Quantum Walks. Karazeev and Kiktenko

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0.1 Quantum walks and Variational algorithm

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- Based on: Quantum Software Master Class Lecturer - Jacob Biamonte TA - Timur Tlyachev email: T.Tlyachev@skoltech.ru DeepQuantum 2018 Skoltech

In [155]:
```
from IPython.display import Image
Image(filename="img1.jpg", width=600)
```

Out[155]:

2 Quantum walks and Variational algorithm

Intro

- *Quantum walk and control of 4 level system.* Let us consider the following Hamiltonian $\mathcal{H} = k + v$, where

$$
\begin{aligned}
k &= |0\rangle\langle 1| + e^{i\alpha_2}|1\rangle\langle 3| + e^{i\alpha_3}|3\rangle\langle 2| + e^{i\alpha_3}|2\rangle\langle 0| + h.c, \\
v &= |3\rangle\langle 3|
\end{aligned}
$$

  1. Plot the probability to find the system at $|0\rangle, |1\rangle, |2\rangle, |3\rangle$ as a function of time and α's.

In [156]:
```
Image(filename="img2.jpg", width=600)
```

Out[156]:

2. Minimize

$$\begin{aligned}\tilde{H} &= \min_{\boldsymbol{\gamma},\boldsymbol{\beta}} \langle \psi(\boldsymbol{\gamma},\boldsymbol{\beta})|H\psi(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle\,, \\ |\psi(\boldsymbol{\gamma},\boldsymbol{\beta})\rangle &= e^{-ik\beta_p}e^{-iv\gamma_p}\ldots e^{-ik\beta_1}e^{-iv\gamma_1}|0\rangle\end{aligned}$$

for some fixed α's. And plot $\tilde{H} - \min_\psi \langle\psi|H\psi\rangle$.

- *Quantum walk and control of 3 level system* The same for

$$\begin{aligned}k &= e^{i\alpha_1}|0\rangle\langle 1| + e^{i\alpha_2}|1\rangle\langle 2| + e^{i\alpha_3}|2\rangle\langle 1| + h.c, \\ v &= |2\rangle\langle 2|.\end{aligned}$$

1 Quantum walks and Variational algorithm

Algorithm steps:

- minimize Hamiltonian h over states for and find this $\min\langle\psi|h\psi\rangle$ where

$$|\psi\rangle = e^{-i*k*params[2p-1]}e^{-i*k*params[2p-2]}\ldots e^{-i*k*params[1]}e^{-i*k*params[0]}|\text{ini\_state}\rangle$$

- prepare state
- Realize phase estimation algorithm to find lowest energy

In [1]:
```
# import packages
import qit
import numpy as np
import scipy.linalg as la
import pandas as pd
import matplotlib
import matplotlib.pyplot as plt
from random import randint
import scipy
%matplotlib inline
```

We are looking for the ground state and ground level energy of the following Hamiltonian (4 level andom walk):

$$h = k + v,$$

where

$$k = e^{i\alpha_0}|0\rangle\langle 1| + e^{i\alpha_1}|1\rangle\langle 3| + e^{i\alpha_2}|3\rangle\langle 2| + e^{i\alpha_3}|2\rangle\langle 0| + h.c,$$

and

$$v = |3\rangle\langle 3|.$$

```
In [2]: # Define states by using qit.state. dim=4, since the system is 4 level.
        zero_state=qit.state('0',dim=4)
        one_state=qit.state('1', dim=4)
        two_state=qit.state('2', dim=4)
        three_state=qit.state('3', dim=4)


        # Function to generate Hamiltonian = k + v.
        def Hamiltonian(alpha: list):
            h = np.exp(1j*alpha[0]) * qit.lmap(np.outer(zero_state.data,one_state.data.ravel()))
                + np.exp(1j*alpha[1]) * qit.lmap(np.outer(one_state.data,three_state.data.ravel(
                + np.exp(1j*alpha[2]) * qit.lmap(np.outer(three_state.data,two_state.data.ravel(
                + np.exp(1j*alpha[3]) * qit.lmap(np.outer(two_state.data,zero_state.data.ravel()
            return h + qit.lmap.ctranspose(h) + qit.state.projector(three_state)
```

First of all we plot the probability to find the system in time t at the three_state if the system starts from zero_state. To this end we use operation

```
u_propagate(la.expm(Hamiltonian(alpha).data*1j*(-t)))
```

which returns state $|\psi(t)\rangle = e^{-iht}|0\rangle$

```
qit.fidelity(state_1,state_2)
```

returns $|\langle state_1|state_2\rangle|$.

```
In [27]: # Probability to find system in time t at the one of the states if the
         # system starts from zero_state.
         def probability(alpha: list, t):
             """
             return 4 probabilities
             """
             state = zero_state.u_propagate(la.expm(Hamiltonian(alpha).data*1j*(-t)))
             return [qit.fidelity(state, zero_state)**2,
                     qit.fidelity(state, one_state)**2,
                     qit.fidelity(state, two_state)**2,
                     qit.fidelity(state, three_state)**2]

         assert sum(probability([1,1,1,1], 1)) == 1.0
```

Use the following parameterization: $\overrightarrow{\alpha} = [\alpha_0, 2\alpha_0, 3\alpha_0, 4\alpha_0]$

```
In [10]: # Calculate probability for different alpha and t.
         alpha_x = np.linspace(0, np.pi, 100)
         time_y = np.linspace(0, 10, 500)

         X, Y = np.meshgrid(alpha_x,time_y)
         df = pd.DataFrame(data={'alpha': X.ravel(), 'time': Y.ravel()})
```

