

An example of non-positivity in the Redfield equation

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In this notebook, we will construct an example where the Redfield equation becomes non-positive. We will also show how to use the positivity-check routine to stop the solver when this happens.

0.1 Ohmic bath

We first create an Ohmic bath with the following parameters:

```
using OpenQuantumTools, OrdinaryDiffEq, Plots, Printf, LaTeXStrings
```

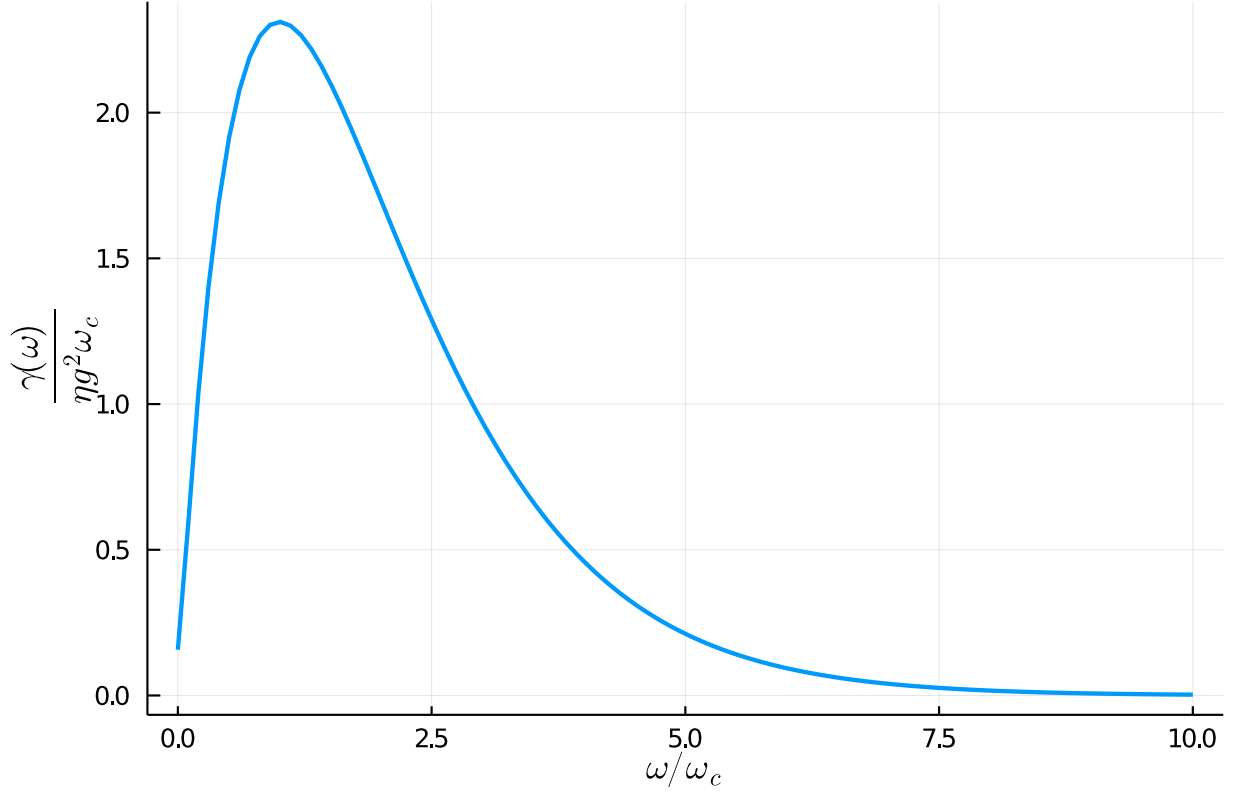
```
 $\beta$  = 4  
T =  $\beta\_2\_temperature(\beta)$   
 $\eta$  = 0.1  
fc= 10/(2 $\pi$ )  
bath = Ohmic( $\eta$ , fc, T)
```

Ohmic bath instance:

```
 $\eta @*(\text{unitless}): 0.1(*@ \omega @*(c \text{ (GHz)}: 1.5915494309189535T \text{ (mK)}: 1.9095587777458247$ 
```

The spectral density γ is plotted below:

```
plot(bath, : $\gamma$ , range(0,10,length=100), linewidth=2, label="")
```



