```
[(2*a, 2*a), (2*a, -2*a), ( -2*a, 2*a), ( -2*a, -2*a)]
```

I get the GKLS form of each of those combinations, as a dictionary

Then I construct the generator by multiplying the appropiate coefficient to each of the GKLS from matrices. Now for the coefficients we have

$$\Gamma_{\alpha,\beta}(\omega,t)=\int_0^t ds e^{i\omega s}\langle B_\alpha^\dagger(t)B_\beta^\dagger(t-s)\rangle_B \tag{15}$$

For convenience we also define

$$\Gamma_{\alpha,\beta}(\omega,\omega',t)=e^{i(\omega'-\omega)t}\int_0^t ds e^{i\omega s}\langle B_\alpha^\dagger(t)B_\beta(t-s)\rangle_B = e^{i(\omega'-\omega)t}\Gamma_{\alpha,\beta}(\omega,t) \tag{16}$$

Since I mainly care about bloch-redfield I make $t\to\infty$ (in the integral) so

$$\Gamma_{\alpha,\beta}(\omega,\omega',t)=e^{i(\omega'-\omega)t}\int_0^\infty ds e^{i\omega s}\langle B(s)B(0)\rangle_B = e^{i(\omega'-\omega)t}\Gamma_{\alpha,\beta}(\omega) \tag{17}$$

Where $\Gamma_{\alpha,\beta}(\omega)$ is the power spectrum

$\Gamma(w)=\frac{2\gamma\lambda^2 w\left(1+\frac{1}{e^{\frac{w}{T}}-1}\right)}{\gamma^2w^2+\left(-w^2+w_0^2\right)^2}$

Next we simply vectorize the density matrix and construct the system of ODES

$\frac{d}{dt}\rho_1(t)=4ac_1\left(c_2\rho_{10}(t)\overline{c_3}+c_2\rho_6(t)\overline{c_2}+c_3\rho_{11}(t)\overline{c_3}+c_3\rho_7(t)\overline{c_2}\right)$

$\frac{d}{dt}\rho_2(t)=c_0\rho_2(t)$

$\frac{d}{dt}\rho_3(t)=c_0\rho_3(t)$

$\frac{d}{dt}\rho_4(t)=4ac_1\left(-\rho_{10}(t)\overline{c_3}^2+\rho_{11}(t)\overline{c_2c_3}-\rho_6(t)\overline{c_2c_3}+\rho_7(t)\overline{c_2}^2\right)$

$\frac{d}{dt}\rho_5(t)=ac_1\left(4c_2^2\rho_2(t)+4c_2c_3\rho_3(t)-4c_2\rho_{14}(t)\overline{c_3}-4c_3\rho_{15}(t)\overline{c_3}-2.0\left(c_2\overline{c_2}+c_3\overline{c_3}\right)\rho_5(t)e^{4iat}\right)e^{-4iat}$

$\frac{d}{dt}\rho_6(t)=2c_0\rho_6(t)$

$\frac{d}{dt}\rho_7(t)=2c_0\rho_7(t)$

$\frac{d}{dt}\rho_8(t)=ac_1\left(-4c_2\rho_2(t)\overline{c_3}+4c_2\rho_3(t)\overline{c_2}-2.0\left(c_2\overline{c_2}+c_3\overline{c_3}\right)\rho_8(t)e^{4iat}+4\rho_{14}(t)\overline{c_3}^2-4\rho_{15}(t)\overline{c_2c_3}\right)e^{-4iat}$

$\frac{d}{dt}\rho_9(t)=ac_1\left(4c_2c_3\rho_2(t)+4c_2\rho_{14}(t)\overline{c_2}+4c_3^2\rho_3(t)+4c_3\rho_{15}(t)\overline{c_2}-2.0\left(c_2\overline{c_2}+c_3\overline{c_3}\right)\rho_9(t)e^{4iat}\right)e^{-4iat}$

$\frac{d}{dt}\rho_{10}(t)=2c_0\rho_{10}(t)$

$\frac{d}{dt}\rho_{11}(t)=2c_0\rho_{11}(t)$

$\frac{d}{dt}\rho_{12}(t)=ac_1\left(-4c_3\rho_2(t)\overline{c_3}+4c_3\rho_3(t)\overline{c_2}-2.0\left(c_2\overline{c_2}+c_3\overline{c_3}\right)\rho_{12}(t)e^{4iat}-4\rho_{14}(t)\overline{c_2c_3}+4\rho_{15}(t)\overline{c_2}^2\right)e^{-4iat}$

$\frac{d}{dt}\rho_{13}(t)=4ac_1\left(c_2^2\rho_{10}(t)+c_2c_3\rho_{11}(t)-c_2c_3\rho_6(t)-c_3^2\rho_7(t)\right)$

$\frac{d}{dt}\rho_{14}(t)=c_0\rho_{14}(t)$

$\frac{d}{dt}\rho_{15}(t)=c_0\rho_{15}(t)$

$\frac{d}{dt}\rho_{16}(t)=4ac_1\left(-c_2\rho_{10}(t)\overline{c_3}+c_2\rho_{11}(t)\overline{c_2}+c_3\rho_6(t)\overline{c_3}-c_3\rho_7(t)\overline{c_2}\right)$

Let me make a few change of variables, and call the new variables c_k

$c_0=\frac{2.0a\gamma\lambda^2\left(-b_0^2-b_1^2-b_2^2-b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}$

$c_1=\frac{\gamma\lambda^2}{4a^2\gamma^2+\left(4a^2-w_0^2\right)^2}$

$c_2=b_0+ib_1$

$c_3=b_2+ib_3$

By substituting these into the differential equation we obtain

$\frac{d}{dt}\rho_1(t)=4ac_1\left(c_2\rho_{10}(t)\overline{c_3}+c_2\rho_6(t)\overline{c_2}+c_3\rho_{11}(t)\overline{c_3}+c_3\rho_7(t)\overline{c_2}\right)$

$\frac{d}{dt}\rho_2(t)=c_0\rho_2(t)$

$\frac{d}{dt}\rho_3(t)=c_0\rho_3(t)$

$\frac{d}{dt}\rho_4(t)=4ac_1\left(-\rho_{10}(t)\overline{c_3}^2+\rho_{11}(t)\overline{c_2c_3}-\rho_6(t)\overline{c_2c_3}+\rho_7(t)\overline{c_2}^2\right)$

$\frac{d}{dt}\rho_5(t)=ac_1\left(4c_2^2\rho_2(t)+4c_2c_3\rho_3(t)-4c_2\rho_{14}(t)\overline{c_3}-4c_3\rho_{15}(t)\overline{c_3}-2.0\left(c_2\overline{c_2}+c_3\overline{c_3}\right)\rho_5(t)e^{4iat}\right)e^{-4iat}$

$\frac{d}{dt}\rho_6(t)=2c_0\rho_6(t)$

$\frac{d}{dt}\rho_7(t)=2c_0\rho_7(t)$

$\frac{d}{dt}\rho_8(t)=ac_1\left(-4c_2\rho_2(t)\overline{c_3}+4c_2\rho_3(t)\overline{c_2}-2.0\left(c_2\overline{c_2}+c_3\overline{c_3}\right)\rho_8(t)e^{4iat}+4\rho_{14}(t)\overline{c_3}^2-4\rho_{15}(t)\overline{c_2c_3}\right)e^{-4iat}$

$\frac{d}{dt}\rho_9(t)=ac_1\left(4c_2c_3\rho_2(t)+4c_2\rho_{14}(t)\overline{c_2}+4c_3^2\rho_3(t)+4c_3\rho_{15}(t)\overline{c_2}-2.0\left(c_2\overline{c_2}+c_3\overline{c_3}\right)\rho_9(t)e^{4iat}\right)e^{-4iat}$

$\frac{d}{dt}\rho_{10}(t)=2c_0\rho_{10}(t)$

$\frac{d}{dt}\rho_{11}(t) = 2c_0\rho_{11}(t)$
$\frac{d}{dt}\rho_{12}(t) = ac_1\left(-4c_3\rho_2(t)\overline{c_3} + 4c_3\rho_3(t)\overline{c_2} - 2.0\left(c_2\overline{c_2} + c_3\overline{c_3}\right)\rho_{12}(t)e^{4iat} - 4\rho_{14}(t)\overline{c_2c_3} + 4\rho_{15}(t)\overline{c_2}^2\right)e^{-4iat}$
$\frac{d}{dt}\rho_{13}(t) = 4ac_1\left(c_2^2\rho_{10}(t) + c_2c_3\rho_{11}(t) - c_2c_3\rho_6(t) - c_3^2\rho_7(t)\right)$
$\frac{d}{dt}\rho_{14}(t) = c_0\rho_{14}(t)$
$\frac{d}{dt}\rho_{15}(t) = c_0\rho_{15}(t)$
$\frac{d}{dt}\rho_{16}(t) = 4ac_1\left(-c_2\rho_{10}(t)\overline{c_3} + c_2\rho_{11}(t)\overline{c_2} + c_3\rho_6(t)\overline{c_3} - c_3\rho_7(t)\overline{c_2}\right)$