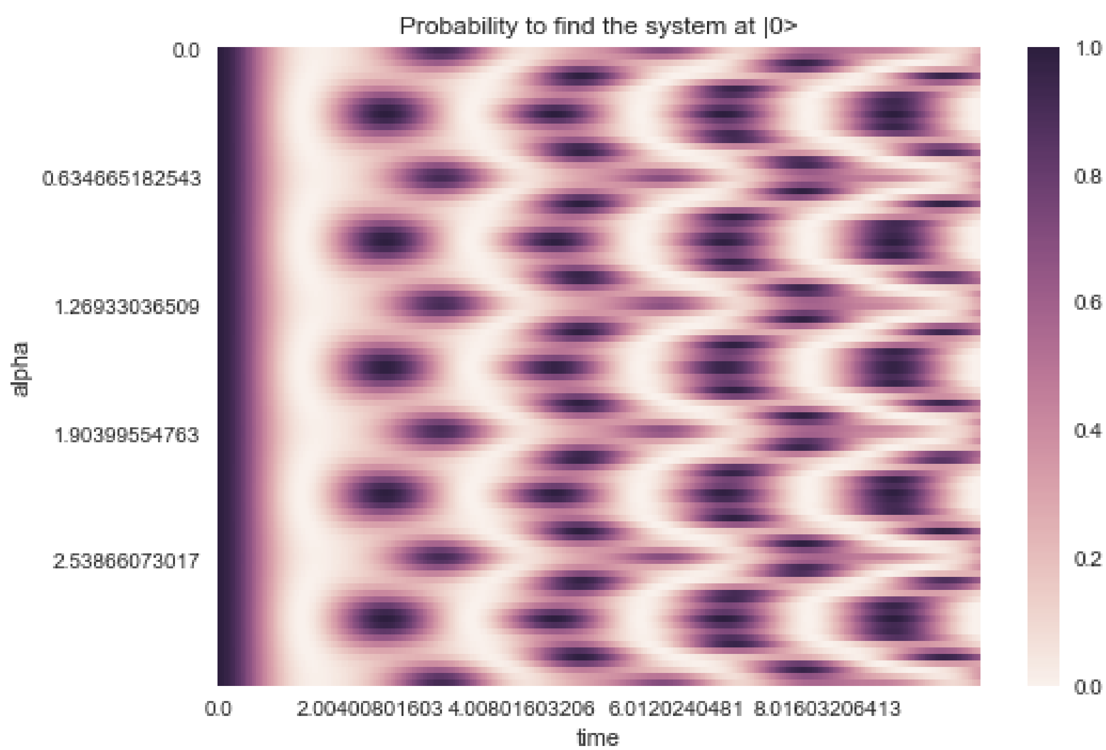
```
df['probability'] = df.apply(lambda x: probability([x.alpha, 2*x.alpha,
                                                     3*x.alpha, 4*x.alpha],
                                                    x.time), axis=1)
```

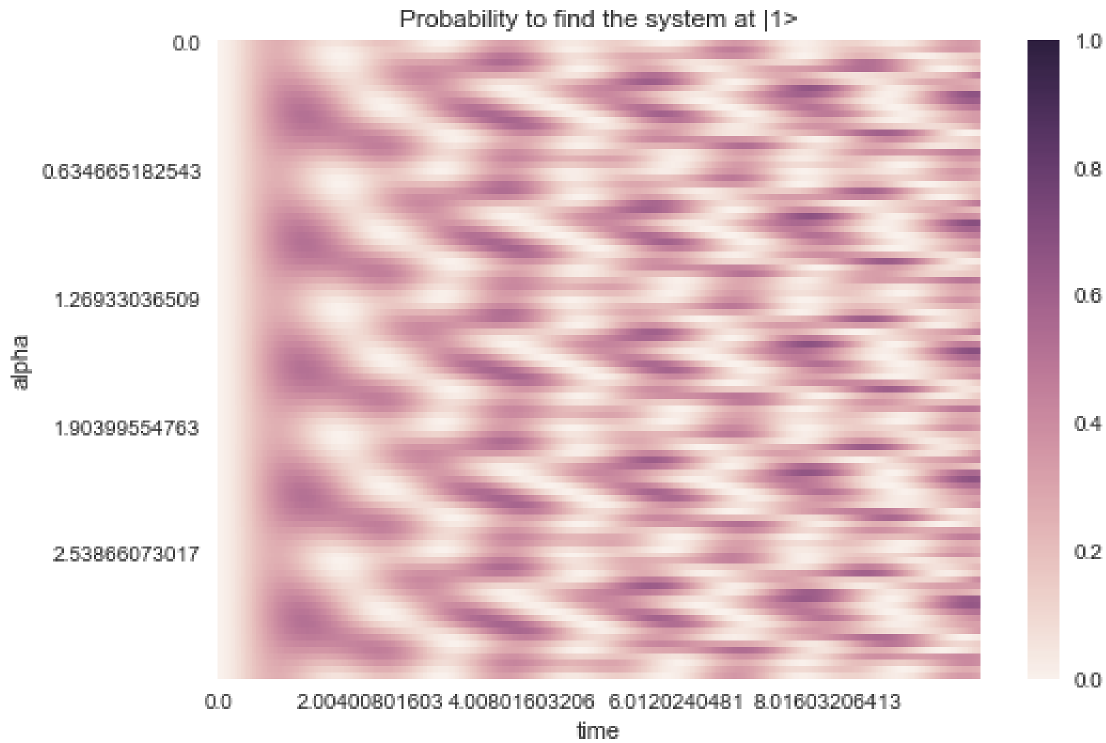
In [11]:
```
for i in range(4):
    df['prob{}'.format(i)] = list(map(lambda x: x[i], df['probability']))

df.head()
```

