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PH413 / k_cnot.py

```
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1 contributor
```

```
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                                                                                                                          Raw
                 History
840 lines (713 sloc) 24.1 KB
      # # Optimization of a State-to-State Transfer in a Two-Level-System
     from krotov.shapes import flattop
     # from krotov import Objective
     from krotov import optimize_pulses, gate_objectives
 5
     from krotov.propagators import expm
 6
     # from krotov.functionals import chis_re
     from krotov.info_hooks import print_table
     from krotov.convergence import check_monotonic_error, Or, value_below
 8
 9
     # from krotov.functionals import J_T_re
 10
     from krotov.functionals import chis_ss
     from krotov.functionals import J_T_ss
     from krotov.structural_conversions import pulse_onto_tlist
 14
     # from qutip.control import grape_unitary,
     from qutip.control import plot_grape_control_fields
 16
     from qutip.control import grape_unitary_adaptive
      from qutip.ui.progressbar import TextProgressBar
 18
      # from cw import crude_writer
      from qutip.operators import sigmax, sigmaz
      from qutip.operators import sigmay, identity
      from qutip.qip.gates import cnot
      from qutip.tensor import tensor
 24
     from qutip.states import basis
     from qutip import ket, ket2dm
     from numpy import linspace, array
      # from numpy import zeros
     from numpy import pi
 29
     from numpy import savez
     # from math import sqrt
     from os import getcwd, mkdir, chdir
     # from sys import stdout
      from mcf import plot_compare
      from numpy.random import random_sample
      from tej_plotter import tej_plotter
 36
      from cf2u import cf2u
      from matplotlib import use
     from matplotlib.pyplot import figure, axes
 39
     from matplotlib.pyplot import subplots
 40
     from matplotlib import rcParams
 41
      from matplotlib.pyplot import style
```

```
from matplotlib.pyplot import cla, close
43
44
      use("TkAgg")
      pgf_with_rc_fonts = {"pgf.texsystem": "pdflatex"}
46
      rcParams.update(pgf_with_rc_fonts)
      style.use('seaborn-whitegrid')
47
48
49
     print("Please input a run_no ")
     print("Only integers allowed")
     run_no = int(input())
      run_dir_name = 'autorun' + str(run_no)
     mkdir(run_dir_name)
54
     chdir(run_dir_name)
55
     print("Current directory")
     print(getcwd())
     f = open('workfile.txt', 'w')