The time scales (defined in [1] Completely positive master equation for arbitrary driving and small level spacing) of the bath are:

```

 $\tau_{sb}$ , err_ $\tau_{sb}$  =  $\tau_{SB}((x) \rightarrow correlation(x, bath))$ 
@printf(" $\tau_{sb}$  of the Ohmic bath is %.6f with error estimation %.2e \n",  $\tau_{sb}$ , err_ $\tau_{sb}$ )
 $\tau_b$ , err_ $\tau_b$  =  $\tau_B((x) \rightarrow correlation(x, bath), 100, \tau_{sb})$ 
@printf(" $\tau_b$  of the Ohmic bath is %.6f with error estimation %.2e \n",  $\tau_b$ , err_ $\tau_b$ )

```

```

 $\tau_0 * ((@_{sb}$  of the Ohmic bath is 0.666454 with error estimation 6.48e-09
 $\tau_0 * ((@_b$  of the Ohmic bath is 0.201395 with error estimation 1.91e-10

```

0.2 Evolution

We construct the Hamiltonian by:

```

Hp = 0.5* $\sigma_z \otimes \sigma_i$  - 0.7* $\sigma_i \otimes \sigma_z$  + 0.3* $\sigma_z \otimes \sigma_z$ 
Hd = standard_driver(2)
H = DenseHamiltonian([(s)  $\rightarrow$  1-s, (s)  $\rightarrow$  s], [-Hd, Hp], unit=: $\hbar$ )

```

```

DenseHamiltonian with Complex{Float64}
with size: (4, 4)

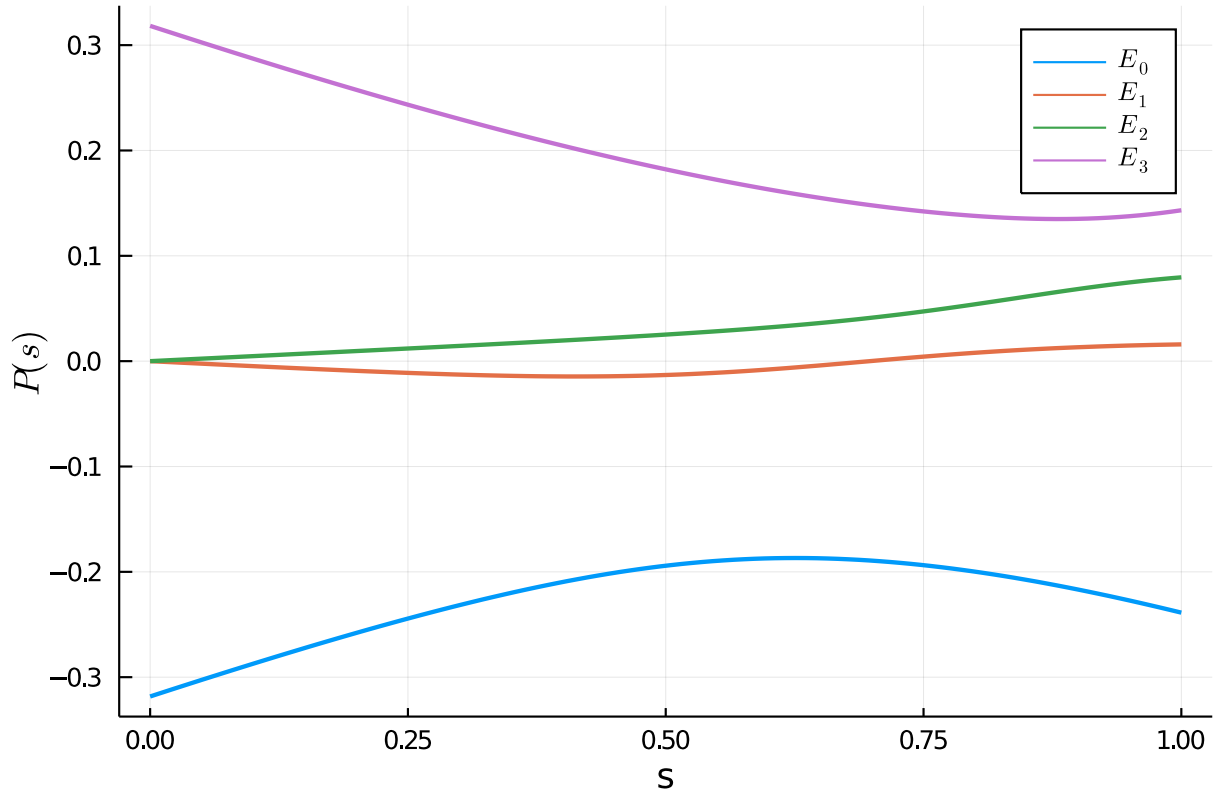
```

The spectrum of the Hamiltonian during the evolution is

```

plot(H, range(0,1,length=100), 4, linewidth=2)
xlabel!(" $s$ ")
ylabel!(" $L^p(s)$ ")