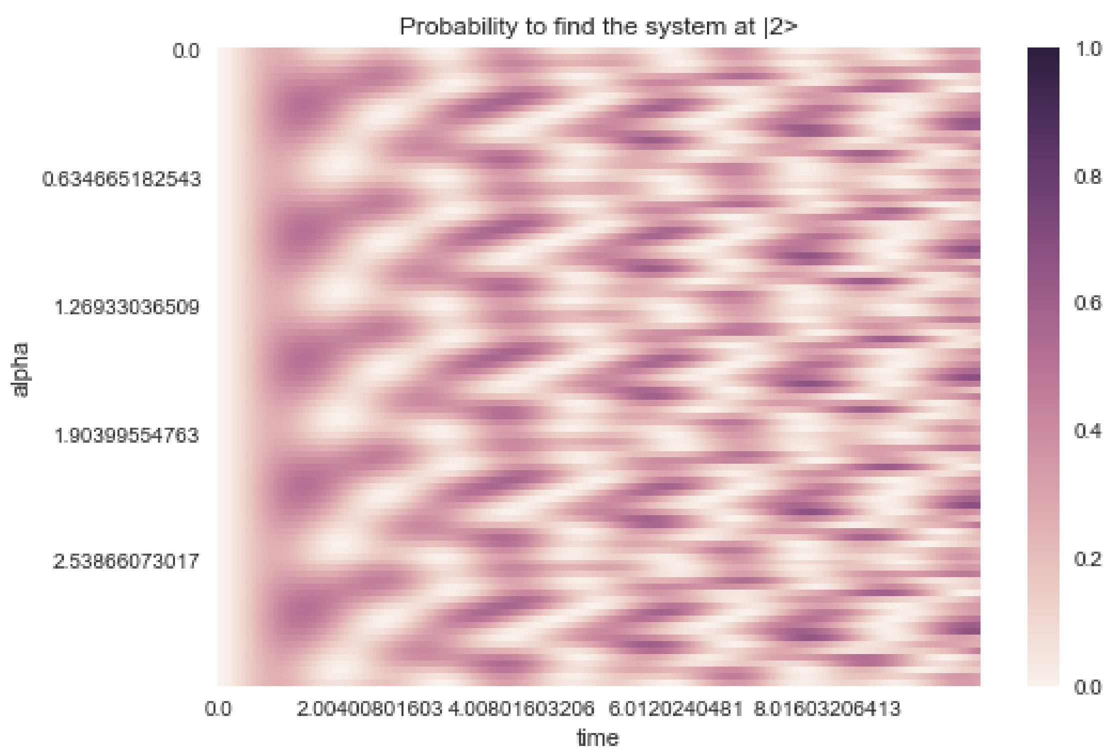
Out[11]:

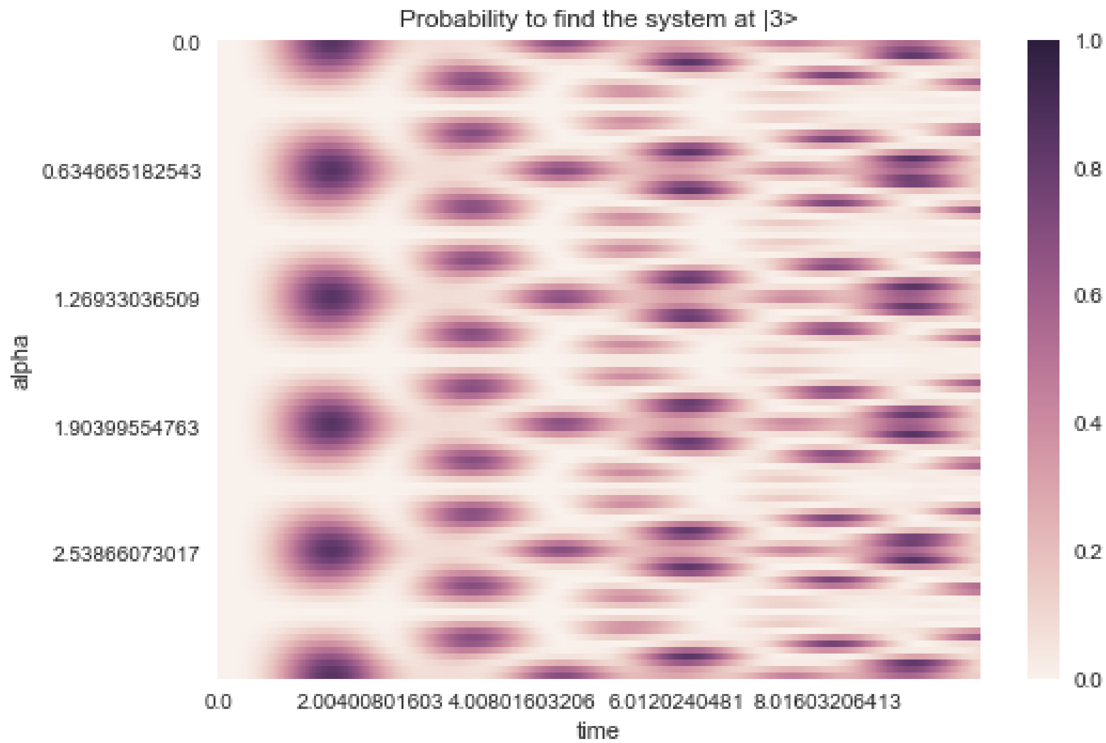
	alpha	time	probability	prob0	prob1	prob2	prob3
0	0.000000	0.0	[1.0, 0.0, 0.0, 0.0]	1.0	0.0	0.0	0.0
1	0.031733	0.0	[1.0, 0.0, 0.0, 0.0]	1.0	0.0	0.0	0.0
2	0.063467	0.0	[1.0, 0.0, 0.0, 0.0]	1.0	0.0	0.0	0.0
3	0.095200	0.0	[1.0, 0.0, 0.0, 0.0]	1.0	0.0	0.0	0.0
4	0.126933	0.0	[1.0, 0.0, 0.0, 0.0]	1.0	0.0	0.0	0.0