With The number of symbols reduced the symbolic computation is feasible. However the default solver with initial conditions yields

$$\rho_5(t) = 1.0C_9e^{-t(2.0ac_1c_2\overline{c_2}+2.0ac_1c_3\overline{c_3})} + \left(4.0C_3ac_1c_2^2 + 4.0C_4ac_1c_2c_3 - 4.0C_7ac_1c_2\overline{c_3} - 4.0C_8ac_1c_3\overline{c_3}\right)\left(\begin{cases}\frac{8.0e^{c_0t}e^{-4.}}{16.0ac_1c_2\overline{c_2}}\\ t\end{cases}\right.$$

Unfortunately there's a bug in the sympy analytical solver when substituting the initial value conditions to obtain the constants It's not so bad because it is evidend that the weird term is zero. But I check it with manual substitutions anyway below

> **Warning**
> It's only evident if the solution of the equation is a valid density matrix

The initial state considered is

$$\rho(0) = \begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 0.5 & 0.5i & 0\\ 0 & -0.5i & 0.5 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}$$

The solution to the system of equations is
$\rho_1(t) = 1.0C_1 + 1.0C_2e^{2.0c_0t}$
$\rho_2(t) = C_3e^{c_0t}$
$\rho_3(t) = C_4e^{c_0t}$
$\rho_4(t) = 1.0C_5 + 1.0C_6e^{2.0c_0t}$
$\rho_5(t) = 1.0C_9e^{-t(2.0ac_1c_2\overline{c_2}+2.0ac_1c_3\overline{c_3})} + \left(4.0C_3ac_1c_2^2 + 4.0C_4ac_1c_2c_3 - 4.0C_7ac_1c_2\overline{c_3} - 4.0C_8ac_1c_3\overline{c_3}\right)\left(\begin{cases}\frac{8.0e^{c_0t}e^{-4.}}{16.0ac_1c_2\overline{c_2}}\\ t\end{cases}\right.$
$\rho_6(t) = \left(\frac{C_{10}c_0c_3\overline{c_3}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} - \frac{C_{11}c_0\overline{c_2c_3}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} + \frac{C_2c_0c_2\overline{c_2}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} - \frac{}{ac_1\left(\right.}\right.$
$\rho_7(t) = -\left(\frac{C_{10}c_0c_2\overline{c_3}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} + \frac{C_{11}c_0\overline{c_3}^2}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} - \frac{C_2c_0c_2\overline{c_3}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} - \frac{}{ac}\right.$
$\rho_8(t) = 1.0C_{12}e^{-t(2.0ac_1c_2\overline{c_2}+2.0ac_1c_3\overline{c_3})} - \left(4.0C_3ac_1c_2\overline{c_3} - 4.0C_4ac_1c_2\overline{c_2} - 4.0C_7ac_1\overline{c_3}^2 + 4.0C_8ac_1\overline{c_2c_3}\right)\left(\begin{cases}\frac{8.0e^{c_0t}e^{}}{16.0ac_1c_2}\\ t\end{cases}\right.$
$\rho_9(t) = 1.0C_{13}e^{-t(2.0ac_1c_2\overline{c_2}+2.0ac_1c_3\overline{c_3})} + \left(4.0C_3ac_1c_2c_3 + 4.0C_4ac_1c_3^2 + 4.0C_7ac_1c_2\overline{c_2} + 4.0C_8ac_1c_3\overline{c_2}\right)\left(\begin{cases}\frac{8.0e^{c_0t}e^{-}}{16.0ac_1c_2\overline{c}}\\ t\end{cases}\right.$
$\rho_{10}(t) = -\left(\frac{C_{10}c_0c_3\overline{c_2}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} - \frac{C_{11}c_0\overline{c_2}^2}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} - \frac{C_2c_0c_3\overline{c_2}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} + \right.$
$\rho_{11}(t) = \left(\frac{C_{10}c_0c_2\overline{c_2}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} + \frac{C_{11}c_0\overline{c_2c_3}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} + \frac{C_2c_0c_3\overline{c_3}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)} + \frac{}{ac_1}\right.$
$\rho_{12}(t) = 1.0C_{14}e^{-t(2.0ac_1c_2\overline{c_2}+2.0ac_1c_3\overline{c_3})} - \left(4.0C_3ac_1c_3\overline{c_3} - 4.0C_4ac_1c_3\overline{c_2} + 4.0C_7ac_1\overline{c_2c_3} - 4.0C_8ac_1\overline{c_2}^2\right)\left(\begin{cases}\frac{8.0e^{c_0t}}{16.0ac_1}\\ t\end{cases}\right.$
$\rho_{13}(t) = 1.0C_{11}e^{2.0c_0t} + 1.0C_{15}$
$\rho_{14}(t) = C_7e^{c_0t}$
$\rho_{15}(t) = C_8e^{c_0t}$
$\rho_{16}(t) = 1.0C_{10}e^{2.0c_0t} + 1.0C_{16}$
Then by substituting this into the solution we obtain to find the constants we obtain
$\rho_1(t) = \frac{1.0ac_1(c_2\overline{c_2} - ic_2\overline{c_3} + ic_3\overline{c_2} + c_3\overline{c_3})e^{2.0c_0t}}{c_0} - \frac{1.0ac_1(c_2\overline{c_2} - ic_2\overline{c_3} + ic_3\overline{c_2} + c_3\overline{c_3})}{c_0}$
$\rho_2(t) = 0$
$\rho_3(t) = 0$

$$\rho_4(t) = \frac{1.0iac_1\left(\overline{c_2}^2+\overline{c_3}^2\right)e^{2.0c_0t}}{c_0} - \frac{1.0iac_1\left(\overline{c_2}^2+\overline{c_3}^2\right)}{c_0}$$

$$\rho_5(t) = 0$$

$$\rho_6(t) = \frac{c_0\left(-\frac{iac_1c_2c_3\left(\overline{c_2}^2+\overline{c_3}^2\right)}{c_0}+\frac{ac_1c_2(c_2\overline{c_2}-ic_2\overline{c_3}+ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_2}}{c_0}+\frac{1.0ac_1c_3(c_2\overline{c_2}+ic_2\overline{c_3}-ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_3}}{c_0}-\frac{iac_1\left(-c_2^2-c_3^2\right)\overline{c_2c_3}}{c_0}\right)e^{2.0c_0t}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)}$$

$$\rho_7(t) = \frac{c_0\left(\frac{iac_1c_2^2\left(\overline{c_2}^2+\overline{c_3}^2\right)}{c_0}+\frac{ac_1c_2(c_2\overline{c_2}-ic_2\overline{c_3}+ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_3}}{c_0}-\frac{1.0ac_1c_2(c_2\overline{c_2}+ic_2\overline{c_3}-ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_3}}{c_0}-\frac{iac_1\left(-c_2^2-c_3^2\right)\overline{c_3}^2}{c_0}\right)e^{2.0c_0t}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)}$$

$$\rho_8(t) = 0$$

$$\rho_9(t) = 0$$

$$\rho_{10}(t) = \frac{c_0\left(-\frac{iac_1c_3^2\left(\overline{c_2}^2+\overline{c_3}^2\right)}{c_0}+\frac{ac_1c_3(c_2\overline{c_2}-ic_2\overline{c_3}+ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_2}}{c_0}-\frac{1.0ac_1c_3(c_2\overline{c_2}+ic_2\overline{c_3}-ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_2}}{c_0}+\frac{iac_1\left(-c_2^2-c_3^2\right)\overline{c_2}^2}{c_0}\right)e^{2.0c_0t}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)}$$

$$\rho_{11}(t) = \frac{c_0\left(\frac{iac_1c_2c_3\left(\overline{c_2}^2+\overline{c_3}^2\right)}{c_0}+\frac{1.0ac_1c_2(c_2\overline{c_2}+ic_2\overline{c_3}-ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_2}}{c_0}+\frac{ac_1c_3(c_2\overline{c_2}-ic_2\overline{c_3}+ic_3\overline{c_2}+c_3\overline{c_3})\overline{c_3}}{c_0}+\frac{iac_1\left(-c_2^2-c_3^2\right)\overline{c_2c_3}}{c_0}\right)e^{2.0c_0t}}{ac_1\left(2.0c_2^2\overline{c_2}^2+4.0c_2c_3\overline{c_2c_3}+2.0c_3^2\overline{c_3}^2\right)}$$

$$\rho_{12}(t) = 0$$

$$\rho_{13}(t) = \frac{1.0iac_1\left(-c_2^2-c_3^2\right)e^{2.0c_0t}}{c_0} - \frac{1.0iac_1\left(-c_2^2-c_3^2\right)}{c_0}$$

$$\rho_{14}(t) = 0$$

$$\rho_{15}(t) = 0$$

$$\rho_{16}(t) = \frac{1.0ac_1(c_2\overline{c_2}+ic_2\overline{c_3}-ic_3\overline{c_2}+c_3\overline{c_3})e^{2.0c_0t}}{c_0} - \frac{1.0ac_1(c_2\overline{c_2}+ic_2\overline{c_3}-ic_3\overline{c_2}+c_3\overline{c_3})}{c_0}$$