      # This first example illustrates the basic use of the `krotov`
      # package by solving
     # a simple canonical optimization problem: the transfer of
     # population in a two
     # level system.
63
64
     # ## Two-level-Hamiltonian
     # We consider the Hamiltonian \phi\{H\}_{0} = - \frac{\Delta}{2}
67
     # \op{\sigma}_{z}$, representing
     # a simple qubit with energy level splitting $\omega$ in the basis
     #  {\ket{0},\ket{1}\}$. The control field $\epsilon(t)$ is assumed to
     # couple via
71
     # the Hamiltonian \operatorname{H}_{1}(t) = \operatorname{Con}(t) \operatorname{Sigma}_{x}\ to the
      # i.e., the control field effectively drives transitions between both
 74
     # qubit states.
76
     # In[20]:
     T = 1 # 1 # 5
78
     tlist = linspace(0, T, 500)
     # T = 1
     # tlist = linspace(0, T, 100)
     def hamiltonian(omega=1.0, ampl0=0.2):
84
          """Two-level-system Hamiltonian
85
          Aras:
              omega (float): energy separation of the qubit levels
             ampl0 (float): constant amplitude of the driving field
89
91
          H_ops = [tensor(sigmax(), identity(2)),
92
                   tensor(sigmay(), identity(2)),
                   tensor(sigmaz(), identity(2)),
                   tensor(identity(2), sigmax()),
                   tensor(identity(2), sigmay()),
96
                   tensor(identity(2), sigmaz()),
                   tensor(sigmax(), sigmax()) +
98
                   tensor(sigmay(), sigmay()) +
                   tensor(sigmaz(), sigmaz())]
          H0 = 0 * pi * (tensor(sigmax(), identity(2)) + tensor(identity(2),
          \# H0 = -0.5 * omega * sigmaz()
          # H0 = 1 * pi * sigmaz()
106
          # H1 = sigmax()
          def guess_control(t, args):
              return ampl0 * flattop(
                  t, t_start=0, t_stop=T, t_rise=0.3*T/5, func="sinsq"
```

```
)
          H_qutip_list = [H0]
114
         for h in H_ops:
             H_qutip_list.append([h, guess_control])
         # [H0, [H1, guess_control]]
         return H_qutip_list
     # H = hamiltonian(ampl0=2 * pi) # pass no change
123
     # H = hamiltonian() # fail
     # H = hamiltonian(ampl0=1.0) # fail
124
     # H = hamiltonian(ampl0=2.0) # fail
     H = hamiltonian(ampl0=3.0)
128
     U = cnot()
     \# U = sigmax()
130
     # The control field here switches on from zero at $t=0$
     # to it's maximum amplitude
     # 0.2 within the time period 0.3 (the switch-on shape
     # is half the first period of
134
     # a $\sin^2$ function). It switches off again in the time period 0.3
     # before the
     # final time $T=5$). We use a time grid with 500 time steps between 0
     # and $T$:
138
     def plot_pulse(pulse, tlist, result_string='r', rounding_limit=5):
141
          plot of the pulse
142
          Inputs:
146
          rounding_limit : int
                           The no of digits to which the file no should be
                           fixed to. Default is 5
          111
          # the random number
154
         t_r_no = str(round(random_sample(), rounding_limit))
          gp_fig = figure()
          gp_ax = axes()
          # gp_fig, gp_ax = subplots()
         if callable(pulse):
159
             pulse = array([pulse(t, args=None) for t in tlist])
          gp_ax.plot(tlist, pulse)
          gp_ax.set_xlabel('time')
          gp_ax.set_ylabel('pulse amplitude')
          gp_ax.set(title='Plot of ' + result_string + 'pulse')
164
         fig_rand_name = result_string + 'pulse' + t_r_no + '.pdf'
          # Could also use date time
166
          # fig_path_name = path + fig_name
          gp_fig.savefig(fig_rand_name)
         cla()
         close(gp_fig)
         # plt.show(fig)
          return gp_fig, gp_ax
174
175
     gp_fig, gp_ax = plot_pulse(H[1][1], tlist, result_string='guess')
     # ## Optimization target
178
```

```
# The `krotov` package requires the goal of the optimization to be
181
     # list of `Objective` instances. In this example, there is only a single
     # objective: the state-to-state transfer from initial state
184
     # $\ket{\Psi_{\init}} =
     # \ket{0}$ to the target state \ket{Psi_{tgt}} = \ket{1}$,
     # under the dynamics
     # of the Hamiltonian \infty\{H\}(t):
189
191
     objectives = [
         Objective(
             initial_state=ket("0"), target=ket("1"), H=H
     ]
     2qubit_basis_states = [tensor(ket("0"), ket("0")),
                            tensor(ket("0"), ket("1")),
199
                             tensor(ket("1"), ket("0")),
                            tensor(ket("1"), ket("1")), ]
     objectives = gate_objectives(
         basis_states=2qubit_basis_states,
         gate=U,
         H=H
         )
     print("objectives[0]\n", objectives[0])
     print("objectives[1]\n", objectives[1])
209
     # print("objectives[2]\n", objectives[2])
210
     print("objectives\n", objectives, file=f)
214
     # In addition, we would like to maintain the property of the control
     # field to be
     \# zero at t=0 and t=T, with a smooth switch-on and switch-off.