In [12]:
```
# Plot probability as a function of alpha and t.
import seaborn as sns

for i in range(4):
    data=df.pivot('alpha', 'time', 'prob{}'.format(i))

    sns.heatmap(data, vmin=0, vmax=1, xticklabels=100, yticklabels=20,)
    plt.title('Probability to find the system at |{}>'.format(i))
    plt.show()
```




Probability to find the system at |1>
0.0
0.634665182543
1.26933036509
1.90399554763
2.53866073017
alpha
0.0
2.00400801603
4.00801603206
6.0120240481
8.01603206413
time
1.0
0.8
0.6
0.4
0.2
0.0


Probability to find the system at |2>
0.0
0.634665182543
1.26933036509
1.90399554763
2.53866073017
alpha
0.0
2.00400801603
4.00801603206
6.0120240481
8.01603206413
time
1.0
0.8
0.6
0.4
0.2
0.0



1.0.1 Variational solver

Lets fix $\overrightarrow{\alpha} = [0.5, 0.6, 0.7, 0.8]$ and define k and v

```
In [13]: alpha = [0.5, 0.6, 0.7, 0.8]

         pre_k = np.exp(1j*alpha[0]) * qit.lmap(np.outer(zero_state.data,one_state.data.ravel())
                + np.exp(1j*alpha[1]) * qit.lmap(np.outer(one_state.data,three_state.data.ravel
                + np.exp(1j*alpha[2]) * qit.lmap(np.outer(three_state.data,two_state.data.ravel
                + np.exp(1j*alpha[3]) * qit.lmap(np.outer(two_state.data,zero_state.data.ravel(

         k = pre_k + qit.lmap.ctranspose(pre_k)
         v = qit.state.projector(three_state)
```

function

```
variational_step(state, params)
```

returns $e^{-i*k*params[1]}e^{-i*v*params[0]}|\text{state}\rangle$, which corresponds to $e^{-i*k*\gamma}e^{-i*v*\beta}|\text{state}\rangle$

```
In [15]: def variational_step(state, params):
             state = state.propagate(v.data, params[0])
             return state.propagate(k.data, params[1])
```

function

`F_function(p, params, ini_state)`

returns the expectation value of Hamiltonian

$$\langle\psi|h\psi\rangle,$$

where

$$|\psi\rangle = e^{-i*k*params[2p-1]}e^{-i*k*params[2p-2]}\dots e^{-i*k*params[1]}e^{-i*k*params[0]}|\text{ini\_state}\rangle$$

and returns $|\psi\rangle$

```
In [16]: def F_function(p, params, ini_state):
             """
             p - number of steps
             """
             global alpha

             for i in range(p):
                 ini_state = variational_step(ini_state, params=[params[2*i], params[2*i+1]])  #
             return ini_state.ev(Hamiltonian(alpha=alpha).data), ini_state
```

function

`get_params(p, ini_state)`

returns the array of params which minimizes the expectation value of Hamiltonian

$$\min_{params}\langle\psi(\text{params})|h\psi(\text{params})\rangle,$$

```
In [17]: def get_params(p, ini_state):
             # Function to optimimize.
             def fun(x):
                 # We minimize f to find max for F.
                 return F_function(p=p, ini_state=ini_state, params=x)[0]

             # Starting point.
             params_0   = [0.25 * np.pi for i in range(2*p)]
             params_min = [0 for i in range(2*p)]
             params_max = [2*np.pi if i%2 == 0 else np.pi for i in range(2*p)]

             # The bounds required by L-BFGS-B.
             bounds = [(low, high) for low, high in zip(params_min, params_max)]

             # Use method L-BFGS-B because the problem is smooth and bounded.
             minimizer_kwargs = dict(method="L-BFGS-B", bounds=bounds)

             result = scipy.optimize.basinhopping(fun, params_0, minimizer_kwargs=minimizer_kwar

             return result.x
```

Calculate

$$\min_{params} \langle \psi(\text{params}) | h\psi(\text{params}) \rangle,$$

for different number of iterations p, if initial state is zero_state

```
In [18]: %%time
         h_ev = []
         iteration = []

         # Changing p.
         for i in range(1, 6):
             h_ev.append(F_function(p=i, params=get_params(i, zero_state), ini_state=zero_state)
             iteration.append(i)
             print(i)
```

```
1
2
3
4
5
CPU times: user 3min 52s, sys: 1.81 s, total: 3min 54s
Wall time: 3min 59s
```