By reverting the change of variables. The analytical answer of the Bloch redfield equation is given by

$$\rho_1(t) = \frac{0.5\left(e^{\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}-1\right)\left(16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4\right)((b_0-ib_1)(b_0+ib_1)+i(b_0-ib_1)(b_2+ib_3)-i(b_0+ib_1)(b_2-}{\left(4a^2\gamma^2+\left(4a^2-w_0^2\right)^2\right)\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}$$

$$\rho_2(t) = 0$$

$$\rho_3(t) = 0$$

$$\rho_4(t) = \frac{0.5i\left((b_0-ib_1)^2+(b_2-ib_3)^2\right)\left(e^{\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}-1\right)\left(16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4\right)e^{-\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1}}}{\left(4a^2\gamma^2+\left(4a^2-w_0^2\right)^2\right)\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}$$

$$\rho_5(t) = 0$$

$$\rho_6(t) = 0.5e^{-\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}$$

$$\rho_7(t) = 0.5ie^{-\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}$$

$$\rho_8(t) = 0$$

$$\rho_9(t) = 0$$

$$\rho_{10}(t) = -0.5ie^{-\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}$$

$$\rho_{11}(t) = 0.5e^{-\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}$$

$$\rho_{12}(t) = 0$$

$$\rho_{13}(t) = \frac{0.5i\left(1-e^{\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}\right)\left((b_0+ib_1)^2+(b_2+ib_3)^2\right)\left(16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4\right)e^{-\frac{4.0a\gamma\lambda^2t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+}}}{\left(4a^2\gamma^2+\left(4a^2-w_0^2\right)^2\right)\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}$$

$$\rho_{14}(t) = 0$$

$$\rho_{15}(t) = 0$$

$$\rho_{16}(t) = \frac{0.5\left(e^{\frac{4.0a\gamma\lambda^2 t\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}{16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4}}-1\right)\left(16.0a^4+4.0a^2\gamma^2-8.0a^2w_0^2+1.0w_0^4\right)((b_0-ib_1)(b_0+ib_1)-i(b_0-ib_1)(b_2+ib_3)+i(b_0+ib_1)(b_2}{\left(4a^2\gamma^2+\left(4a^2-w_0^2\right)^2\right)\left(b_0^2+b_1^2+b_2^2+b_3^2\right)}$$

We can then substitute the numerical values for example for the case we explored above

$$\rho(t) = \begin{bmatrix} 0.55247613848278\left(e^{0.946799658168 26t}-1.0\right)e^{-0.946799658168 26t} & 0 \\ 0 & 0.5e^{-0.946799} \\ 0 & -0.5ie^{-0.9467} \\ \left(-0.486572940196368-0.102435485836685i\right)\left(1.0-e^{0.946799658168 26t}\right)e^{-0.946799658168 26t} & 0 \end{bmatrix}$$

Then we may evaluate for long times

$$\rho(50) = \begin{bmatrix} 0.55247613848278 & 0 & 0 & 0.486572940196368-0.102435485836685i \\ 0 & 0.0 & 0 & 0 \\ 0 & 0 & 0.0 & 0 \\ 0.486572940196368+0.102435485836685i & 0 & 0 & 0.44752386151722 \end{bmatrix}$$

I believe I was careful enough to use the same convention used in the other equations (Pseudomodes, Cumulant and redfield) but currently reviewing the derivations to make sure there's no inconsistencies. The derivations in question are in https://master–gsuarezthesis.netlify.app/redfield . I do think it is now safe to assume that BR/Redfield breaksdown and that it is not a bug in the code, so maybe we can write a paper on redfield breaking down, cumulant/global being good once we figure out why it happens. Though it seems to be about the coupling and not the degeneracies

About Pictures
Technically the above matrix is not correct as it is in the interaction picture and not the Schrodinger picture. In this case it does not make a difference, however, let us do the rotation

```
U=exp(I*H*t)
```

$$U = \begin{bmatrix} e^{-iat} & 0 & 0 & 0 \\ 0 & e^{iat} & 0 & 0 \\ 0 & 0 & e^{iat} & 0 \\ 0 & 0 & 0 & e^{-iat} \end{bmatrix}$$

$$U\rho U^\dagger = \begin{bmatrix} \rho_1 & \rho_2 e^{-2iat} & \rho_3 e^{-2iat} & \rho_4 \\ e^{2iat}\overline{\rho_2} & \rho_6 & \overline{\rho_{10}} & \rho_8 e^{2iat} \\ e^{2iat}\overline{\rho_3} & \rho_{10} & \rho_{11} & \rho_{12}e^{2iat} \\ \overline{\rho_4} & e^{-2iat}\overline{\rho_8} & e^{-2iat}\overline{\rho_{12}} & -\rho_1-\rho_{11}-\rho_6+1 \end{bmatrix}$$

```
rhoss=U*roundMatrix(ans.subs(num_values).subs(t,150).evalf(),18)*Dagger(U)
```

$$\rho(50) = \begin{bmatrix} 0.55247613848278 & 0 & 0 & 0.486572940196368-0.102435485836685i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0.486572940196368+0.102435485836685i & 0 & 0 & 0.44752386151722 \end{bmatrix}$$

0.2.1 RC picture of the Hamiltonian

For the RC I simply follow one of your papers https://arxiv.org/pdf/1511.05181

So If I didn't misunderstand it then

$$\Omega = w_0 \tag{18}$$

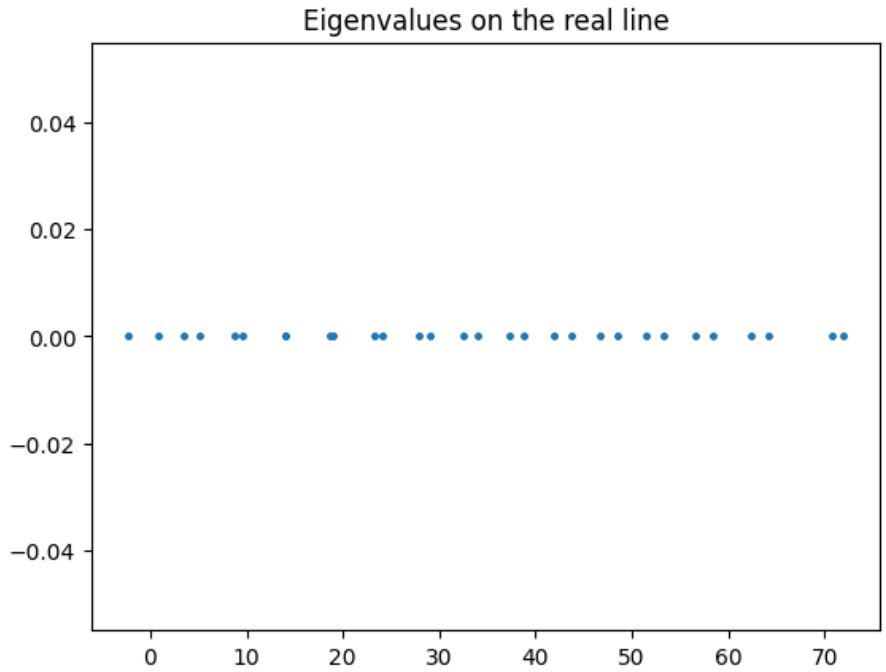
$$\lambda_{rc} = \sqrt{\frac{\pi}{2w_0}}\lambda \tag{19}$$

Not actually sure if π should be there, but does not seem to be relevant for the question we are asking

Not sure how many levels to take here, but let us guess 15 is enough
Then I construct the RC Hamiltonian

```
NHRC=HRC.subs(num_values).evalf()
```

```
plt.scatter(np.real(eigenvalues),np.round(np.imag(eigenvalues),10),s=5)
plt.title("Eigenvalues on the real line")
plt.show()
```



Propably I shopuld have done the partial trace so

```
qHRC.ptrace(0)
```

```
Quantum object: dims=[[4], [4]], shape=(4, 4), type='oper', isherm=True
Qobj data =
[[471.25867623   0.           0.           0.        ]
 [  0.         536.71867623   0.           0.        ]
 [  0.           0.         536.71867623   0.        ]
 [  0.           0.           0.         471.25867623]]
```