```



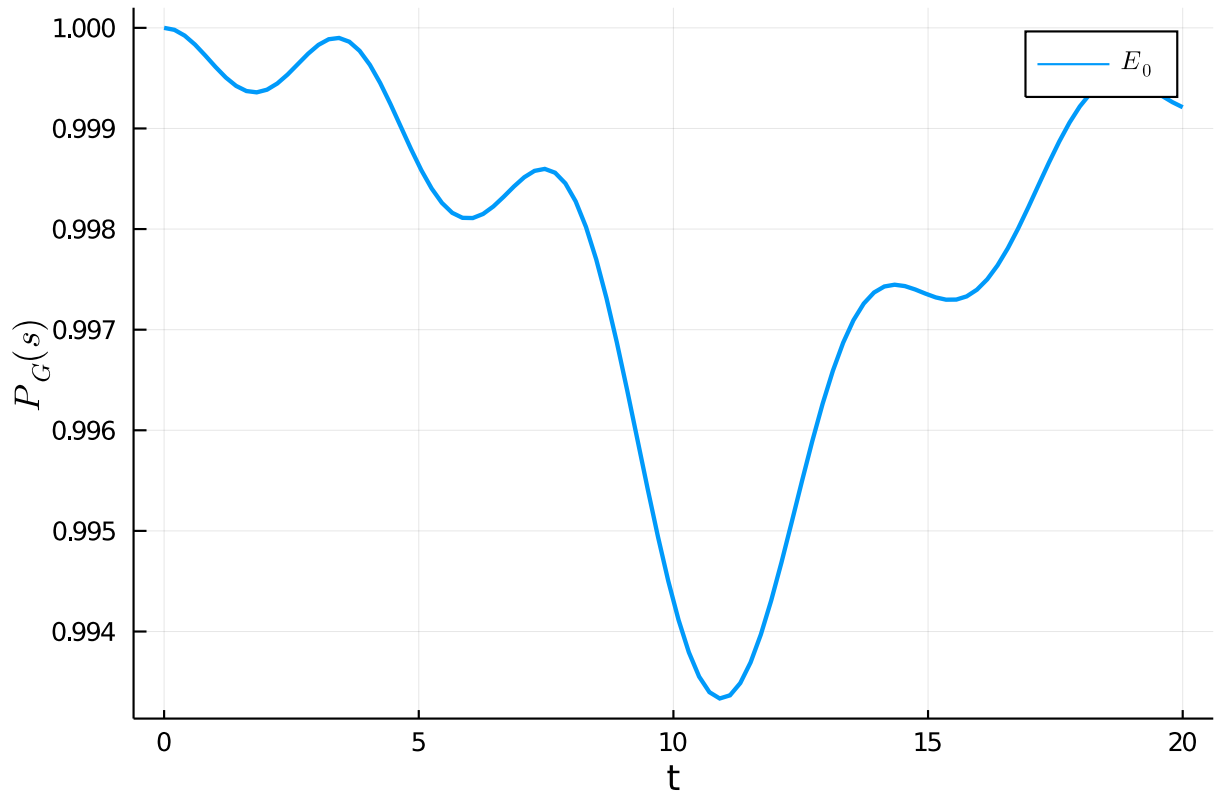
0.2.1 Closed system

We now run the closed-system simulation:

```
tf = 20
ρ0 = (σi+σx)⊗(σi+σx)/4
coupling = ConstantCouplings([σz⊗σi, σi⊗σz], unit=ħ)
annealing = Annealing(H, ρ0, bath=bath, coupling=coupling)
close_sol = solve_von_neumann(annealing, tf, alg = Tsit5(), abstol=1e-6, reltol=1e-6);
```