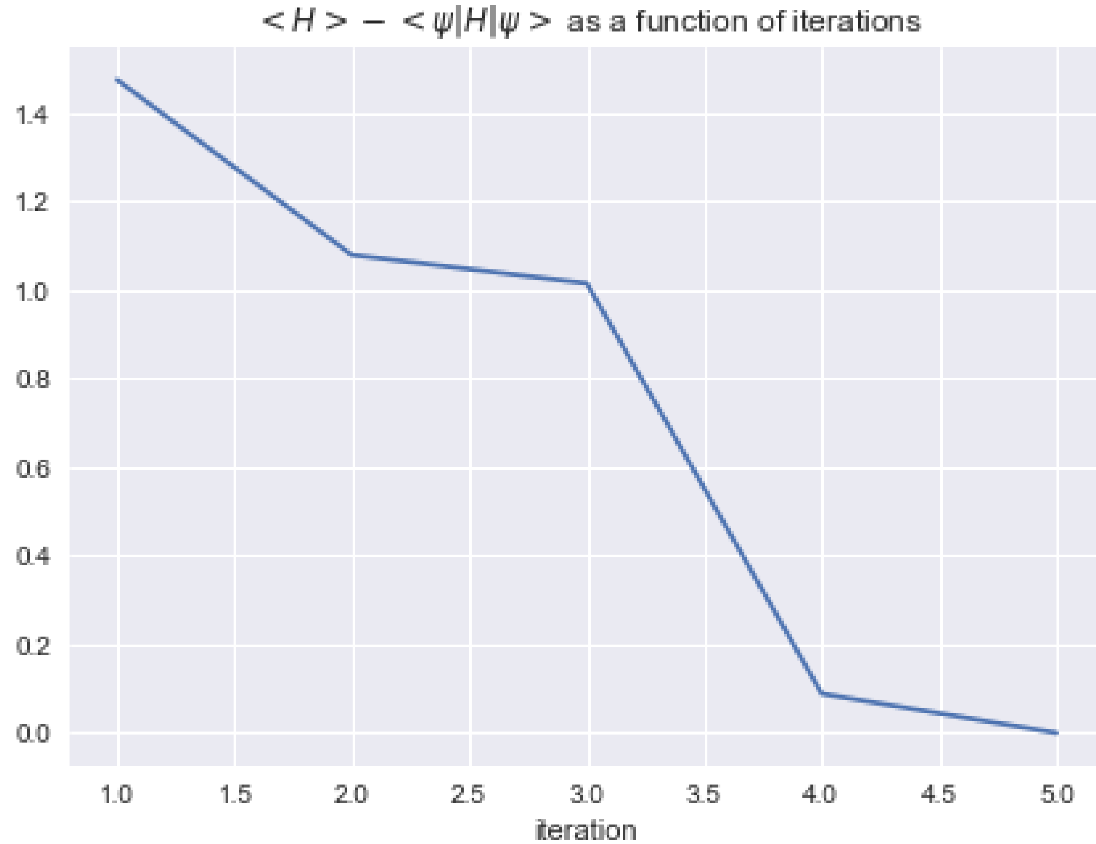
Plot

$$\min_{params} \langle \psi(\text{params}) | h\psi(\text{params}) \rangle$$

as a function of p

```
In [19]: h_ev = np.array(h_ev)
```

```
In [21]: eigenvalue, eigenvectors = np.linalg.eigh(Hamiltonian(alpha).data)

         plt.figure(figsize=(7,5))
         plt.plot(iteration, h_ev - eigenvalue[0])  # Subtract lowest eigenvalue of H
         plt.title('$<H> - <\psi|H|\psi>$ as a function of iterations')
         plt.xlabel('iteration')

         plt.show()
```



Let us fix ψ as function that minimizes

$$\min_{params} \langle \psi(\text{params}) | h\psi(\text{params}) \rangle,$$

at step $p = 5$

In [22]:
```
psi = F_function(5, get_params(5, ini_state=zero_state), ini_state=zero_state)[1]
psi
```

Out[22]:
```
 +(0.6338+0.1911j) |0> +(-0.5064-0.03706j) |1> +(-0.3492-0.3687j) |2> +(0.1893+0.1017j)
dim: (4,) <- (1,)
```

2 Quantum Walk and Control of 3 level system

We are looking for the ground state and ground level energy of the following Hamiltonian (3 level andom walk):

$$h = k + v,$$

where

$$k = e^{i\alpha_0}|0\rangle\langle 1| + e^{i\alpha_1}|1\rangle\langle 2| + e^{i\alpha_2}|2\rangle\langle 0| + h.c,$$

and

$$v = |2\rangle\langle 2|.$$

In [24]:
```
# Function to generate Hamiltonian = k + v.
def Hamiltonian(alpha: list):
    h = np.exp(1j*alpha[0]) * qit.lmap(np.outer(zero_state.data,one_state.data.ravel())
        + np.exp(1j*alpha[1]) * qit.lmap(np.outer(one_state.data,two_state.data.ravel()
        + np.exp(1j*alpha[2]) * qit.lmap(np.outer(two_state.data,zero_state.data.ravel(
    return h + qit.lmap.ctranspose(h) + qit.state.projector(two_state)
```