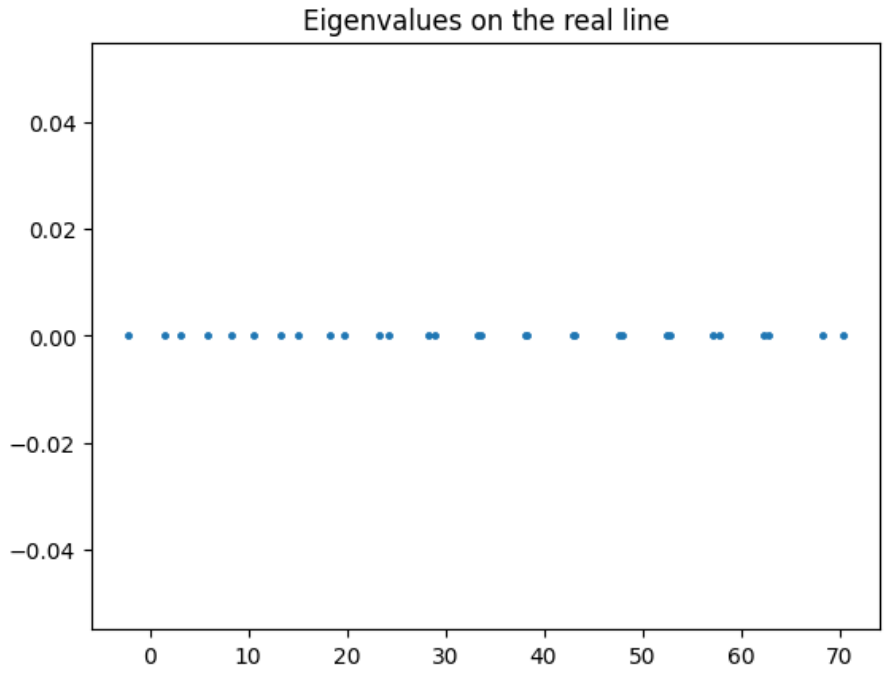
Still degenerate
Let us try the other coupling which does not break bloch redfield

```
qHRC.ptrace(0)
```

```
Quantum object: dims=[[4], [4]], shape=(4, 4), type='oper', isherm=True
Qobj data =
[[471.25867623   0.           0.           0.        ]
 [  0.         536.71867623   0.           0.        ]
 [  0.           0.         536.71867623   0.        ]
 [  0.           0.           0.         471.25867623]]
```

```
eigenvalues, eigenvectors = np.linalg.eig(ans)
```

```
plt.scatter(np.real(eigenvalues), np.round(np.imag(eigenvalues), 10), s=5)
plt.title("Eigenvalues on the real line")
plt.show()
```



There doesn't seem to be much change in the Hamiltonian if any

0.3 Hamiltonian Simulation

0.3.1 When the Hamiltonian is Physical

When the Hamiltonian is physical we can take the same steps as people who simulate the Lindblad master equation. I followed the Lin Lin paper. Here's a bit of the paper but instead of using SDE schemes, I do it on the ensemble. To obtain the Krauss operators (I also only do it to first order, because it is simplest and should work when $dt \to 0$ but probably one should consider higher orders).

0.3.2 Krauss Operator from a Lindbladian

> **Warning**
> This might be a mistake from the very beginning as Pseudomodes is not a CPTP map.However numerically, I've never seen any issue with positivity when enough levels are considered in the modes. So from here I'm assumming it will be CPTP

The logic here is to start from the master equation

$$\dot{\rho(t)} = \mathcal{L}(\rho(t)) \tag{20}$$

From the definition of derivative this means

$$\lim_{dt\to 0} \frac{\rho(t+dt) - \rho(t)}{dt} = \mathcal{L}(\rho(t)) \tag{21}$$

For now let us forget about the limit, but work our quantities approximately and to order $\mathcal{O}(dt^2)$ so that

$$\rho(t+dt) \approx \rho(t) + \mathcal{L}(\rho(t))dt + \mathcal{O}(dt^2) \tag{22}$$

Since the map is CPTP then it must have a sum operator representation (Krauss representation) so

$$\rho(t+dt) = \sum_k M_k \rho(t) M_k^\dagger \tag{23}$$

What's left now is to find what the krauss operators should be. This is known and can be seen for example in Lidar's lecture notes. Here I do some extra algebra to illustrate how to generalize to higher order schemes

Since this is lowest order then, we propose the Krauss operators

$$M_0 = \infty + Adt \tag{24}$$

$$M_k = \sqrt{dt} B_k \tag{25}$$

Then we find that

> **Warning**
> I did these calculations by hand, but I am really lazy when it comes to latexing so I decided to use sympy for intermediate steps, if there's any inconsistency I can just latex those steps

$\rho(dt+t) = \sum_{k=1}^{N} dt B_k \rho(t) B_k^\dagger + \rho(t) + dt\rho(t)A^\dagger + dtA\rho(t) + O\left(dt^2\right)$

Notice the series of Krauss operators we used have identical contributions (in their form, and could be represented as a sum). Notice on the other hand we have

$$\rho(t+dt) \approx \rho(t) + \mathcal{L}(\rho(t))dt + \mathcal{O}(dt^2) \tag{26}$$

By replacing the lindbladian one obtains

$$\rho(t+dt) \approx \rho(t) + \left(-i[H,\rho(t)] + \sum_k L_k \rho(t) L_k^\dagger - \frac{\{L_k^\dagger L_k, \rho(t)\}}{2} \right) dt \tag{27}$$

where the L_k are the jump operators. Then by comparison we can find the required Krauss operators, First let us note That to generate a commutator A must be an Anti-Hermitian matrix, and to generate an anticommutator A must be Hermitian. If we choose A to be a sum of a Hermitian and Anti-hermitian matrix then

$A = -iH + K$

$\rho(dt+t) = \sum_{k=1}^N dt B_k \rho(t) B_k^\dagger + \rho(t) + dt\rho(t)K + idt\rho(t)H + dtK\rho(t) - idtH\rho(t) + O\left(dt^2\right)$

Which we can simplify to

$\rho(dt+t) = \sum_{k=1}^N dt L\rho(t)L^\dagger + \rho(t) - \frac{dt\left(\sum_{k=1}^N L_k^\dagger L_k\right)\rho(t)}{2} - \frac{dt\rho(t)\sum_{k=1}^N L_k^\dagger L_k}{2} + idt\rho(t)H - idtH\rho(t) + O\left(dt^2\right)$

At this point notice that if we select the B_k to be the jump operators and K to be the corresponding anticommutator term

$\rho(dt+t) = \sum_{k=1}^N dt L\rho(t)L^\dagger + \rho(t) - \frac{dt\left(\sum_{k=1}^N L_k^\dagger L_k\right)\rho(t)}{2} - \frac{dt\rho(t)\sum_{k=1}^N L_k^\dagger L_k}{2} + idt\rho(t)H - idtH\rho(t) + O\left(dt^2\right)$

We have obtained the First order scheme to obtain the Linblad master equation Krauss operators. To obtain Higher order schemes One can notice that the solution to the master equation is

$$\rho(t) = e^{\mathcal{L}t}\rho(0) \tag{28}$$

and

$$\rho(t+dt) = e^{\mathcal{L}(t+dt)}\rho(0) = e^{\mathcal{L}dt}\rho(t) \tag{29}$$

And then expand the series of the exponential. Similarly one should increase the order of the krauss operator guess by one and find the appropiate operators

0.3.3 Notice We could have not guess K and use the Completeness relation of krauss operators

In this case it was not needed but it might be useful to find relations in higher order schemes and to check the krauss operators are ok. So next we find K this way

The completeness relation indicates

$$\sum_k M_k^\dagger M_k = 1 \tag{30}$$

Since in our schemes we are numerically approximating to $\mathcal{O}(dt^2)$ then

$$\sum_k M_k^\dagger M_k = 1 + \mathcal{O}(dt^2) \tag{31}$$

$1 = 1 + dt\sum_{k=1}^N L_k^\dagger L_k + 2dtK + O\left(dt^2\right)$

Which we can solve to find

$K = -\frac{\sum_{k=1}^N L_k^\dagger L_k}{2} + O\left(dt\right)$

Now that we have found the Krauss operators one may simply ask if one can follow the same scheme to obtain the Krauss operators of a pseudomode equation. Since I have not seen positivity issues I do think it's possible. but the naive approach to it yields and inconsistency

0.3.4 Same derivation with a non-Hermitian Hamiltonian

Any non-Hermitian matrix can be split into the sum of a Hermitian and Anti-Hermitian Matrix such that I can write the unphysical Hamiltonian H as

$$H = H_0 + iH_u \tag{32}$$

Then the Lindblad equation turns into

$$\rho(t+dt) \approx \rho(t) + \left(-i[H_0, \rho(t)] + [H_u, \rho(t)] + \sum_k L_k \rho(t) L_k^\dagger - \frac{\{L_k^\dagger L_k, \rho(t)\}}{2} \right) dt \tag{33}$$

Following the same strategy as before only A changes (the part that generated the commutator), so the change is only on M_0 We neglect the part that contains K as that one does not change

$\rho(t) + idt\rho(t)H^\dagger - idtH\rho(t) + O\left(dt^2\right)$

Substitute

$$H = H_0 + iH_u \tag{34}$$

$\rho(t) + dt\left(H_u\rho(t) + \rho(t)H_u - i\left[H_0, \rho(t)\right]\right) + O\left(dt^2\right)$

By comparison we would need

$$\{H_u, \rho(t)\} = [H_u, \rho(t)] \tag{35}$$

Which cannot be satisfied

Even though this calculation was a failure. Perhaps one would need to use higher orders, or reorder the terms in another Fashion. I do believe it would be easier if I don't use the general formulation but the jump operators as a and $a^\dagger$ and the unphysical part of the Hamiltonian to have the form $\sum_k \omega_k a_k^\dagger a_k$ where ω_k is complex.