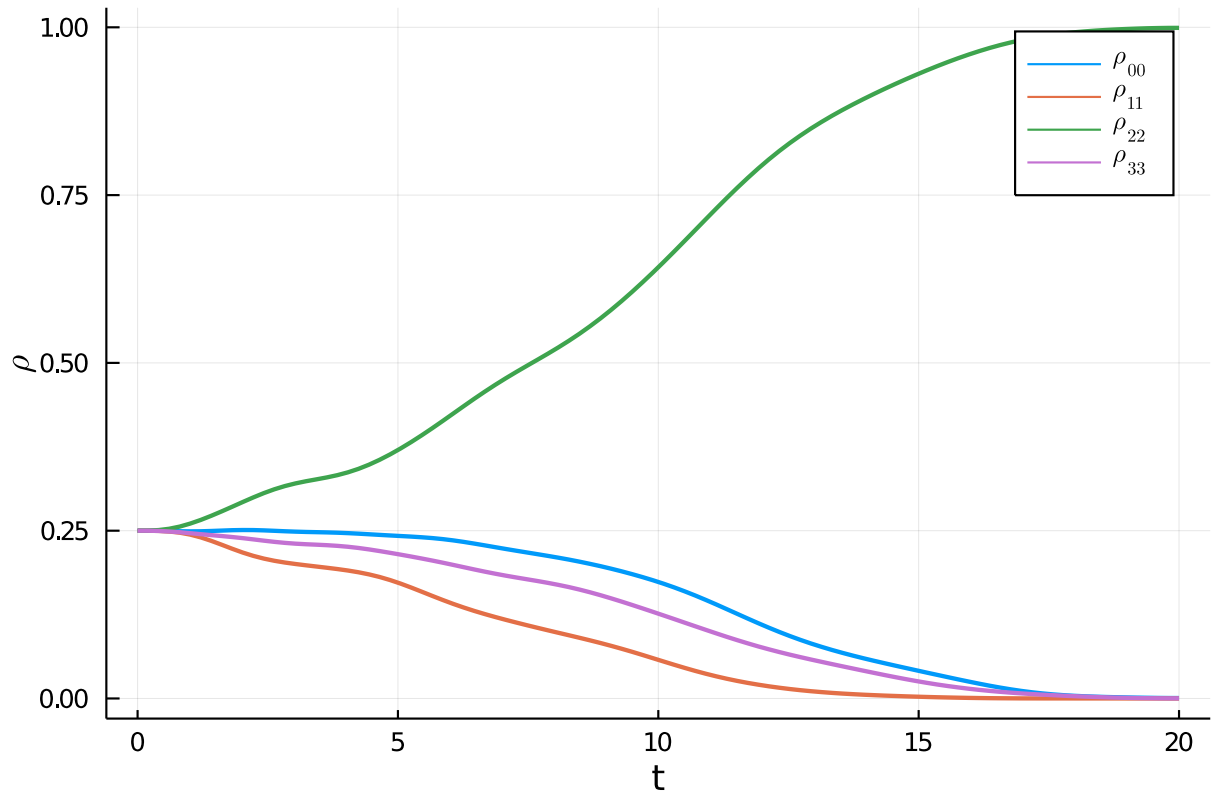
The population of the instantaneous ground state is:

```
plot(close_sol, H, 1, range(0,tf,length=100), linewidth=2)
xlabel!("t")
ylabel!(L"P_G(s)")
```



The populations of the computational states are:

```
t_axis = range(0,tf,length=100)
p_computational_basis = [real(diag(close_sol(s))) for s in t_axis]
p_computational_basis = hcat(p_computational_basis...)
plot(t_axis, p_computational_basis', linewidth=2, label=[L"\rho_{00}" L"\rho_{11}"
L"\rho_{22}" L"\rho_{33}"])
xlabel!("t")
ylabel!(L"\rho")
```