In [28]:
```
# Probability to find system in time t at the one of the states if the
# system starts from zero_state.
def probability(alpha: list, t):
    """
    return 3 probabilities
    """
    state = zero_state.u_propagate(la.expm(Hamiltonian(alpha).data*1j*(-t)))
    return [qit.fidelity(state, zero_state)**2,
            qit.fidelity(state, one_state)**2,
            qit.fidelity(state, two_state)**2]

assert sum(probability([1,1,1], 1)) == 1.0
```

Use the following parameterization: $\overrightarrow{\alpha} = [\alpha_0, 2\alpha_0, 3\alpha_0]$

In [29]:
```
# Calculate probability for different alpha and t.
alpha_x = np.linspace(0, np.pi, 100)
time_y = np.linspace(0, 10, 500)

X, Y = np.meshgrid(alpha_x,time_y)
df = pd.DataFrame(data={'alpha': X.ravel(), 'time': Y.ravel()})

df['probability'] = df.apply(lambda x: probability([x.alpha, 2*x.alpha, 3*x.alpha],
                                                    x.time), axis=1)
```

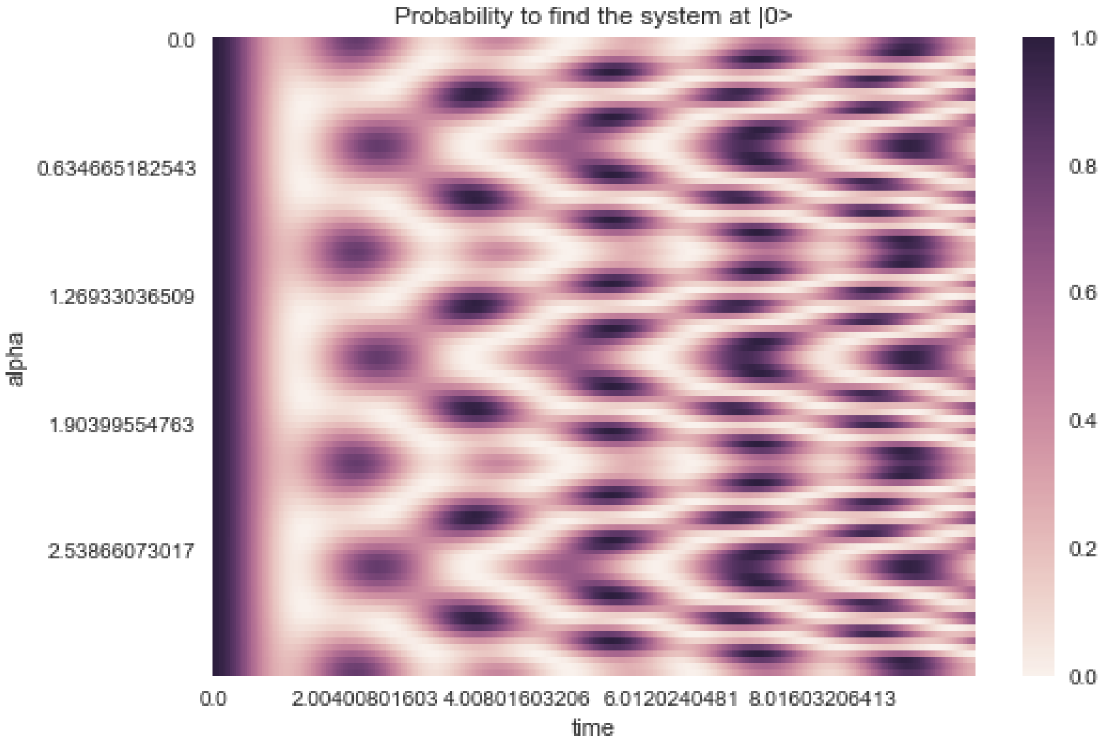
In [30]:
```
for i in range(3):
    df['prob{}'.format(i)] = list(map(lambda x: x[i], df['probability']))

df.head()
```

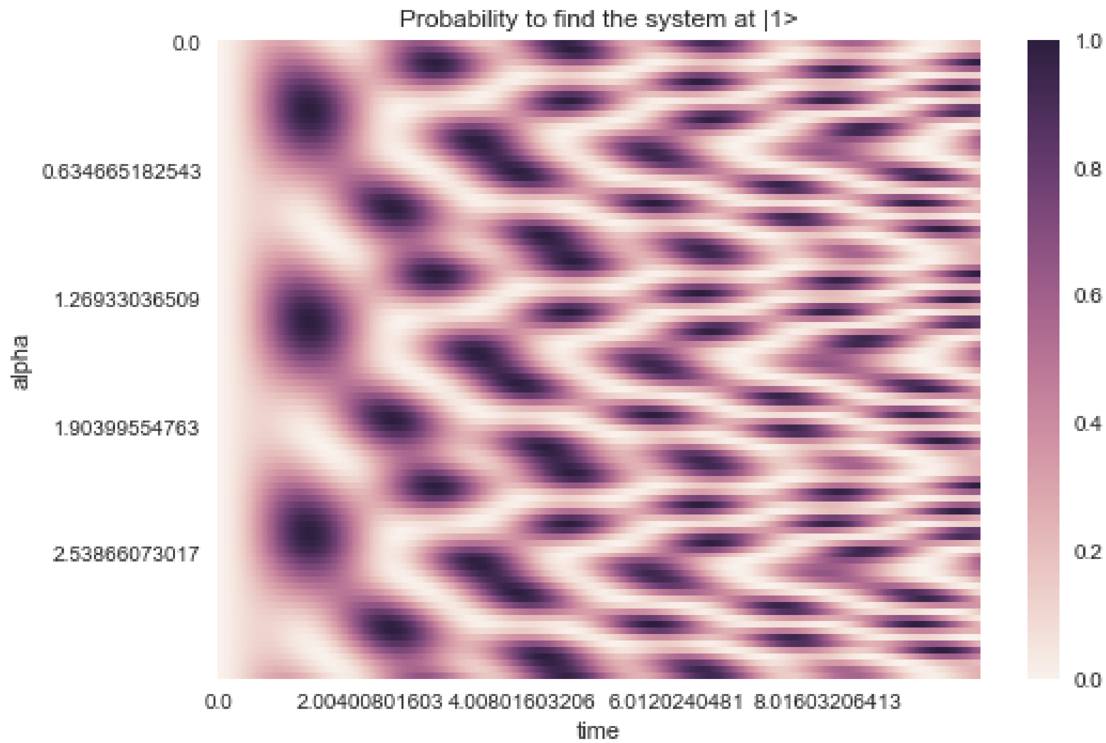
Out[30]:

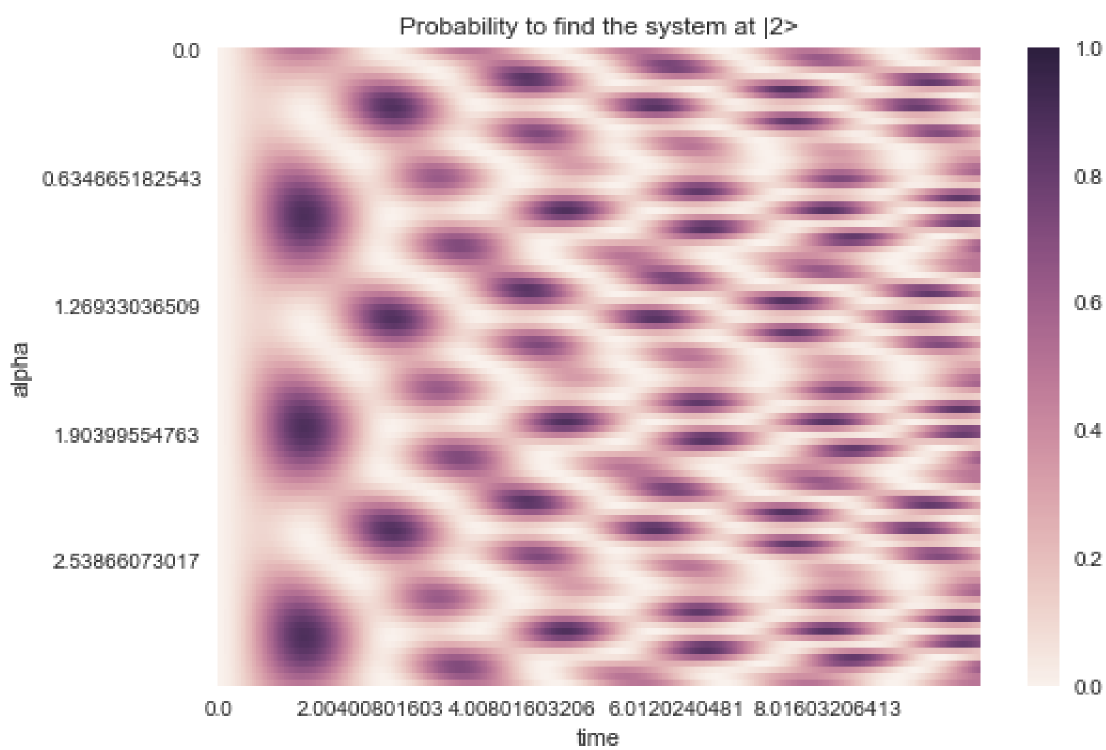
	alpha	time	probability	prob0	prob1	prob2
0	0.000000	0.0	[1.0, 0.0, 0.0]	1.0	0.0	0.0
1	0.031733	0.0	[1.0, 0.0, 0.0]	1.0	0.0	0.0
2	0.063467	0.0	[1.0, 0.0, 0.0]	1.0	0.0	0.0
3	0.095200	0.0	[1.0, 0.0, 0.0]	1.0	0.0	0.0
4	0.126933	0.0	[1.0, 0.0, 0.0]	1.0	0.0	0.0

In [31]:
```
# Plot probability as a function of alpha and t.
import seaborn as sns

for i in range(3):
    data=df.pivot('alpha', 'time', 'prob{}'.format(i))
```

```
sns.heatmap(data, vmin=0, vmax=1, xticklabels=100, yticklabels=20,)
plt.title('Probability to find the system at |{}>'.format(i))
plt.show()
```




Probability to find the system at |1>
0.0
0.634665182543
1.26933036509
1.90399554763
2.53866073017
alpha
0.0
2.00400801603
4.00801603206
6.0120240481
8.01603206413
time
1.0
0.8
0.6
0.4
0.2
0.0


Probability to find the system at |2>
0.0
0.634665182543
1.26933036509
1.90399554763
2.53866073017
alpha
0.0
2.00400801603
4.00801603206
6.0120240481
8.01603206413
time
1.0
0.8
0.6
0.4
0.2
0.0