While I look into it. Asume the Hamiltonian is Physical and then extrapolation is done. One has several schemes to simulate Krauss operators in a quantum circuit simulator. Let us go with the scheme in the Lin Lin paper

Even though in their case is not so bad, Here I illustrate why I don't like this Hamiltonian approach in the first order. Perhaps it is better to use the other 2nd Lin Lin paper though I think the number of ancillas needed will be bigger. I also need to try the Hush et al. [2015]

0.3.5 Hamiltonian Simulation From Krauss Operators

In this section all traces are partial traces with respect to the ancilla

The paper suggests using the Stinespring representation of the Krauss Operators Namely. Finding an ancilla and a matrix μ such that

$$Tr(\mu) = \sum_k M_k \rho(t) M_k^\dagger \tag{36}$$

To achieve this we can use the matrix μ

$$\mu = \begin{pmatrix} M_0\rho(t)M_0^\dagger & M_0\rho(t)M_1^\dagger & \dots & M_0\rho(t)M_k^\dagger \\ M_1\rho(t)M_0^\dagger & M_1\rho(t)M_1^\dagger & \dots & M_1\rho(t)M_k^\dagger \\ \vdots & \vdots & \ddots & \vdots \\ M_k\rho(t)M_0^\dagger & \dots & \dots & M_k\rho(t)M_k^\dagger \end{pmatrix} \tag{37}$$

Which can be easily constructed by requiring one ancilla qubit for each jump operator. We consider all the ancillas to be on the ground state such that the state of the ancillas is

$$00 = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix}$$

Then one can obtain μ by

$$\mu = A00 \otimes \rho A^\dagger \tag{38}$$

Where

$$A = \begin{pmatrix} M_0 & M_1^\dagger & \dots & M_k^\dagger \\ M_1 & 0 & \dots & 0 \\ \vdots & 0 & \dots & 0 \\ M_k & 0 & \dots & 0 \end{pmatrix} \tag{39}$$

Then one can express the operator sum representation as

$$Tr(A00 \otimes \rho A^\dagger) = \sum_k M_k \rho(t) M_k^\dagger \tag{40}$$

To have a Hamiltonian simulation of the Krauss representation we want to find a unitary such that

$$Tr(U00 \otimes \rho U^\dagger) = Tr(A00 \otimes \rho A^\dagger) = \sum_k M_k \rho(t) M_k^\dagger \tag{41}$$

Or at least to order $\mathcal{O}(dt^2)$. One of the insights of the paper is to write U as

$$U = e^{-i\sqrt{dt}\bar{H}} \tag{42}$$

Where

$$\bar{H} = \begin{pmatrix} H_0 & H_1^\dagger & \dots & H_k^\dagger \\ H_1 & 0 & \dots & 0 \\ \vdots & 0 & \dots & 0 \\ H_k & 0 & \dots & 0 \end{pmatrix} \tag{43}$$

with Hermitian H_0. Then One can obtain $\bar{H}$ from taylor expanding the exponential and matching the same order terms. For simplicity here I do it for 4 jump operators

While at first order in the exponential we have

$$exp(x) \approx 1 + x \tag{44}$$

$$U = \begin{bmatrix} -i\sqrt{dt}H_0 + 1 & -i\sqrt{dt}H_1^\dagger & -i\sqrt{dt}H_2^\dagger & -i\sqrt{dt}H_3^\dagger & -i\sqrt{dt}H_4^\dagger \\ -i\sqrt{dt}H_1 & 1 & 0 & 0 & 0 \\ -i\sqrt{dt}H_2 & 0 & 1 & 0 & 0 \\ -i\sqrt{dt}H_3 & 0 & 0 & 1 & 0 \\ -i\sqrt{dt}H_4 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Again the goal is to have this emulate the krauss operators, which emulate the master equation

$\rho(dt+t) = \sum_{k=1}^N dt L\rho(t)L^\dagger + \rho(t) - \frac{dt\left(\sum_{k=1}^N L_k^\dagger L_k\right)\rho(t)}{2} - \frac{dt\rho(t)\sum_{k=1}^N L_k^\dagger L_k}{2} + idt\rho(t)H - idtH\rho(t) + O\left(dt^2\right)$

By using

$U\rho U^\dagger = \sqrt{dt}\left(i\rho(t)H_0 - iH_0\rho(t)\right) + dt\left(H_0\rho(t)H_0 + H_1\rho(t)H_1^\dagger + H_2\rho(t)H_2^\dagger + H_3\rho(t)H_3^\dagger + H_4\rho(t)H_4^\dagger\right) + \rho(t)$

We further simiplify it to be

$U\rho U^\dagger = -i\sqrt{dt}\left[H_0, \rho(t)\right] + dt\left(H_0\rho(t)H_0 + \sum_{k=1}^4 H_k\rho(t)H_k\right) + \rho(t)$

To approximate the master equation notice that we can have

$H_0 = \sqrt(dt)H$

$H_k = L_k$

Which is the first order in the Lin Lin paper and results in

$U\rho U^\dagger = dt\left(dtH\rho(t)H + \sum_{k=1}^4 L_k\rho(t)L_k\right) - idt\left[H, \rho(t)\right] + \rho(t)$

Then neglecting higher order terms one has
$U\rho U^\dagger = \rho(t) + dt\sum_{k=1}^{4} L_k\rho(t)L_k - idt\,[H,\rho(t)] + O\left(dt^2\right)$
But this neglects the anticommutator bit This is what I don't like but it can be fixed by higher orders does not seem to affect accuracy too much

TO DO!

- Use higher order Schemes, and try to have a non-Hermitian Hamiltonian
- Test pseudomodes being CPTP by calculating $\tau := (\mathcal{L}\otimes \mathrm{id}_d)(|\Omega\rangle\langle\Omega|)$ where Ω is the maximally entangled state (if CPTP $\tau \geq 0$)
- Check other simulation schemes like the other lin lin paper or Clover's paper
- Actually do the Hamiltonian simulation, The ancillas need to be reset every timestep but this suceeds with probabulity one in theory

---

title: 1/f Noise date: 2024-08-08 authors:

- name: Gerardo Suarez

0.4 Dertivation of $\frac{1}{f}$ Noise based on 1 and 2

Nearly all optical and electronic systems, are subject to the so called $\frac{1}{f}$ noise. While a physical mechanism for $\frac{1}{f}$ noide is yet to be identified. There are specific physical models that give rise to $\frac{1}{f}$ noise. However, those are not necessarily unique.

Perhaps the Most relevant one, is $\frac{1}{f}$ arising from a superposition of train pulses.

0.4.1 Superposition of train pulses

A Noisy waveform

Consider a Noisy waveform $x(t)$ with a band pass filtered such that the power spectral density

$$S(\omega) = \begin{cases} \frac{\alpha}{\omega}, & \text{for } \omega_L \leq \omega \leq \omega_H \\ 0, & \text{otherwise} \end{cases} = \frac{\alpha}{\omega}\theta(\omega_H - \omega)\theta(\omega - \omega_L) \tag{45}$$

Then the auto-correlation function of $x(t)$ is then given by

$$C(\tau) = \langle x(t)x(t+\tau)\rangle \tag{46}$$

Let us remember that the power spectrum and the correlation function are related by

$$S(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} C(t) \qquad = \mathcal{F}(C(t)) \tag{47}$$

Then

$$\mathcal{F}^{-1}(S(\omega)) = \mathcal{F}^{-1}(\mathcal{F}(C(t))) = C(t) \tag{48}$$

So finally we can write

$$C(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega t} S(\omega) \tag{49}$$

By substituting the power spectrum Eq. (**??**) then

$$C(t) = \frac{\alpha}{2\pi}\int_{\omega_L}^{\omega_H} \frac{d\omega}{\omega} e^{-i\omega t} \tag{50}$$

Which results in

$$C(t) = \frac{\alpha}{2\pi}\left(E_i(\omega_H t) - E_i(\omega_L t)\right) \tag{51}$$

where E_i is the exponential integral function.

Warning
At this stage we are going to assume that this is a scalar stationary process, this means that the correlation function is even, which is not necessarily the case. In fact this model does not mathematically follow this. One could consider the imaginary (Quantum part of the noise as well)

Then

$$C(t) = \frac{C(t) - C(-t)}{2} = \frac{\alpha}{2\pi} \int_{\omega_L}^{\omega_H} \frac{d\omega}{\omega} \cos(\omega t) \tag{52}$$

and

$$C(t) = \frac{\alpha}{2\pi} \left(C_i(\omega_H t) - C_i(\omega_L t) \right) \tag{53}$$

where C_i is the cosine integral function.