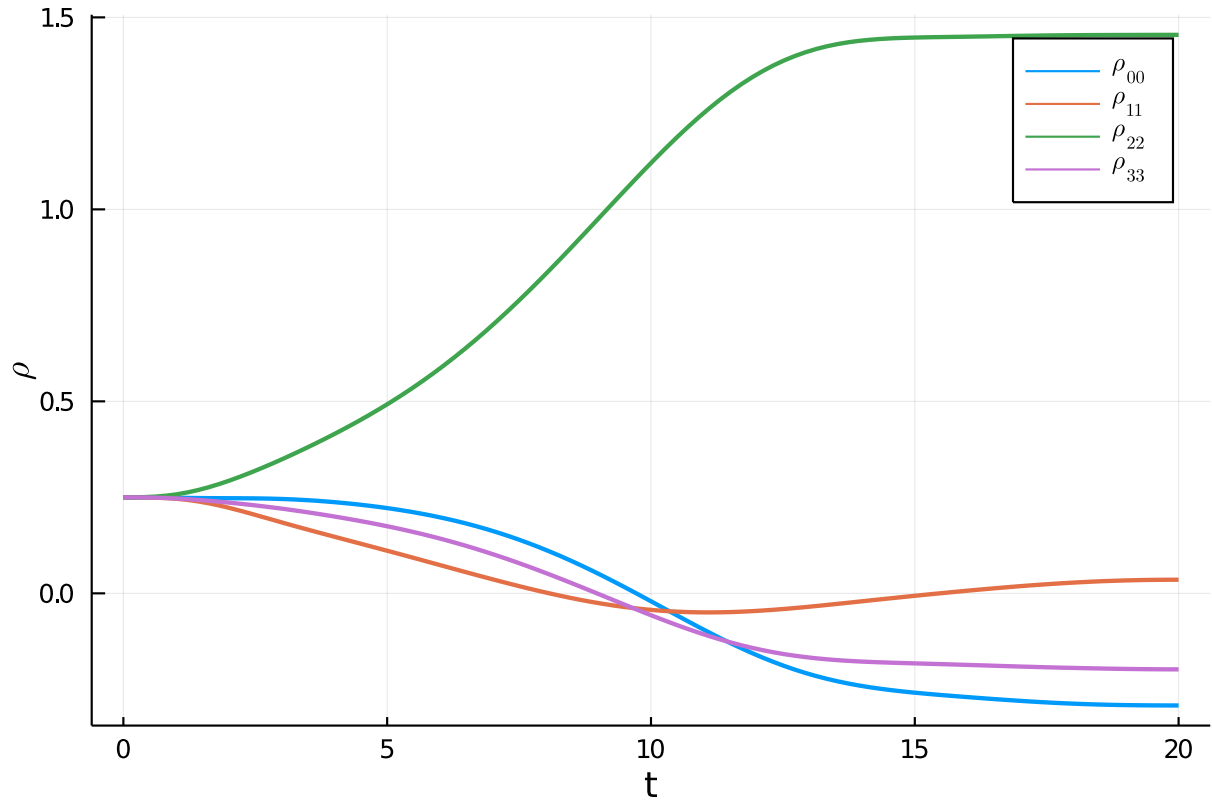
0.2.2 Redfield equation

We solve the Redfield equation:

```
tf = 20
U = solve_unitary(annealing, tf, alg = Tsit5(), abstol=1e-7, reltol=1e-7);
redfield_sol = solve_redfield(annealing, tf, U, alg = Tsit5(), abstol=1e-7, reltol=1e-7);
```

We plot the populations of the computational basis states:

```
t_axis = range(0,tf,length=100)
p_computational_basis = [real(diag(redfield_sol(s))) for s in t_axis]
p_computational_basis = hcat(p_computational_basis...)
plot(t_axis, p_computational_basis', linewidth=2, label=[L"\rho_{00}" L"\rho_{11}"
L"\rho_{22}" L"\rho_{33}"])
xlabel!("t")
ylabel!(L"\rho")
```



We can see that the density matrix becomes negative during evolution.

0.2.3 Positivity check

We can add a callback to stop the ODE solver when the density matrix becomes negative.

```
redfield_sol = solve_redfield(annealing, tf, U, alg = Tsit5(), abstol=1e-7, reltol=1e-7,
callback=PositivityCheckCallback())
```

```
retcode: Terminated
```

```
Interpolation: specialized 4th order "free" interpolation
```

```
t: 38-element Array{Float64,1}:
```

```
0.0
9.999999999999999e-5
0.0010999999999999998
0.00786551568397621
0.016932240388251633
0.026303763546061412
0.03727043304206125
0.049257562452163145
0.06292827203759598
0.07875976726667351
```

```
:@*(1.67134486024115051.86388132982545042.06457517970948872.2742129686106532.49221591759457932.7193240
```

```
38-element Array{*@{Array{Complex{Float64},2},1}:
```

```
[0.25 + 0.0im 0.25 + 0.0im 0.25 + 0.0im 0.25 + 0.0im; 0.25 + 0.0im 0.25 +
0.0im 0.25 + 0.0im 0.25 + 0.0im; 0.25 + 0.0im 0.25 + 0.0im 0.25 + 0.0im 0.2
5 + 0.0im; 0.25 + 0.0im 0.25 + 0.0im 0.25 + 0.0im 0.25 + 0.0im]
[0.24999999999999667 + 0.0im 0.2499999499008545 + 4.9999990174512035e-11im
0.2499999499008645 - 9.999997925042628e-11im 0.24999989980172238 + 2.49999
8989472679e-11im; 0.2499999499008545 - 4.9999990174512035e-11im 0.249999999
```

