

An example of non-positivity in Redfield equation

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0.1 Ohmic bath

We first create Ohmic bath with the following parameters

```
using QuantumAnnealingTools, OrdinaryDiffEq, Plots, Printf, LaTeXStrings
```

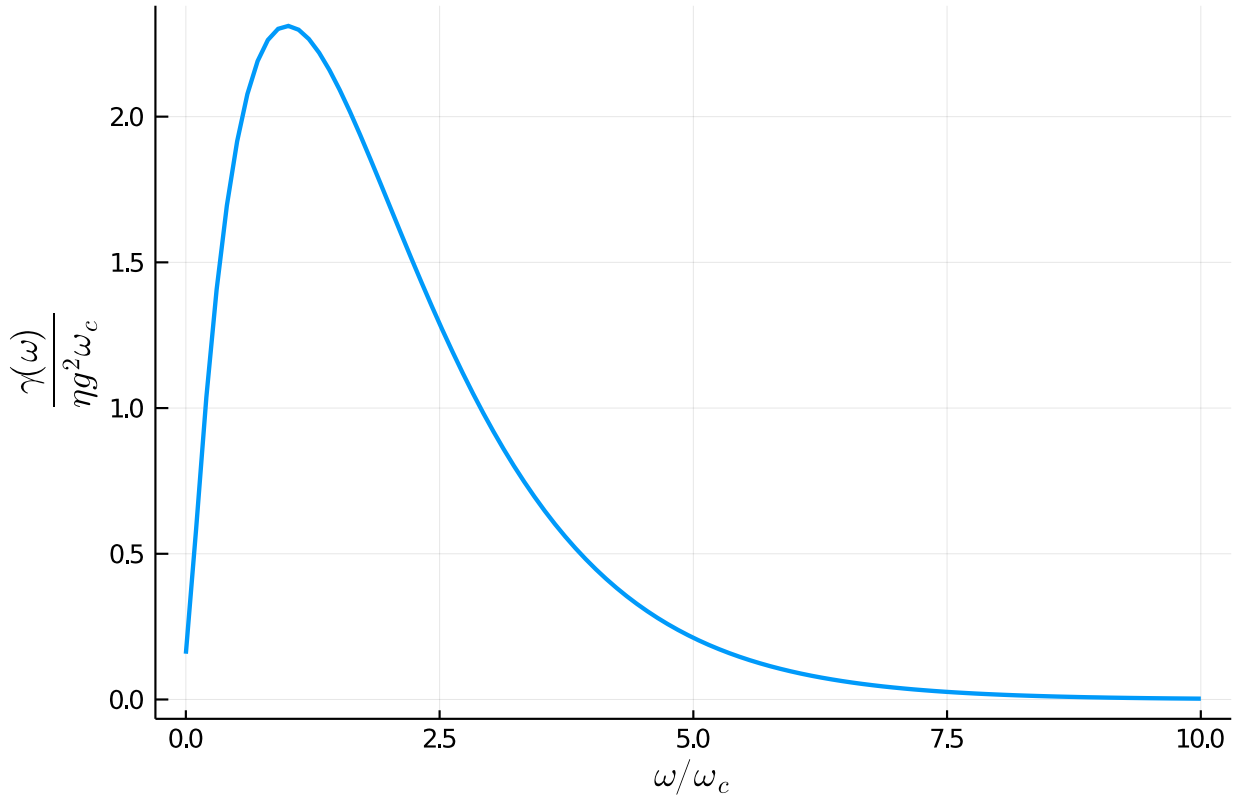
```
 $\beta$  = 4  
T =  $\beta\_2\_temperature(\beta)$   
 $\eta$  = 0.1  
fc= 10/(2 $\pi$ )  
bath = Ohmic( $\eta$ , fc, T)
```

Ohmic bath instance:

```
 $\eta$  (unitless): 0.1  
 $\omega_c$  (GHz): 1.5915494309189535  
T (mK): 1.9095587777458247
```

The spectrum γ is plotted below:

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



and the properties of the bath are

```
τsb, err_τsb = τ_SB((x)->correlation(x, bath))
@printf("τ_sb of the Ohmic bath is %.6f with error estimation %.2e \n", τsb, err_τsb)
```

```
τ_sb of the Ohmic bath is 0.666454 with error estimation 6.48e-09
```

```
τb, err_τb = τ_B((x)->correlation(x, bath), 100, τsb)
@printf("τ_b of the Ohmic bath is %.6f with error estimation %.2e \n", τb, err_τb)
```

```
τ_b of the Ohmic bath is 0.201395 with error estimation 1.91e-10
```

0.2 Annealing

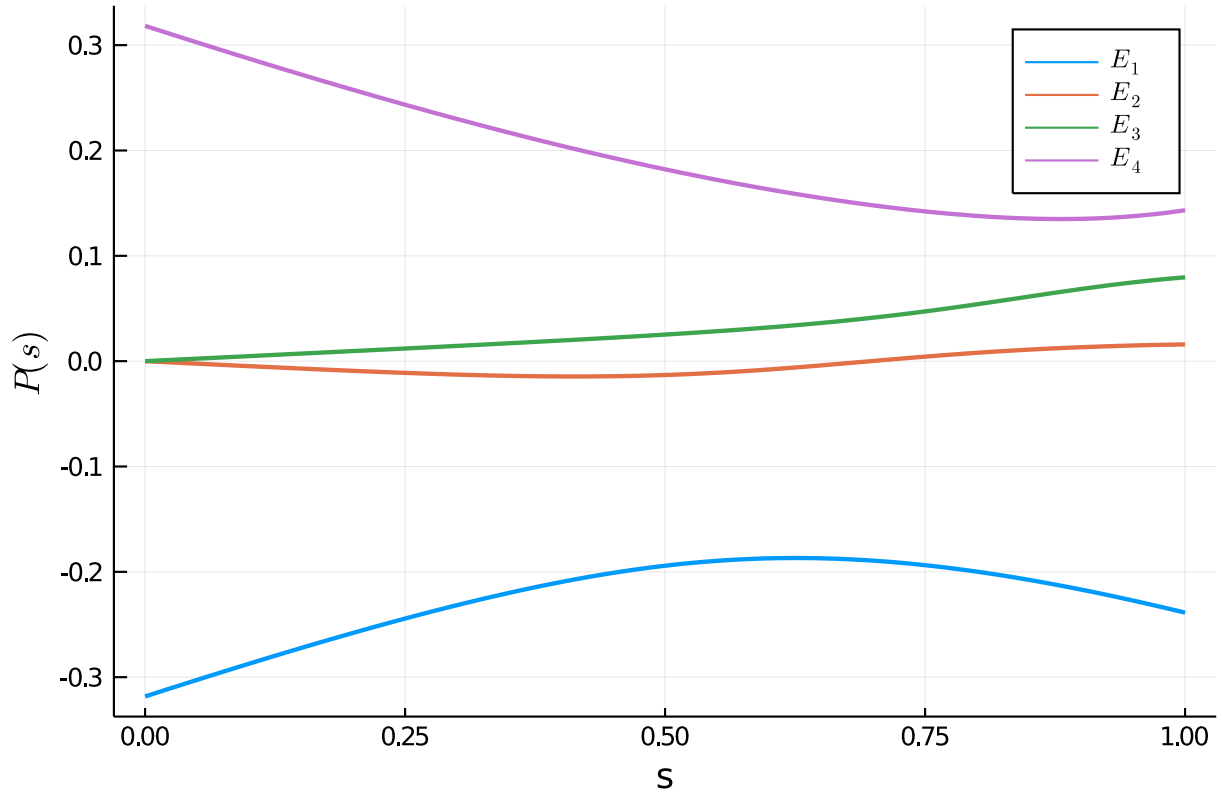
We define the annealing process as

```
Hp = 0.5*σz⊗σi - 0.7*σi⊗σz + 0.3*σz⊗σz
Hd = standard_driver(2)
H = DenseHamiltonian([(s)->1-s, (s)->s], [-Hd, Hp], unit=:ħ)
```

```
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)")
```