0.4.2 The noisy waveform in terms of Train pulses (From Lorentzians)

Let us consider the waveform behaves like an exponential relaxation process. This would mean that our autocorrelatio function is given by

$$C(\tau) = \begin{cases} A_0 e^{-\lambda t} & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases} \tag{54}$$

It's Fourier transform is given by

$$\mathcal{F}(C(\tau)) = \int_{-\infty}^{\infty} e^{i\omega t} C(\tau) dt = A_0 \int_0^{\infty} e^{-(\lambda - i\omega)t} dt = \frac{A_0}{\lambda - i\omega} \tag{55}$$

If instead of a pulse we have a train of pulses

$$C(\tau) = \sum_k C(t, t_k) = \sum_k \begin{cases} A_0 e^{-\lambda(t - t_k)} & \text{for } t > t_k \\ 0 & \text{for } t < t_k \end{cases} \tag{56}$$

Then it's Fourier transform is given by

$$\mathcal{F}(C(\tau)) = \int_{-\infty}^{\infty} e^{i\omega t} C(\tau) dt = A_0 \int_0^{\infty} e^{-(\lambda - i\omega)t} dt = \frac{A_0}{\lambda - i\omega} \sum_k e^{i\omega t_k} \tag{57}$$

From here we can find the power spectrum via averaging

$$S(\omega) = lim_{T\to\infty} \frac{1}{T} \langle |\mathcal{F}(C(\tau))|^2 \rangle = \frac{A_0^2}{\lambda^2 + \omega^2} lim_{T\to\infty} \frac{\langle |\sum_k e^{i\omega t_k}|^2 \rangle}{T} \tag{58}$$

If

$$n = lim_{T\to\infty} \frac{\langle |\sum_k e^{i\omega t_k}|^2 \rangle}{T} \tag{59}$$

Then we can write

$$S(\omega) = \frac{A_0^2 n}{\lambda^2 + \omega^2} \tag{60}$$

By identifying $\tau_z = \lambda^{-1}$ as the time scale of the pulses, and $g(\tau_z) = A_0^2 n \tau_z^2$ as the pulse generation details we may write the more popular expression

$$S(\omega) = \frac{g(\tau_z)}{1 + (\tau_z \omega)^2} \tag{61}$$

This is indeed a power spectrum, but it does not behave as $\frac{1}{f}$. However, suppose now that the noisy waveform we are considering is made out of a linear superposition of such processes and that it's decay time scales are between τ_1 and τ_2 with probability density $P(\tau_z)$ then the power spectrum of such superposition is given by

$$S(\omega) = \int_{\tau_1}^{\tau_2} d\tau_z P(\tau_z) \frac{g(\tau_z)}{1 + (\tau_z \omega)^2} \tag{62}$$

If we now assume that $P(\tau_z)g(\tau_z) \propto 1$. Meaning that it is independent of the decay time scale. Then

$$S(\omega) = \int_{\tau_1}^{\tau_2} d\tau_z \frac{\alpha}{1 + (\tau_z \omega)^2} = \frac{\alpha}{\omega} \left(\tan^{-1}(\omega \tau_2) - \tan^{-1}(\omega \tau_1) \right) \tag{63}$$

Finally when $\omega \tau_2 \gg 1$ and $0 < \omega \tau_1 \ll 1$ we have

$$\tan^{-1}(\omega \tau_2) \approx \frac{\pi}{2} \quad \tan^{-1}(\omega \tau_2) \approx 0 \tag{64}$$

So that in this regime, the superposition of different relaxation processes gives rise to the $\frac{1}{f}$ spectrum

$$S(\omega) = \frac{\alpha \pi}{2\omega} \tag{65}$$

On the other hand if $P(\tau_z)g(\tau_z) \propto \tau_z^{\beta - 1}$ then

$$S(\omega) = \int_{\tau_1}^{\tau_2} d\tau_z \frac{\alpha \tau_z^{\beta-1}}{1 + (\tau_z \omega)^2} = \frac{\alpha}{\beta} \left(\tau_2^{\beta} F_1 \left(1, \frac{\beta}{2}, 1 + \frac{\beta}{2}, -\omega^2 \tau_2^2 \right) - \tau_1^{\beta} F_1 \left(1, \frac{\beta}{2}, 1 + \frac{\beta}{2}, -\omega^2 \tau_1^2 \right) \right) \tag{66}$$

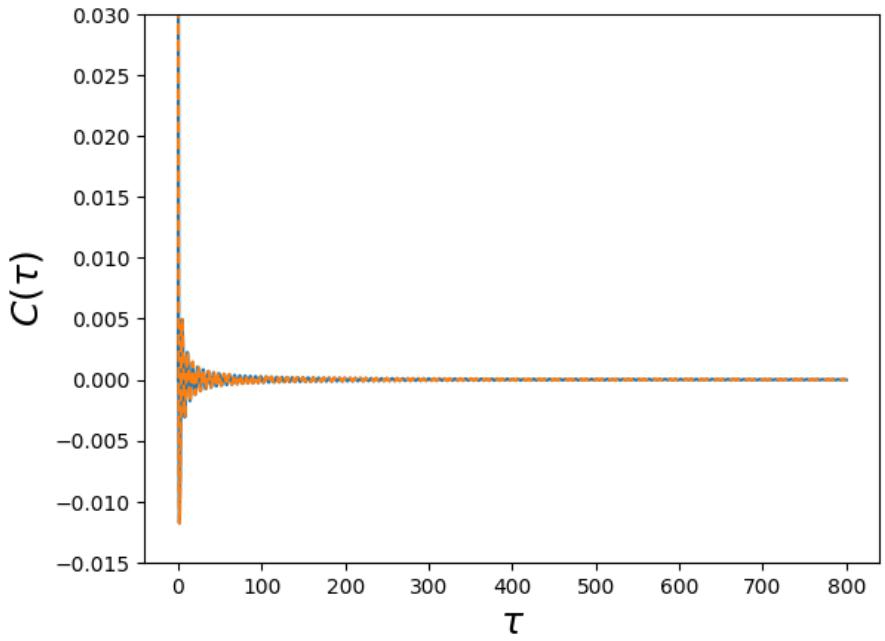
using the same limit

$$S(\omega) \propto \frac{\alpha \pi}{2\omega^{\beta}} \tag{67}$$

```
Fit correlation class instance:

Result of fitting The Real Part Of                                          |Result of fitting The
 the Correlation Function with 10 terms:                                    | Of the Correlation F
                                                                            |
 Parameters|    a     |    b     |    c     |    d                         | Parameters|    a
 1         | 6.22e -02 | -1.58e+00 | -9.16e -01 |1.34e -03                      | 1         | 0.0
 2         | 6.63e -02 | -2.67e+00 | -1.27e -01 | -9.44e -02                     |
 3         | 1.18e -07 | -2.53e -03 | -1.00e+00 | -1.85e -04                     |A  normalized R
 4         | 3.61e -04 | -1.05e -01 | -1.00e+00 | -3.60e -03                     | Of the Correla
 5         | -6.57e -02 | -2.78e+00 | -6.67e -02 | -5.62e -03                    |
 6         | 2.35e -05 | -2.23e -02 | -1.00e+00 | -9.75e -04                     |
 7         | 6.58e -02 | -2.65e+00 | -3.71e -01 | -2.51e -01                     |
 8         | -5.74e -02 | -2.74e+00 | -8.64e -02 |3.70e -02                      |
 9         | 3.25e -03 | -3.81e -01 | -9.91e -01 | -1.05e -02                    |
 10        | -2.34e -02 | -2.79e+00 | -1.37e -01 | -9.64e -02                    |
                                                                            |
A  normalized RMSE of  4.88e -06 was obtained for the The Real Part Of      |
 the Correlation Function                                                   |
 The current fit took  115.358402 seconds                                   | The current fit took
```

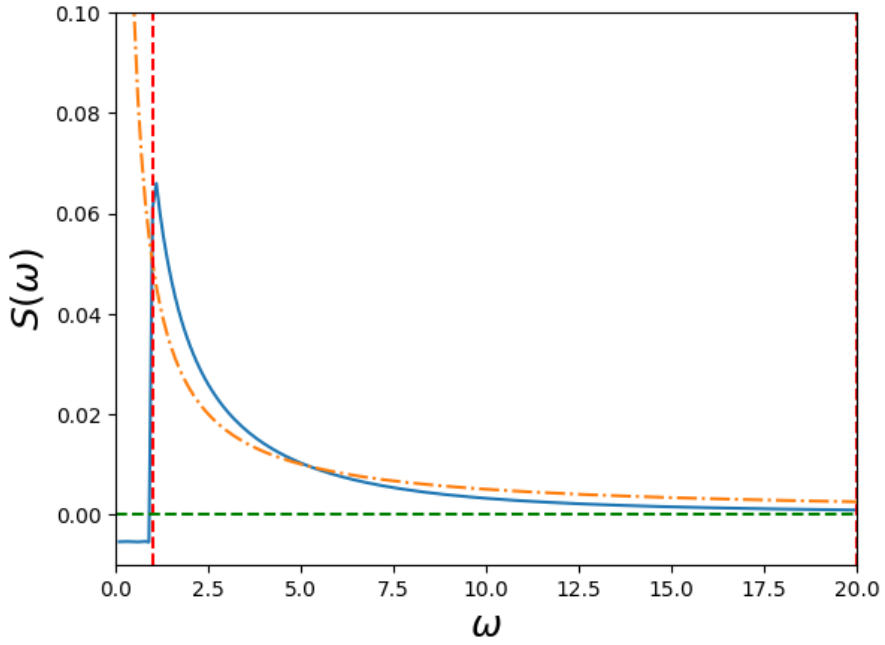
Issue: The correlation function does not decay like one would expect. Most likely this is going to make things difficult, unless one devices how to do it with lorentzians in a limit, or some alternate formulation that yields an easier fit

```
/tmp/ipykernel_67450/1893926815.py:2: RuntimeWarning: invalid value encountered in divide
  return (expi(1j*x)+expi( -1j*x))/2
/tmp/ipykernel_67450/3153800274.py:2: RuntimeWarning: invalid value encountered in subtract
  cc=alpha*(ci(wh*t) -ci(wl*t))/(2)
/home/mcditoos/miniconda3/envs/qutip -dev/lib/python3.12/site -packages/matplotlib/cbook.py:16
  return math.isfinite(val)
/home/mcditoos/miniconda3/envs/qutip -dev/lib/python3.12/site -packages/matplotlib/cbook.py:13
  return np.asarray(x, float)
```