999995 + 0.0im 0.24999989980173237 - 1.499999393743525e-10im 0.249999949900
 85284 - 2.4999995250486812e-11im; 0.2499999499008645 + 9.999997925042628e-1
 1im 0.24999989980173237 + 1.499999393743525e-10im 0.250000000000015 + 0.0im
 0.24999994990086283 + 1.2499997419002007e-10im; 0.24999989980172238 - 2.49
 9998989472679e-11im 0.24999994990085284 + 2.4999995250486812e-11im 0.249999
 94990086283 - 1.2499997419002007e-10im 0.2499999999999334 + 0.0im]
 [0.2499999999556358 + 0.0im 0.24999393848502027 + 6.049856360775496e-9im
 0.24999393849832896 - 1.2099696252796612e-8im 0.2499878771214445 + 3.024852
 0933238623e-9im; 0.24999393848502027 - 6.049856360775496e-9im 0.24999999999
 334538 + 0.0im 0.24998787713475293 - 1.8149112559113315e-8im 0.249993938482
 80216 - 3.0249309250320802e-9im; 0.24999393849832896 + 1.2099696252796612e-
 8im 0.24998787713475293 + 1.8149112559113315e-8im 0.2500000001996386 + 0.0
 im 0.24999393849611065 + 1.5124621688573342e-8im; 0.2499878771214445 - 3.02
 48520933238623e-9im 0.24999393848280216 + 3.0249309250320802e-9im 0.2499939
 3849611065 - 1.5124621688573342e-8im 0.24999999999112718 + 0.0im]
 [0.24999999837975584 + 0.0im 0.24969132975142425 + 3.0895766607337363e-7im
 0.2496913346058523 - 6.178723540242412e-7im 0.24938304222425808 + 1.542809
 468843706e-7im; 0.24969132975142425 - 3.0895766607337363e-7im 0.24999999756
 94084 + 0.0im 0.2493830470804095 - 9.256856939315008e-7im 0.249691328942400
 68 - 1.544859966565001e-7im; 0.2496913346058523 + 6.178723540242412e-7im 0.
 2493830470804095 + 9.256856939315008e-7im 0.25000000729141414 + 0.0im 0.249
 69133379625535 + 7.723440234400316e-7im; 0.24938304222425808 - 1.5428094688
 43706e-7im 0.24969132894240068 + 1.544859966565001e-7im 0.24969133379625535
 - 7.723440234400316e-7im 0.24999999675942158 + 0.0im]
 [0.24999998388874467 + 0.0im 0.24859060513778264 + 1.4255873379732954e-6im
 0.24859065319919907 - 2.8502559946955376e-6im 0.24718917159160642 + 7.0862
 29842403495e-7im; 0.24859060513778264 - 1.4255873379732954e-6im 0.249999975
 82273706 + 0.0im 0.24718921975769031 - 4.251738485634606e-6im 0.24859059712
 85693 - 7.129468101170297e-7im; 0.24859065319919907 + 2.8502559946955376e-6
 im 0.24718921975769031 + 4.251738485634606e-6im 0.25000007251518047 + 0.0im
 0.24859064517772647 + 3.5628965224982478e-6im; 0.24718917159160642 - 7.086
 229842403495e-7im 0.2485905971285693 + 7.129468101170297e-7im 0.24859064517
 772647 - 3.5628965224982478e-6im 0.24999996777333777 + 0.0im]
 [0.2499999399299207 + 0.0im 0.24668618944470977 + 3.414497800430544e-6im 0
 .24668636730601845 - 6.823685348706714e-6im 0.24341636107441625 + 1.6837455
 45732269e-6im; 0.24668618944470977 - 3.414497800430544e-6im 0.2499999098015
 226 + 0.0im 0.24341653992297976 - 1.0102478474120433e-5im 0.246686159807077
 53 - 1.7081341889836474e-6im; 0.24668636730601845 + 6.823685348706714e-6im
 0.24341653992297976 + 1.0102478474120433e-5im 0.2500002704460534 + 0.0im 0.
 2466863375975447 + 8.53004895941865e-6im; 0.24341636107441625 - 1.683745545
 732269e-6im 0.24668615980707753 + 1.7081341889836474e-6im 0.246686337597544
 7 - 8.53004895941865e-6im 0.24999987982250327 + 0.0im]
 [0.2499998306336825 + 0.0im 0.24362670203202597 + 6.771747588244123e-6im 0
 .24362719751451525 - 1.3522344561285555e-5im 0.2374160316205387 + 3.2961215
 160996274e-6im; 0.24362670203202597 - 6.771747588244123e-6im 0.249999745422
 2247 + 0.0im 0.2374165326436156 - 1.9776758343931157e-5im 0.243626619475231
 7 - 3.3894002797073305e-6im; 0.24362719751451525 + 1.3522344561285555e-5im
 0.2374165326436156 + 1.9776758343931157e-5im 0.2500007628880057 + 0.0im 0.2
 4362711467578574 + 1.6904691863948198e-5im; 0.2374160316205387 - 3.29612151
 60996274e-6im 0.2436266194752317 + 3.3894002797073305e-6im 0.24362711467578
 574 - 1.6904691863948198e-5im 0.24999966105608704 + 0.0im]
 [0.24999961384104594 + 0.0im 0.23951637520397615 + 1.1631933549511452e-5im
 0.23951748667756637 - 2.3200383422364576e-5im 0.22947269701460934 + 5.5619
 3874294054e-6im; 0.23951637520397615 - 1.1631933549511452e-5im 0.2499994186
 580527 + 0.0im 0.22947382960870774 - 3.3371747944009756e-5im 0.239516190029
 47735 - 5.826552822401771e-6im; 0.23951748667756637 + 2.3200383422364576e-5
 im 0.22947382960870774 + 3.3371747944009756e-5im 0.2500017406599985 + 0.0im
 0.23951730065779062 + 2.9005764118730046e-5im; 0.22947269701460934 - 5.561
 93874294054e-6im 0.23951619002947735 + 5.826552822401771e-6im 0.23951730065