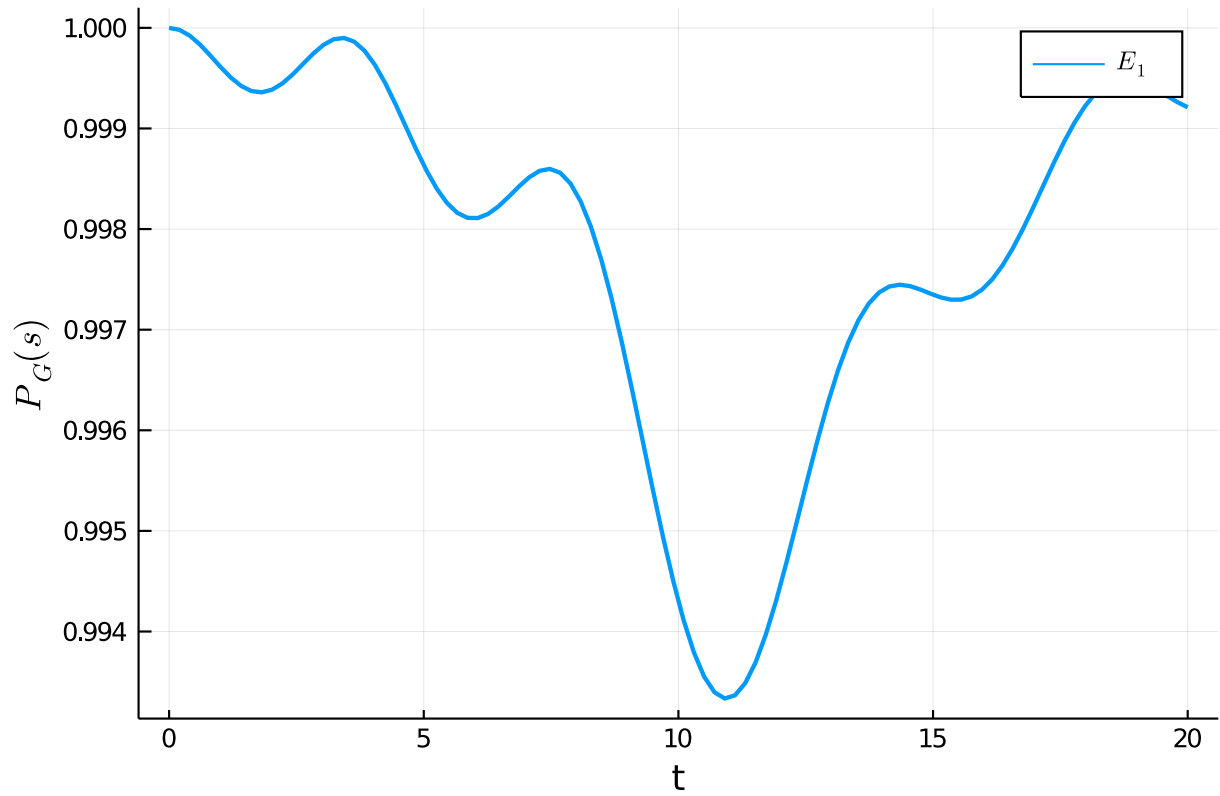
0.2.1 Closed system

We now run 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);
```

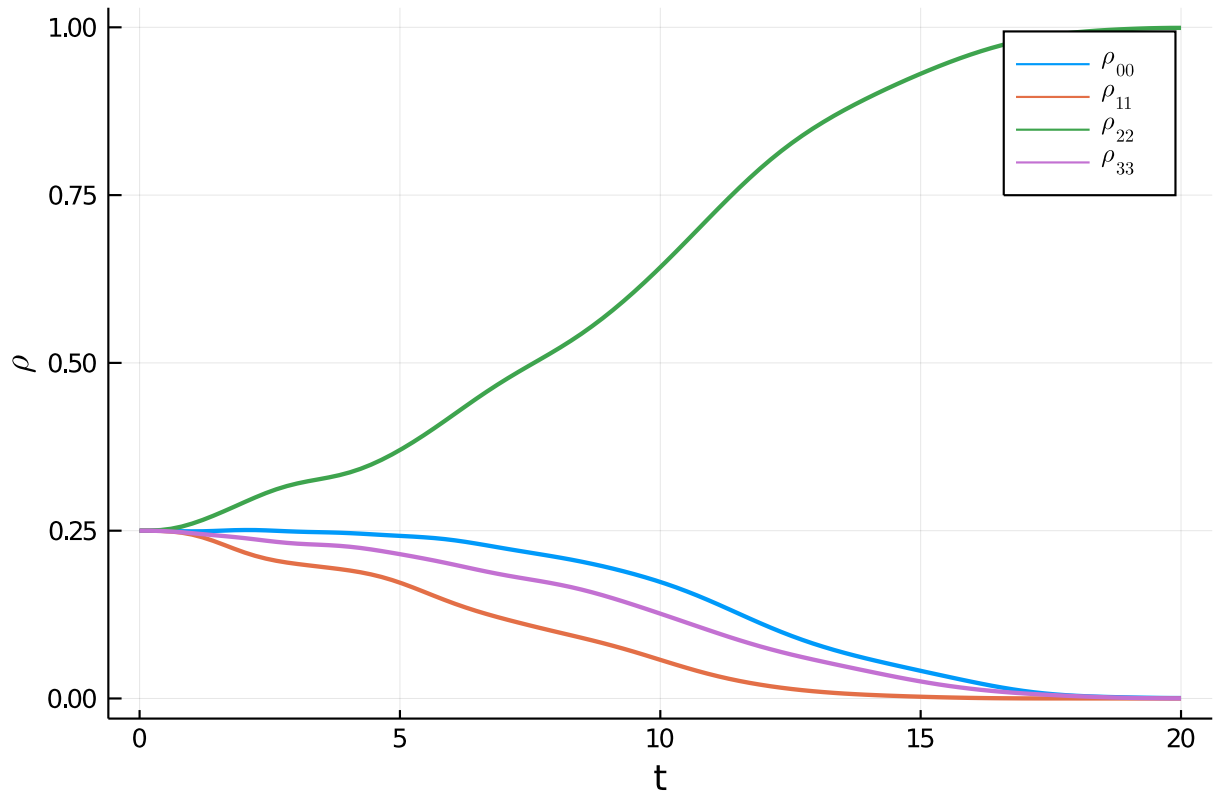
The population of instantaneous ground state is:

```
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")
```



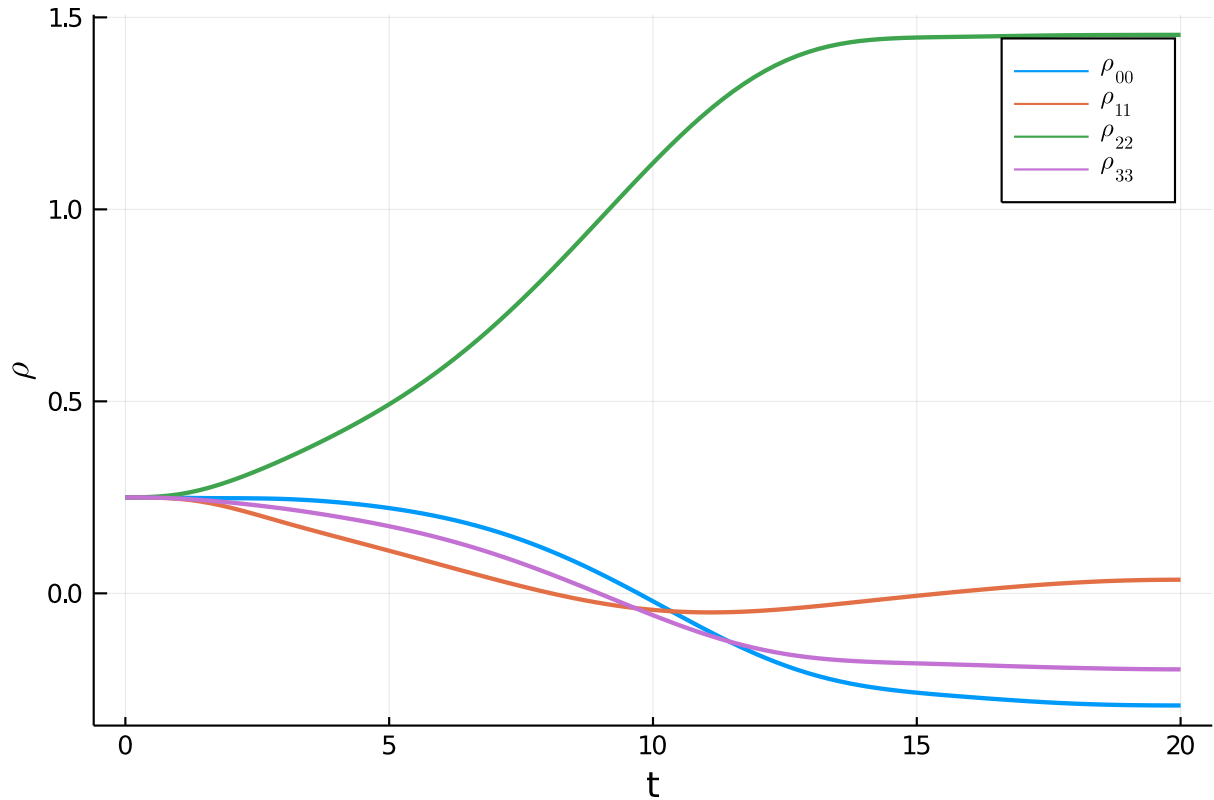
0.2.2 Redfield equation

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 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 the evolution.

0.2.3 Positivity check

We can add a callback to stop the ODE solver when the density matrix become 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
 ⋮
 1.6713448602411505
 1.8638813298254504
 2.0645751797094887
 2.274212968610653
 2.4922159175945793
 2.7193240163467145
 2.9544081226732986
 3.19854539102924
```

```

3.4527816734933183
u: 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 + 4.99999901825347e-11im 0
 .2499999499008645 - 9.999997925042628e-11im 0.2499989980172238 + 2.4999989
 876830957e-11im; 0.2499999499008545 - 4.99999901825347e-11im 0.24999999999
 995 + 0.0im 0.2499989980173237 - 1.4999993939261605e-10im 0.24999994990085
 284 - 2.499999525814185e-11im; 0.2499999499008645 + 9.999997925042628e-11im
 0.2499989980173237 + 1.4999993939261605e-10im 0.2500000000000015 + 0.0im 0
 .24999994990086283 + 1.2499997419002007e-10im; 0.2499989980172238 - 2.4999
 989876830957e-11im 0.24999994990085284 + 2.499999525814185e-11im 0.24999994
 990086283 - 1.2499997419002007e-10im 0.24999999999999334 + 0.0im]
 [0.24999999999556358 + 0.0im 0.24999393848502027 + 6.049856360704342e-9im
 0.24999393849832896 - 1.2099696252661033e-8im 0.2499878771214445 + 3.024852
 0933565355e-9im; 0.24999393848502027 - 6.049856360704342e-9im 0.24999999999
 334538 + 0.0im 0.24998787713475293 - 1.814911255928721e-8im 0.2499939384828
 0216 - 3.0249309249106878e-9im; 0.24999393849832896 + 1.2099696252661033e-8
 im 0.24998787713475293 + 1.814911255928721e-8im 0.25000000001996386 + 0.0im
 0.24999393849611065 + 1.512462168836352e-8im; 0.2499878771214445 - 3.02485
 20933565355e-9im 0.24999393848280216 + 3.0249309249106878e-9im 0.2499939384
 9611065 - 1.512462168836352e-8im 0.24999999999112718 + 0.0im]
 [0.24999999837975584 + 0.0im 0.24969132975142425 + 3.0895766607105096e-7im
 0.2496913346058523 - 6.178723540238896e-7im 0.24938304222425808 + 1.542809
 4688492337e-7im; 0.24969132975142425 - 3.0895766607105096e-7im 0.2499999975