     # We can define
     # an "update shape" $S(t) \in [0, 1]$ for this purpose: Krotov's method
219
     # will
220
     # update the field at each point in time proportionally to $S(t)$;
     # $S(t)$ is zero, the optimization will not change the value of the
     # control from
224
     # the original guess.
     def S(t):
         """Shape function for the field update"""
228
         return flattop(
             t, t_start=0, t_stop=T, t_rise=(0.3*T)/5,
             t_fall=(0.3*T)/5, func='sinsq'
         )
234
     # Beyond the shape, Krotov's method uses a parameter $\lambda_a$
     # for each control
     # field that determines the overall magnitude of the respective field
     # in each
238
     # iteration (the smaller $\lambda_a$, the larger the update;
239
     # specifically, the
     # update is proportional to \frac{S(t)}{\lambda_a}. Both the
241
     \# S(t) and the \lambda a parameter must be passed to the
243
     # optimization routine
     # as "pulse options":
244
245
```

```
247
     pulse_options = {
         H[1][1]: dict(lambda_a=5, shape=S)
249
250
     pulse_options = {
       H[1][1]: dict(lambda_a=5, update_shape=S)
     }
254
     pulse_options = {
         H[i][1]: dict(lambda_a=5, update_shape=S)
         for i in range(1, len(H_{ops}) + 1, 1)
259
     }
     # ## Simulate dynamics under the guess field
263
264
     # Before running the optimization procedure, we first simulate the
     # dynamics under the
     # guess field \epsilon_{0}(t). The following solves equation
     # of motion for the
268
     # defined objective, which contains the initial state
     # $\ket{\Psi_{\init}}$ and
270
     # the Hamiltonian \phi(t) defining its evolution.
     # This delegates to QuTiP's
     # usual `mesolve` function.
274
     # We use the projectors \sup\{P\}_0 = \left\{0\right\}
275
     # and \sigma\{P\}_1 = \left\{1\right\} for calculating the population:
     proj0 = ket2dm((basis(4, 0)))
     proj1 = ket2dm(U*(basis(4, 0)))
281
     proj0 = ket2dm((basis(2, 0) + basis(2, 1))/(1/sqrt(2)))
     proj1 = ket2dm((basis(2, 0) - basis(2, 1))/(1/sqrt(2)))
284
     proj0 = ket2dm(basis(2, 0) + 1j*basis(2, 1))
     proj1 = ket2dm(basis(2, 0) - 1j*basis(2, 1))
     Python 3.7.4 (default, Aug 13 2019, 20:35:49)
288
     [GCC 7.3.0] :: Anaconda, Inc. on linux
289
     Type "help", "copyright", "credits" or "license" for more information.
     >>> import qutip
     >>> basis(0, 2)
     Traceback (most recent call last):
       File "<stdin>", line 1, in <module>
294
     NameError: name 'basis' is not defined
295
     >>> from qutip.operators import basis
296
     Traceback (most recent call last):
       File "<stdin>", line 1, in <module>
     ImportError: cannot import name 'basis' from 'qutip.operators'
      (/home/tejas/anaconda3/envs/krotov/lib/python3.7/site-packages/qutip/
     operators.pv)
     >>> doc
     Traceback (most recent call last):
       File "<stdin>", line 1, in <module>
304
     NameError: name 'doc' is not defined
     >>> doc(qutip)
306
     Traceback (most recent call last):
       File "<stdin>", line 1, in <module>
     NameError: name 'doc' is not defined
     >>> from qutip.states import basis
     >>> basis(0, 2)
     Traceback (most recent call last):
       File "<stdin>", line 1, in <module>
       File
314
        "/home/tejas/anaconda3/envs/krotov/lib/python3.7/site-packages/qutip/
```

```
states.py", line 105, in basis
         raise ValueError("basis vector index need to be in n <= N-1")</pre>
      ValueError: basis vector index need to be in n \le N-1
318
      >>> basis(2, 0)
      Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
      Qobj data =
     [[1.]
      [0.]]
      >>> basis(2, 0) + 1j*basis(2, 1)
      Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
      Qobj data =
     [[1.+0.j]
      [0.+1.j]]
328
     >>> from qutip.operators import sigmay
329
      >>> sigmay()*(basis(2, 0) + 1j*basis(2, 1))
     Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
      Qobj data =
     [[1.+0.j]
      [0.+1.j]]
     >>>
     proj0 = ket2dm(ket("0"))
      proj1 = ket2dm(ket("1"))
339
340
     Python 3.7.4 (default, Aug 13 2019, 20:35:49)
342
     [GCC 7.3.0] :: Anaconda, Inc. on linux
     Type "help", "copyright", "credits" or "license" for more information.
344
     >>> import qutip
     >>> proj0 = qutip.ket2dm(qutip.ket("0"))
346
347
     Traceback (most recent call last):
       File "<stdin>", line 1, in <module>
     NameError: name 'pr' is not defined
350
      >>> proj0
      Quantum object: dims = [[2], [2]], shape = (2, 2), type = oper, isherm = True
      Qobj data =
      [[1. 0.]
354
      [0. 0.]]