779062 - 2.9005764118730046e-5im 0.24999922684090284 + 0.0im]
 [0.2499992083063724 + 0.0im 0.23422939685490862 + 1.857118209719181e-5im 0
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 09 + 0.0im 0.21945653145195324 - 5.204435731894794e-5im 0.23422902521060607
 - 9.313180131653292e-6im; 0.2342316278375741 + 3.697693691826234e-5im 0.21
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 439e-6im 0.23422902521060607 + 9.313180131653292e-6im 0.23423125399318892 -
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 214168369e-5im; 0.22779717326802448 - 2.8299733764945774e-5im 0.24999770176
 659977 + 0.0im 0.20757154511921982 - 7.700079551639141e-5im 0.2277964791051
 7015 - 1.421565901665766e-5im; 0.2278013409290694 + 5.620502986750122e-5im
 0.20757154511921982 + 7.700079551639141e-5im 0.2500068608887103 + 0.0im 0.2
 2780064152368015 + 7.028910412895205e-5im; 0.2075672008837808 - 1.283327721
 4168369e-5im 0.22779647910517015 + 1.421565901665766e-5im 0.227800641523680
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 0.0028255504625640158im; 0.22614229334826394 - 0.009141702321136765im 0.2330924243746943
 + 0.0im 0.22362920899755323 - 0.017763226373053692im 0.22281061467711177 -
 0.006113370951367806im; 0.24727054966668502 + 0.009599467687634727im 0.22362920899755323 +
 0.017763226373053692im 0.2785234665407388 + 0.0im 0.24340395258651612 +
 0.012612805673926053im; 0.21798083067554633 - 0.0028255504625640158im 0.22281061467711177
 + 0.006113370951367806im 0.24340395258651612 - 0.012612805673926053im 0.24046205989483996
 + 0.0im] [0.2477926053255273 + 0.0im 0.2258676285700636 + 0.010495019683078114im
 0.2538406714697561 - 0.010792545758447953im 0.2225107777299921 + 0.0032036757962302202im;
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 0.2868104795604476 + 0.0im 0.24870275451372903 + 0.014162744132238704im;
 0.2225107777299921 - 0.0032036757962302202im 0.2215044558123656 + 0.007099178279177384im
 0.24870275451372903 - 0.014162744132238704im 0.2380803683534121 +
 0.0im] [0.247693583978478 + 0.0im 0.22422790736391682 + 0.011639263951965179im
 0.26008239763459284 - 0.011919290616851416im 0.2253506663841521 +
 0.0035127509359304974im; 0.22422790736391682 - 0.011639263951965179im 0.22057357682004874
 + 0.0im 0.23237159762173387 - 0.02273312186699301im 0.21870318369298308-
 0.007944130972830874im; 0.26008239763459284 + 0.011919290616851416im 0.23237159762173387
 + 0.02273312186699301im 0.2963113557970802 + 0.0im 0.2534763370476774 +
 0.015572838770129124im; 0.2253506663841521 - 0.0035127509359304974im 0.21870318369298308
 + 0.007944130972830874im 0.2534763370476774 - 0.015572838770129124im 0.23542148340439298
 + 0.0im] [0.24755957713243973 + 0.0im 0.2215065857284598 + 0.01251172052097779im
 0.26621368654120264 - 0.012987893694865426im 0.2269457946435507 +
 0.0037404128749102005im; 0.2215065857284598 - 0.01251172052097779im 0.2129508378172507+
 0.0im 0.23459876882193653 - 0.02468402126850542im 0.2147106408079851 -
 0.008598787932615558im; 0.26621368654120264 + 0.012987893694865426im 0.23459876882193653
 + 0.02468402126850542im 0.3070321733242578 + 0.0im 0.2579557812677962 +
 0.016836440019009146im; 0.2269457946435507 - 0.0037404128749102005im 0.2147106408079851 +
 0.008598787932615558im 0.2579557812677962 - 0.016836440019009146im 0.23245741172605164 +
 0.0im] [0.2472983519580838 + 0.0im 0.21796856461239028 + 0.01308349809731773im
 0.2723559082156419 - 0.014009145645186604im 0.22766121123221605 +
 0.0038824934147620883im; 0.21796856461239028 - 0.01308349809731773im 0.20463161310769679
 + 0.0im 0.23597007469967626 - 0.026235623365816724im 0.20982396237589382-
 0.009040034519874514im; 0.2723559082156419 + 0.014009145645186604im 0.23597007469967626 +
 0.026235623365816724im 0.3189048310906175 + 0.0im 0.26229140307850385 +
 0.017957142196730464im; 0.22766121123221605 - 0.0038824934147620883im 0.20982396237589382
 + 0.009040034519874514im 0.26229140307850385- 0.017957142196730464im 0.22916520384360178