 694084 + 0.0im 0.2493830470804095 - 9.256856939283221e-7im 0.24969132894240
 068 - 1.5448599665740338e-7im; 0.2496913346058523 + 6.178723540238896e-7im
 0.2493830470804095 + 9.256856939283221e-7im 0.25000000729141414 + 0.0im 0.2
 4969133379625535 + 7.723440234396483e-7im; 0.24938304222425808 - 1.54280946
 88492337e-7im 0.24969132894240068 + 1.5448599665740338e-7im 0.2496913337962
 5535 - 7.723440234396483e-7im 0.2499999675942158 + 0.0im]
 [0.24999998388874467 + 0.0im 0.24859060513778264 + 1.4255873379703545e-6im
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 9842388839e-7im; 0.24859060513778264 - 1.4255873379703545e-6im 0.2499999758
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 0.24718921975769031 + 4.251738485629021e-6im 0.25000007251518047 + 0.0im 0
 .24859064517772647 + 3.5628965225007135e-6im; 0.24718917159160642 - 7.08622
 9842388839e-7im 0.2485905971285693 + 7.129468101143465e-7im 0.2485906451777
 2647 - 3.5628965225007135e-6im 0.24999996777333777 + 0.0im]
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 0.24668636730601845 - 6.823685348711051e-6im 0.24341636107441625 + 1.683745
 5457302144e-6im; 0.24668618944470977 - 3.4144978004254665e-6im 0.2499999098
 015226 + 0.0im 0.24341653992297976 - 1.0102478474115962e-5im 0.246686159807
 07753 - 1.708134188979452e-6im; 0.24668636730601845 + 6.823685348711051e-6i
 m 0.24341653992297976 + 1.0102478474115962e-5im 0.2500002704460534 + 0.0im
 0.2466863375975447 + 8.530048959419607e-6im; 0.24341636107441625 - 1.683745
 5457302144e-6im 0.24668615980707753 + 1.708134188979452e-6im 0.246686337597
 5447 - 8.530048959419607e-6im 0.24999987982250327 + 0.0im]
 [0.2499998306336825 + 0.0im 0.243626702032026 + 6.7717475882394504e-6im 0.
 24362719751451523 - 1.3522344561290953e-5im 0.2374160316205387 + 3.29612151
 6099427e-6im; 0.243626702032026 - 6.7717475882394504e-6im 0.249999745422224
 7 + 0.0im 0.2374165326436156 - 1.977675834392792e-5im 0.2436266194752317 -
 3.38940027970478e-6im; 0.24362719751451523 + 1.3522344561290953e-5im 0.2374
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 -6im 0.2436266194752317 + 3.38940027970478e-6im 0.24362711467578574 - 1.690
 469186394774e-5im 0.24999966105608704 + 0.0im]