      >>> qutip.ket("0")
      Quantum object: dims = [[2], [1]], shape = (2, 1), type = ket
      Qobj data =
     [[1.]
      [0.]]
      guess_dynamics = objectives[0].mesolve(tlist, e_ops=[proj0, proj1])
364
      # The plot of the population dynamics shows that the guess field
      # does not transfer
      # the initial state \left\{ \right\} = \left\{ 0\right\}  to the desired
      # target state
      # \star \{\P \} = \left\{1\right\}
      \# (so the optimization will have something to do).
      def plot_population(result, result_string='r', rounding_limit=5):
         '''plot of the population dynamics
         Inputs:
         result
378
          result_string : str
379
                           The thing whose population dynamics is
                           being plotted
```

```
rounding_limit : int
                           The no of digits to which the file no should be
                           fixed to. Default is 5
          1.1.1
         # the random number
          t_r_no = str(round(random_sample(), rounding_limit))
          # fig, ax = plt.subplots()
         pop_fig = figure()
         pop ax = axes()
         pop_ax.plot(result.times, result.expect[0], label='0')
          pop_ax.plot(result.times, result.expect[1], label='1')
         pop_ax.legend()
         pop_ax.set_xlabel('time')
         pop_ax.set_ylabel('population')
          pop_ax.set(title='Plot of population dynamics: ' + result_string)
         pop_fig_rand_name = 'popula dynamics ' + result_string + t_r_no + '.pdf'
         # Could also use date time
401
         # fig_path_name = path + fig_name
         pop_fig.savefig(pop_fig_rand_name)
         cla()
405
         close(pop_fig)
         # plt.show(fig)
         return None
409
         # plt.show(fig)
410
411
412
     # In[31]:
413
414
     plot_population(guess_dynamics, result_string='guess')
416
417
     # ## Optimize
418
     # In the following we optimize the guess field \epsilon_{0}(t) such
421
     # that the intended state-to-state transfer
     # $\ket{\Psi_{\init}} \rightarrow
422
423
     # \ket{\Psi_{\tgt}}$ is solved, via the `krotov` package's central
     # `optimize_pulses` routine. It requires, besides the previously
424
     # defined
     # `objectives`, information about the optimization functional
427
     # $J_T$ (implicitly,
428
     # via `chi_constructor`, which calculates the states $\ket{\chi} =
429
     # \frac{J_T}{\bra{\Psi}}$).
431
     # Here, we choose J_T = J_{T, \text{re}} = 1 - F_{\text{re}}
432
     # with $F_{\text{re}}
433
     \# = \Re\{\Pr\{\Pr(T)\}{\footnote{T}}\, with \Re\{\Pr(T)\}\ the forward
     # propagated state of \star \ is not
434
435
     # explicitly
436
     # required for the optimization, it is nonetheless useful to be able
437
     # to calculate
438
     # and print it as a way to provide some feedback about the optimization
439
     # progress.
     # Here, we pass as an `info_hook` the function
440
441
     # `krotov.info_hooks.print_table`,
442
     # using `krotov.functionals.J_T_re` (which implements the above
443
     # functional; the
444
     # `krotov` library contains implementations of all the "standard"
445
     # functionals used in
446
     # quantum control). This `info_hook` prints a tabular overview after
447
448
     # iteration, containing the value of $J_T$,
     # the magnitude of the integrated pulse
```