The fit of the correlation function is good, does this approximation actually show $\frac{1}{f}$ spectrum

```
/home/mcditoos/github/qutip_gsoc_app/qutip/solver/heom/bofin_baths.py:510: RuntimeWarning: inv
  S += 2 * np.real((coeff) / (exp.vk - 1j*w))
/tmp/ipykernel_67450/310120726.py:3: RuntimeWarning: divide by zero encountered in divide
  plt.plot(w, 0.05 * 1/w," -.")
```



it does behave sort of like 1/f as wanted, Maybe using AAA would be better since overthere one actually fits the spectrum. Better support points here and lower/upper/guesses may also yield faster simulations. But for now maybe it's good

```
Quantum object: dims=[[2], [2]], shape=(2, 2), type='oper', isherm=True
Qobj data =
[[1. 0.]
 [0. 0.]]

10.0%. Run time:  15.81s. Est. time left: 00:00:02:22
20.0%. Run time:  30.36s. Est. time left: 00:00:02:01
30.0%. Run time:  45.05s. Est. time left: 00:00:01:45
40.0%. Run time:  59.83s. Est. time left: 00:00:01:29
50.0%. Run time:  73.81s. Est. time left: 00:00:01:13
60.0%. Run time:  88.89s. Est. time left: 00:00:00:59
70.0%. Run time: 103.17s. Est. time left: 00:00:00:44
80.0%. Run time: 117.08s. Est. time left: 00:00:00:29
90.0%. Run time: 128.02s. Est. time left: 00:00:00:14
100.0%. Run time: 139.80s. Est. time left: 00:00:00:00
Total run time: 139.80s
```

0.5 Classical Noise approach

To cross-check results from heom we take the approach outline in Costa-Filho et al. [2017]

Thanks again for the code neill !

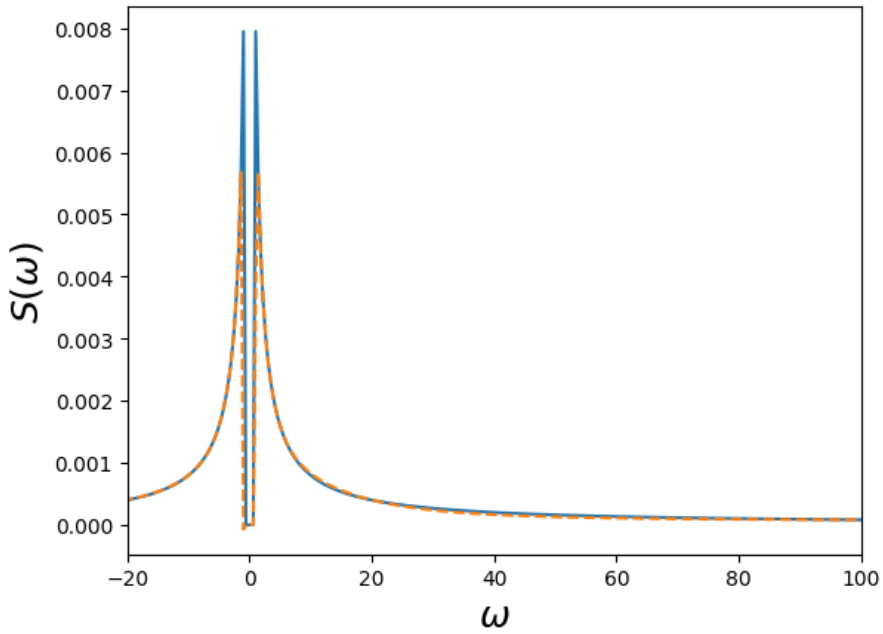
```
Computing rates(tlist)

/tmp/ipykernel_67450/1893926815.py:2: RuntimeWarning: invalid value encountered in scalar divi
  return (expi(1j*x)+expi( -1j*x))/2
/tmp/ipykernel_67450/3153800274.py:2: RuntimeWarning: invalid value encountered in scalar subt
  cc=alpha*(ci(wh*t) -ci(wl*t))/(2)
/tmp/ipykernel_67450/3011102656.py:43: DeprecationWarning: Conversion of an array with ndim >
  C_array[k, i, j] = integral(soft, Deltaij, x_i=0, x_f=t, limit=500)
/home/mcditoos/miniconda3/envs/qutip -dev/lib/python3.12/site -packages/numpy/lib/function_bas
  the requested tolerance from being achieved.  The error may be
  underestimated.
  return self.pyfunc(*the_args, **kwargs)
/home/mcditoos/miniconda3/envs/qutip -dev/lib/python3.12/site -packages/numpy/lib/function_bas
  If increasing the limit yields no improvement it is advised to analyze
  the integrand in order to determine the difficulties.  If the position of a
  local difficulty can be determined (singularity, discontinuity) one will
  probably gain from splitting up the interval and calling the integrator
  on the subranges.  Perhaps a special -purpose integrator should be used.
  return self.pyfunc(*the_args, **kwargs)
/home/mcditoos/miniconda3/envs/qutip -dev/lib/python3.12/site -packages/numpy/lib/function_bas
  return self.pyfunc(*the_args, **kwargs)
```

0.6 Using AAA

AAA works great but to get great fits I need a lot of RAM, For some reason I can't connect to Pitchfork or Torch. So perhaps the results in the section below can be way better

The idea is that since one fits the spectrum directly. It may provide faster and better fits

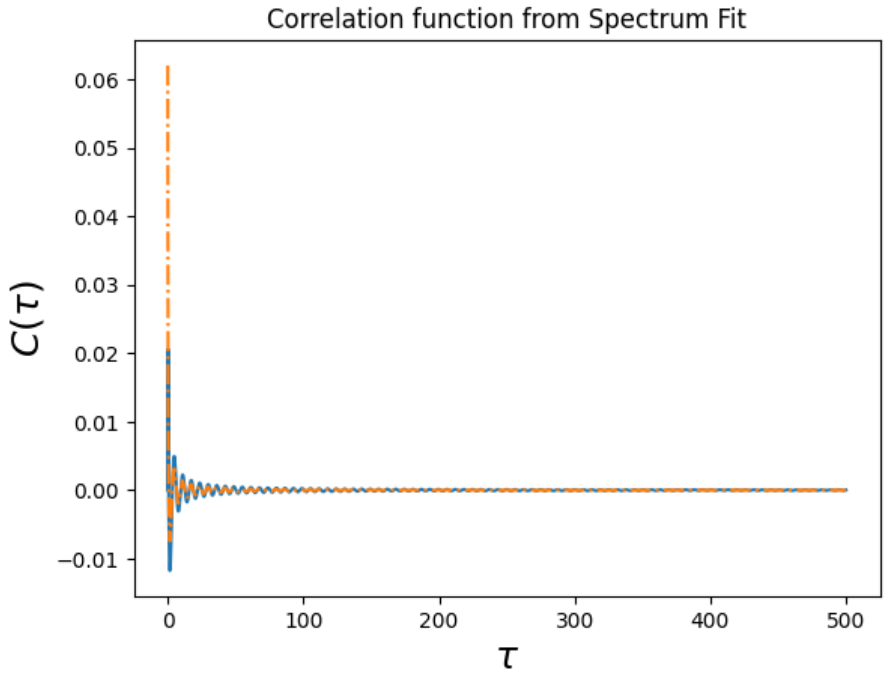
```
/tmp/ipykernel_67450/958776843.py:3: DeprecationWarning: Bitwise inversion '~' on bool is depr
  if ~ (type(F)==np.array):
/tmp/ipykernel_67450/958776843.py:38: ComplexWarning: Casting complex values to real discards
  R[J] = N / D
```



Way better $\frac{1}{f}$ behaviour except at the origin but still great. However, when I limit the number of exponents this is just as bad as the other fitting approach (but a lot faster). Could be better when tried with more RAM, specially since we only care about the spectrum here. Not the correlation function

```
plt.plot(times,correlation(times))
plt.plot(times,correlation_from_exponents(ckAR+1j*ckAI,vkAR+1j*vkAI,times),' -.')
plt.ylabel(r"$C(\tau)$",fontsize=18)
plt.xlabel(r"$\tau$",fontsize=18)
plt.title("Correlation function from Spectrum Fit")
plt.show()
```

```
/tmp/ipykernel_67450/1893926815.py:2: RuntimeWarning: invalid value encountered in divide
  return (expi(1j*x)+expi( -1j*x))/2
/tmp/ipykernel_67450/3153800274.py:2: RuntimeWarning: invalid value encountered in subtract
  cc=alpha*(ci(wh*t) -ci(wl*t))/(2)
```