```

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 $947735 - 5.826552822403158e-6im; \ 0.23951748667756634 + 2.3200383422371203e-$
 $5im \ 0.22947382960870774 + 3.3371747944010006e-5im \ 0.2500017406599985 + 0.0i$
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 $7015 - 1.4215659016653364e-5im; \ 0.22780134092906937 + 5.6205029867506846e-5$
 $im \ 0.20757154511921982 + 7.700079551639064e-5im \ 0.2500068608887103 + 0.0im$
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 97 + 0.0im 0.2372991674457979 - 0.028350796281651484im 0.1982007754785463 -
 0.009376947663321845im; 0.28494348694607957 + 0.015996143250113268im 0.237
 2991674457979 + 0.028350796281651484im 0.3460268587439749 + 0.0im 0.2708999
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 020758921591130946im 0.21690594616018874 + 0.0im]
 [0.2429052406629345 + 0.0im 0.19861358798823284 + 0.01327397369931864im 0.
 29790191810671135 - 0.01808286738386583im 0.22557911333857417 + 0.003815779
 6038409166im; 0.19861358798823284 - 0.01327397369931864im 0.167534670904856
 35 + 0.0im 0.2375026103925509 - 0.029826691438890867im 0.184845035298351 -
 0.00937795208934614im; 0.29790191810671135 + 0.01808286738386583im 0.237502
 6103925509 + 0.029826691438890867im 0.3776671806178616 + 0.0im 0.2795334438
 51181 + 0.021656108687892774im; 0.22557911333857417 - 0.0038157796038409166
 im 0.184845035298351 + 0.00937795208934614im 0.279533443851181 - 0.02165610
 8687892774im 0.21189290781434758 + 0.0im]