```
450
      \# update, and information on how much J_T (and the full Krotov
451
      # functional $J$)
452
      \# changes between iterations. It also stores the value of J_T
453
      # internally in the
454
      # `Result.info_vals` attribute.
455
456
     # The value of $J_T$ can also be used to check the convergence.
457
     # In this example.
458
     # we limit the number of total iterations to 10, but more generally,
459
      # we could use
460
     # the `check_convergence` parameter to stop the optimization
     # when $J_T$ falls below
461
462
     # some threshold. Here, we only pass a function that checks that
463
     # the value of
464
     # $J T$ is monotonically decreasing. The
      # `krotov.convergence.check_monotonic_error` relies on
465
466
      # `krotov.info_hooks.print_table` internally having stored the value
467
      # of $J_T$ to
      # the `Result.info_vals` in each iteration.
470
      # In[32]:
471
472
473
474
      oct_result = optimize_pulses(
475
          objectives,
476
          pulse_options=pulse_options,
477
          tlist=tlist,
478
          propagator=expm,
479
          chi_constructor=chis_re,
480
          info_hook=print_table(J_T=J_T_re, out=f),
481
          check_convergence=check_monotonic_error,
482
          iter_stop=20,
      )
484
485
      opt_result = optimize_pulses(
          objectives,
          pulse_options=pulse_options,
488
          tlist=tlist,
489
          propagator=expm,
          chi_constructor=chis_ss,
491
          info_hook=print_table(J_T=J_T_ss, out=f),
492
          check_convergence=0r(
493
              value_below('1e-3', name='J_T'),
              check_monotonic_error,
495
          ),
496
          store_all_pulses=True,
      )
      111
499
      opt_result = optimize_pulses(
          objectives,
          pulse_options=pulse_options,
          tlist=tlist,
          propagator=expm,
          chi_constructor=chis_ss,
506
          info_hook=print_table(J_T=J_T_ss, ),
          check convergence=Or(
              value_below('1e-3', name='J_T'),
              check_monotonic_error,
          ),
          store_all_pulses=True,
512
514
      # In[33]:
```

```
print("opt_result\n", opt_result)
     # print
     print("opt_result\n", opt_result, file=f)
     # ## Simulate the dynamics under the optimized field
     # Having obtained the optimized control field, we can now plot it and
     # calculate the population dynamics under this field.
524
     # In[34]:
     opt_pulse_index = 0
     for pulse in opt_result.optimized_controls:
529
          plot_pulse(pulse, tlist,
                    result_string='opt' + str(opt_pulse_index))
          opt_pulse_index = opt_pulse_index + 1
     # print("\n opt_result.optimized_controls[0]",
534
           opt_result.optimized_controls[0], file=f)
     # print("type of opt_result.optimized_controls[0]",
             type(opt_result.optimized_controls[0]))
     # In contrast to the dynamics under the guess field,
     # the optimized field indeed
     # drives the initial state $\ket{\Psi_{\init}} = \ket{0}$
     # to the desired target
     # state $\ket{\Psi_{\tgt}} = \ket{1}$.
     # In[35]:
     opt_dynamics = opt_result.optimized_objectives[0].mesolve(
          tlist, e_ops=[proj0, proj1])
     # In[36]:
     for i in range(len()):
     plot_population(opt_dynamics,
                      result_string=' optimized control')
558
     To gain some intuition on how the controls and the dynamics
     change throughout the optimization procedure,
     we can generate a plot of the control fields and the dynamics
     after each iteration of the optimization algorithm.
     This is possible because we set `store_all_pulses=True`
564
     in the call to `optimize_pulses`,
566
     which allows to recover the optimized controls from each
     iteration from `Result.all_pulses`.
     The flag is not set to True by default,
     as for long-running optimizations with thousands or
570
     tens of thousands iterations,
     the storage of all control fields may require significant memory.
574
     def plot_iterations(opt_result):
576
          """Plot the control fields in population dynamics over all iterations.
          This depends on ``store_all_pulses=True`` in the call to
579
          `optimize_pulses`.