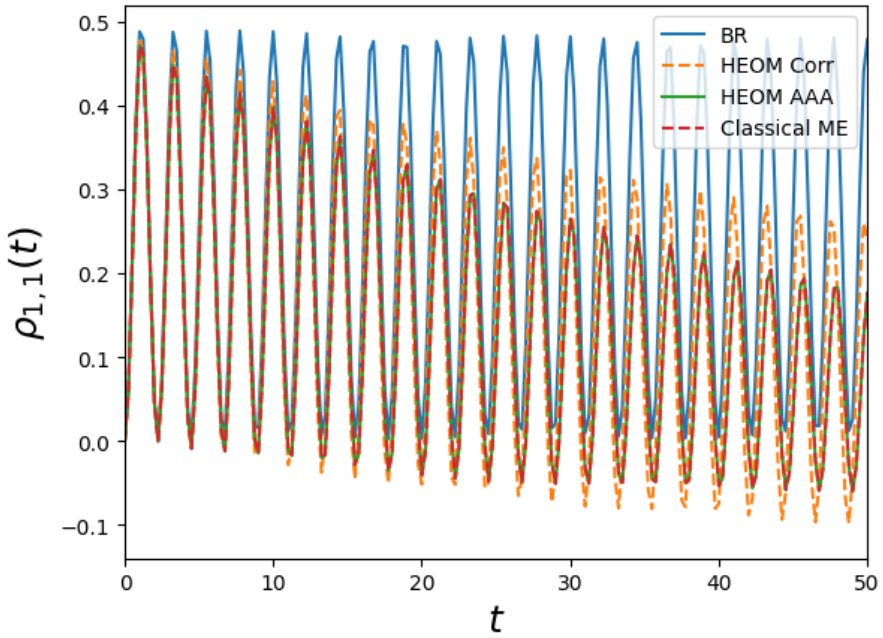


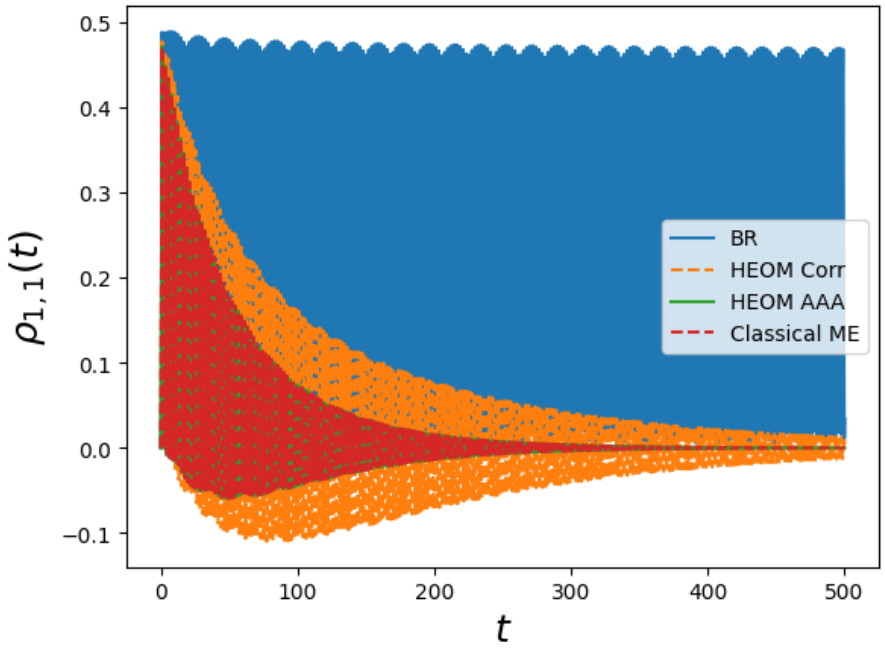
There's two problems here

1. The exponents generated from the fit are complex, They give rise to 1/F. But from this fitting I don't see how to make them real for now
2. The correlation function is definetely off by a constant factor

```
10.0%. Run time:   0.68s. Est. time left: 00:00:00:06
20.0%. Run time:   1.24s. Est. time left: 00:00:00:04
30.0%. Run time:   1.68s. Est. time left: 00:00:00:03
40.0%. Run time:   2.18s. Est. time left: 00:00:00:03
50.0%. Run time:   2.65s. Est. time left: 00:00:00:02
60.0%. Run time:   3.11s. Est. time left: 00:00:00:02
70.0%. Run time:   3.55s. Est. time left: 00:00:00:01
80.0%. Run time:   3.99s. Est. time left: 00:00:00:00
90.0%. Run time:   4.43s. Est. time left: 00:00:00:00
100.0%. Run time:   4.88s. Est. time left: 00:00:00:00
Total run time:   4.88s
```

Note this is fast even when the number of exponents is higher, probably due to the combine feature





Well the classical bit is pretty good. AAA works nicely in this regime because we only care about the spectrum. And there's difficulties using the correlation function. Perhaps making it mire efficient would be the way to go. AAA is fast ~3s per simulation. I bet rescaling would make it faster :). Since there's at least one situation where AAA is better (without too much ram). We should perhaps implement spira which is a better version of AAA for this. While here I tried prony but did not like it :(

0.6.1 Using the spectral density

Probably not the best idea, because the number of exponents would grow drastically as this behaves like $T = 0$. I just want to check whether one can fit the corresponding power spectrum using

$$S(\omega) = 2J(\omega)\,(n(\omega) + 1) \tag{68}$$

At $T = 0$

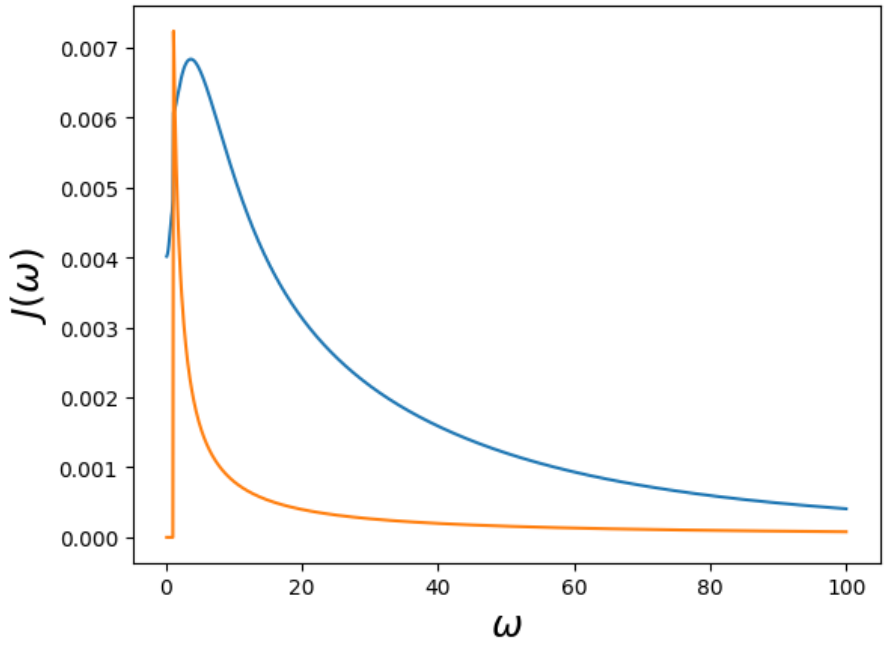
$$S(\omega) = 2J(\omega) \tag{69}$$

so now one may see if it's easy to fit or whether it requires many exponents

```
Result of fitting The Spectral Density with 10 terms:

 Parameters|   lam    |  gamma   |   w0
 1         | -1.25e -01 | 1.10e -01 |1.23e+00
 2         | -2.31e -01 | 1.90e -01 |1.23e+00
 3         | 1.31e -01 | 2.23e -01 |1.24e+00
 4         | 7.23e -01 | 4.13e+01 |5.87e -01
 5         | -5.06e -02 | 1.25e+01 |3.05e+01
 6         | 8.57e -02 | 1.02e+01 |1.13e -01
 7         | 7.42e -02 | 3.36e+00 |1.44e+00
 8         | 6.97e -02 | 1.68e+00 |1.27e+00
 9         | 2.28e -01 | 1.29e -01 |1.22e+00
 10        | -1.06e -01 | 2.31e+00 |4.96e -01

A  normalized RMSE of  8.83e -05 was obtained for the The Spectral Density
 The current fit took  8.219971 seconds
```

```
plt.plot(w2,sbath.spectral_density_approx(w2)/(2*np.pi))
plt.plot(w2,spectrum_f(w2))
plt.ylabel(r"$J(\omega)$",fontsize=18)
plt.xlabel(r"$\omega$",fontsize=18)
plt.show()
```

```
/home/mcditoos/github/qutip_gsoc_app/qutip/solver/heom/bofin_baths.py:425: RuntimeWarning: ove
  return (1 / (np.exp(w / self.T) - 1))
```



While the fit is ok, really hard to converge on the number of exponents as expected.

Bibliography

J. I. Costa-Filho, R. B. B. Lima, R. R. Paiva, P. M. Soares, W. A. M. Morgado, R. L. Franco, and D. O. Soares-Pinto. Enabling quantum non-Markovian dynamics by injection of classical colored noise. *Physical Review A*, 95(5), 5 2017. ISSN 2469-9934. doi: 10.1103/physreva.95.052126. URL http://dx.doi.org/10.1103/PhysRevA.95.052126.

M. R. Hush, I. Lesanovsky, and J. P. Garrahan. Generic map from non-Lindblad to Lindblad master equations. *Physical Review A*, 91(3), 3 2015. ISSN 1094-1622. doi: 10.1103/physreva.91.032113. URL http://dx.doi.org/10.1103/PhysRevA.91.032113.