+ 0.0im] [0.24680090479436495 + 0.0im 0.21380216512832234 +
 0.013375854961349213im 0.27860392689281405 - 0.015005986890265562im 0.22776506696147508 +
 0.0039454154643364025im; 0.21380216512832234 - 0.013375854961349213im 0.19577120834353381
 + 0.0im 0.23680669722002734 - 0.027431962260960088im 0.20425696144245825 -
 0.009284171233671807im; 0.27860392689281405 + 0.015005986890265562im 0.23680669722002734 +
 0.027431962260960088im 0.33193353142130866 + 0.0im 0.266598903477385 +
 0.01896143884360183im; 0.22776506696147508 - 0.0039454154643364025im 0.20425696144245825
 + 0.009284171233671807im 0.266598903477385- 0.01896143884360183im 0.2254943554407925 +
 0.0im] [0.24596348831664838 + 0.0im 0.2091626422505489 + 0.013447396939781394im
 0.2849434869460782 - 0.015996143250113358im 0.22741593914979108 + 0.003942598186544016im;
 0.2091626422505489 - 0.013447396939781394im 0.18658503638407722 + 0.0im
 0.23729916744579543 - 0.028350796281651023im 0.19820077547854548- 0.009376947663321962im;
 0.2849434869460782 + 0.015996143250113358im 0.23729916744579543 + 0.028350796281651023im
 0.34602685874397515 + 0.0im 0.27089996792142595 + 0.019879208900483822im;
 0.22741593914979108 - 0.003942598186544016im 0.19820077547854548 + 0.009376947663321962im
 0.27089996792142595- 0.019879208900483822im 0.2214246165552992 +
 0.0im] [0.24469136963824628 + 0.0im 0.20410097866522758 + 0.01338365121078571im
 0.2913811139938835 - 0.017009984064360276im 0.22668480983402695 + 0.003892713193799888im;
 0.20410097866522758 - 0.01338365121078571im 0.1771615207174667 + 0.0im 0.2375325475036707
 - 0.029108003661788548im 0.19172586000076142 -0.009385184752227061im; 0.2913811139938835 +
 0.017009984064360276im 0.2375325475036707 + 0.029108003661788548im 0.36124116348409824 +
 0.0im 0.2752142009683333 + 0.02075892159113134im; 0.22668480983402695 -
 0.003892713193799888im 0.19172586000076142 + 0.009385184752227061im 0.2752142009683333 -
 0.02075892159113134im 0.21690594616018874 + 0.0im] [0.24290524066293354 + 0.0im
 0.19861358798823017 + 0.013273973699318457im 0.29790191810670746 - 0.018082867383866618im
 0.22557911333856914 + 0.003815779603840782im; 0.19861358798823017 -
 0.013273973699318457im 0.16753467090485658 + 0.0im 0.23750261039254483 -
 0.02982669143889128im 0.18484503529834903 - 0.009377952089346392im; 0.29790191810670746 +
 0.018082867383866618im 0.23750261039254483 + 0.02982669143889128im 0.3776671806178623 +
 0.0im 0.2795334438511778 + 0.021656108687892934im; 0.22557911333856914 -
 0.003815779603840782im 0.18484503529834903 + 0.009377952089346392im 0.2795334438511778
 -0.021656108687892934im 0.21189290781434753 + 0.0im]