          0.00
          it_fig, [ax_ctr, ax_dyn] = subplots(nrows=2, figsize=(8, 10))
          n_iters = len(opt_result.iters)
          for (iteration, pulses) in zip(opt_result.iters, opt_result.all_pulses):
              controls = [
```

```
pulse_onto_tlist(pulse)
                  for pulse in pulses
587
              objectives = opt_result.objectives_with_controls(controls)
              dynamics = objectives[0].mesolve(
                  opt_result.tlist, e_ops=[proj0, proj1]
              )
              if iteration == 0:
                  ls = '--' # dashed
                  alpha = 1 # full opacity
                  ctr_label = 'guess'
                  pop_labels = ['0 (guess)', '1 (guess)']
597
              elif iteration == opt_result.iters[-1]:
                 ls = '-' # solid
                  alpha = 1 # full opacity
                  ctr_label = 'optimized'
                  pop_labels = ['0 (optimized)', '1 (optimized)']
              else:
                  ls = '-' # solid
                  alpha = 0.5 * float(iteration) / float(n_iters) # max 50%
605
                  ctr_label = None
                  pop_labels = [None, None]
              ax_ctr.plot(
                  dynamics.times,
                  controls[0],
                  label=ctr_label,
                  color='black',
612
                  ls=ls,
                  alpha=alpha,
              )
615
              ax_dyn.plot(
616
                  dynamics.times,
                  dynamics.expect[0],
                  label=pop_labels[0],
                  color='#1f77b4', # default blue
                  ls=ls,
                  alpha=alpha,
              )
              ax_dyn.plot(
                  dynamics.times,
                  dynamics.expect[1],
626
                  label=pop_labels[1],
                  color='#ff7f0e', # default orange
627
                  ls=ls,
                  alpha=alpha,
          ax_dyn.legend()
          ax_dyn.set_xlabel('time')
633
          ax_dyn.set_ylabel('population')
          ax_ctr.legend()
          ax_ctr.set_xlabel('time')
          ax_ctr.set_ylabel('control amplitude')
          # plt.show(fig)
          # ax.set(title='iterations: ')
640
          it_fig_rand_name = 'Iterations.pdf'
641
          it_fig.savefig(it_fig_rand_name)
          cla()
644
          close(it_fig)
645
647
      plot_iterations(opt_result)
648
649
     The initial guess (dashed) and final optimized (solid)
      control amplitude and resulting dynamics are shown with full opacity,
      whereas the curves corresponding intermediate iterations
```

```
are shown with decreasing transparency.
      ...
654
     Traceback (most recent call last):
       File "k5.py", line 499, in <module>
         [], tlist)
       File "/home/tejas/Dropbox/Lab computer code to run/gkrape/krotov-try/
       k5/cf2unitary.py", line 68, in cf2unitary
         for U in U_list_tej:
       File "/home/tejas/Dropbox/Lab computer code to run/gkrape/krotov-try/
       k5/cf2unitary.py", line 66, in <genexpr>
664
         for idx in range(M-1))
       File "/home/tejas/Dropbox/Lab computer code to run/gkrape/krotov-try/
       k5/cf2unitary.py", line 45, in A tej
         H = H0 + sum([ug[j, idx] * H_ops[j] for j in range(J)])
       File "/home/tejas/Dropbox/Lab computer code to run/gkrape/krotov-try/
        k5/cf2unitary.py", line 45, in <listcomp>
         H = H0 + sum([ug[j, idx] * H_ops[j] for j in range(J)])
     IndexError: too many indices for array
671
672
673
674
     >>> from numpy import array, arange
675
     >>> yahoo = arange(5)
676
     >>> yahoo
     array([0, 1, 2, 3, 4])
     >>> yar = array(yahoo)
678
679
     >>> yar
     array([0, 1, 2, 3, 4])
     >>> yar.shape()
     Traceback (most recent call last):
      File "<stdin>", line 1, in <module>
684
     TypeError: 'tuple' object is not callable
     >>> yar.shape()
     Traceback (most recent call last):
      File "<stdin>", line 1, in <module>
     TypeError: 'tuple' object is not callable
     >>> yar.shape
     (5,)
     >>> yar_list = list(yar, yar + 2)
     Traceback (most recent call last):
693
      File "<stdin>", line 1, in <module>
     TypeError: list expected at most 1 arguments, got 2
     >>> yar_list = list([^[[Cyar, yar + 2])
       File "<stdin>", line 1
         yar_list = list([ yar, yar + 2])
698
     SyntaxError: invalid syntax
     >>> yar_list = [yar, yar + 2]
     >>> yar_list
     [array([0, 1, 2, 3, 4]), array([2, 3, 4, 5, 6])]
     >>> aarr_yar_list = array(yar_list)
704
     >>> aarr_yar_list
     array([[0, 1, 2, 3, 4],
            [2, 3, 4, 5, 6]])
     >>> lonely_yar_list = [yar]
     >>> ar_lonely_yar_list = array(lonely_yar_list)
709
     >>> ar_lonely_yar_list
     array([[0, 1, 2, 3, 4]])
     >>> ar_lonely_yar_list.shape
     (1, 5)
     >>> aarr_yar_list.shape
714
     (2, 5)
716
718
     111
719
```

```
a = zeros()
     U_kopt = cf2unitary(array(array(opt_result.optimized_controls[0])),
                          H[0], [H[1][1]],
724
                          [], tlist)
     tej_plotter(U, 'U')
     tej_plotter(U_kopt, 'U_kopt')
726
     krotov_opt_controls = array([array(opt_result.optimized_controls[0]), ])
     print('krotov_opt_controls.shape', krotov_opt_controls.shape)
730
     U_kopt = cf2u(krotov_opt_controls,
                   H[0], [H[1][0]],
                    tlist)
734
736
     def _overlap(A, B):
         return (A.dag() * B).tr() / A.shape[0]
         # return cy_overlap(A.data, B.data)
741
     krotov_fid = _overlap(U, U_kopt)
     abs_kf = abs(krotov_fid)
743
     print("krotov_fid", krotov_fid)
744
     print("krotov_fid", krotov_fid, file=f)
     print('absolute value of krotov_fid', abs_kf,)
     print('absolute value of krotov_fid', abs_kf, file=f)
747
     tej_plotter(U, 'U')
748
     tej_plotter(U_kopt, 'U_kopt')
750
     savez('krotov-opt',
           krotov_field=array(opt_result.optimized_controls[0])
           )
754
     if opt_result.all_pulses:
         savez('krotov_extra',
                krotov_field_all_iter=opt_result.all_pulses)
759
     # GRAPE begins
761
     print('\n\n GRAPE begins')
     u_limits = None # [0, 1 * 2 * pi]
762
     alpha = None
     R = 600 # 150, 500
764
     # Increasing no of of iterations improves fidelity
     # H_labels = [r'$u_{1}$', ]
768
     H_labels = [r'$u_{1x}$', r'$u_{1y}$', r'$u_{1z}$',
769
                 r'$u_{2x}$', r'$u_{1y}$', r'$u_{2z}$',
770
                  r'$u_{xx}$',
                  r'$u_{yy}$',
                  r'$u_{zz}$',
774
     # eps = 2*pi, None, pi, 3*pi, 10*pi
775
     # Apparently lower the eps lower the absolute value of the fidelity.
     # this fails if we increase the value of the eps to 10*pi
776
     # Can also change to grape unitary adaptive, increase eps to 3*pi, 10*pi
     grape_result = grape_unitary_adaptive(U, H[0], [H[1][0]],
779
                                            R, tlist,
                                            u_start=krotov_opt_controls,
                                            u limits=u limits,
                                            eps=3.5*pi,
                                            alpha=alpha,
784
                                            phase_sensitive=False,
                                            progress_bar=TextProgressBar()
```

```
787
      grape_result = grape_unitary(U, H[0], [H[1][0]],
                                   R, tlist,
                                   u_start=krotov_opt_controls,
                                   u_limits=u_limits,
                                   eps=4*pi*1,
794
                                   alpha=alpha,
                                   phase_sensitive=False,
796
                                   progress_bar=TextProgressBar()
799
800
     # Plotting the control field
     gr_f_fig, gr_f_axes = plot_grape_control_fields(tlist,
                                                      grape_result.u,
803
                                                      H_labels,
804
                                                      uniform_axes=True)
807
     f_rand_name = 'f' + str(random_sample()) + '.pdf'
808
     # Could also use date time
     # fig_path_name = path + fig_name
     gr_f_fig.savefig(f_rand_name)
     cla()
812
     close(gr_f_fig)
814
     tej_plotter(grape_result.U_f, 'U_gr')
815
     savez('grape_result',
816
            resultu=grape_result.u, resultU_f=grape_result.U_f.full())
817
818
819
     U_gopt = cf2u(grape_result.u,
                    H[0], [H[1][0]],
821
                    tlist)
     111
822
     print('grape_result.shape', grape_result.u.shape)
823
824
     grape_fid = _overlap(U, grape_result.U_f)
825
     abs_gf = abs(grape_fid)
826
     print("grape_fid", grape_fid)
     print("grape_fid", grape_fid, file=f)
828
     print('absolute value of grape_fid', abs_gf)
829
     print('absolute value of grape_fid', abs_gf, file=f)
830
     # tej_plotter(U, 'U')
     # tej_plotter(U_gopt, 'U_gopt')
     # plot_compare(tlist, kcf, gcf_full, rounding_limit=5)
833
834
     plot_compare(tlist, krotov_opt_controls,
835
                   grape_result.u, rounding_limit=5)
836
837
     chdir('../')
839
     print('We are in' + getcwd())
```