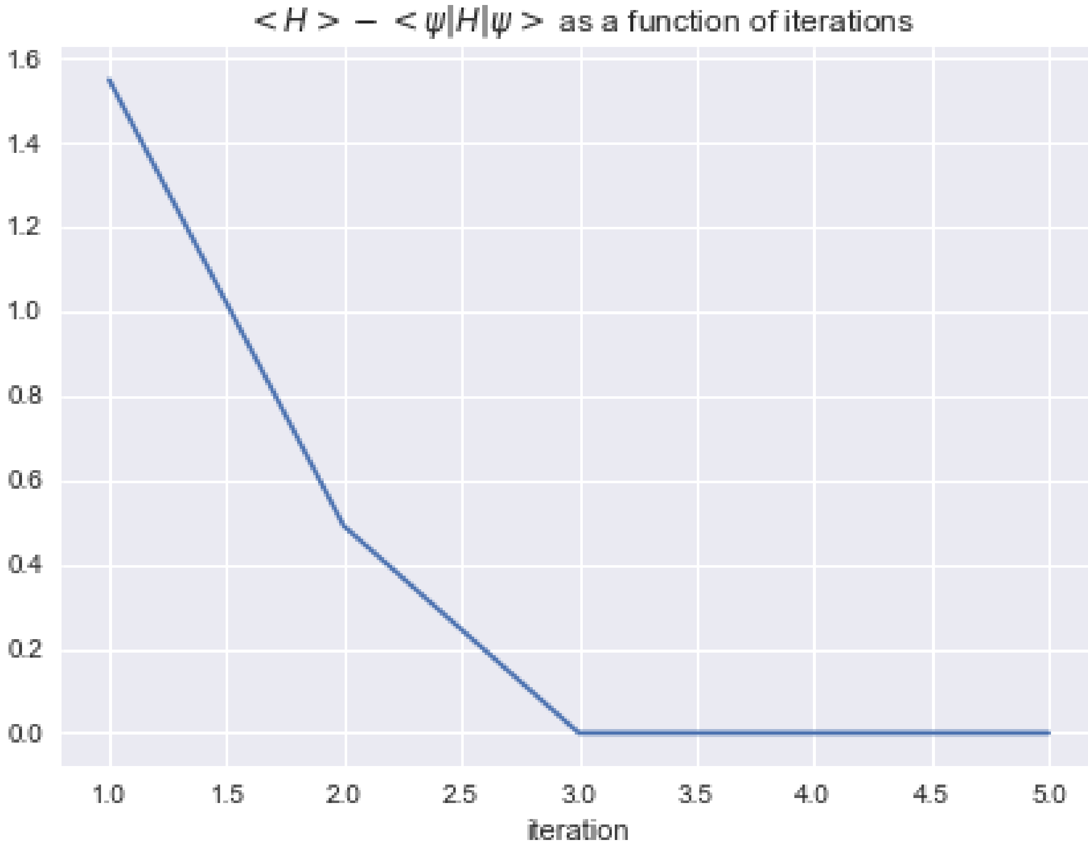
Lets fix $\overrightarrow{\alpha} = [0.5, 0.6, 0.7]$ and define k and v

```
In [32]: alpha = [0.5, 0.6, 0.7]

         pre_k = np.exp(1j*alpha[0]) * qit.lmap(np.outer(zero_state.data,one_state.data.ravel())
                + np.exp(1j*alpha[1]) * qit.lmap(np.outer(one_state.data,two_state.data.ravel()
                + np.exp(1j*alpha[2]) * qit.lmap(np.outer(two_state.data,zero_state.data.ravel(

         k = pre_k + qit.lmap.ctranspose(pre_k)
         v = qit.state.projector(two_state)

In [33]: def variational_step(state, params):
             state = state.propagate(v.data, params[0])
             return state.propagate(k.data, params[1])


         def F_function(p, params, ini_state):
             """
             p - number of steps
             """
             global alpha

             for i in range(p):
                 ini_state = variational_step(ini_state, params=[params[2*i], params[2*i+1]])  #
             return ini_state.ev(Hamiltonian(alpha=alpha).data), ini_state


         def get_params(p, ini_state):
             # Function to optimimize.
             def fun(x):
                 # We minimize f to find max for F.
                 return F_function(p=p, ini_state=ini_state, params=x)[0]

             # Starting point.
             params_0   = [0.25 * np.pi for i in range(2*p)]
             params_min = [0 for i in range(2*p)]
             params_max = [2*np.pi if i%2 == 0 else np.pi for i in range(2*p)]

             # The bounds required by L-BFGS-B.
             bounds = [(low, high) for low, high in zip(params_min, params_max)]

             # Use method L-BFGS-B because the problem is smooth and bounded.
             minimizer_kwargs = dict(method="L-BFGS-B", bounds=bounds)

             result = scipy.optimize.basinhopping(fun, params_0, minimizer_kwargs=minimizer_kwar

             return result.x

In [34]: %%time
```

```
h_ev = []
iteration = []

# Changing p.
for i in range(1, 6):
    h_ev.append(F_function(p=i, params=get_params(i, zero_state), ini_state=zero_state)
    iteration.append(i)
    print(i)
```

```
1
2
3
4
5
CPU times: user 2min 15s, sys: 1.07 s, total: 2min 16s
Wall time: 2min 21s
```

In [35]:
```
h_ev = np.array(h_ev)

eigenvalue, eigenvectors = np.linalg.eigh(Hamiltonian(alpha).data)

plt.figure(figsize=(7,5))
plt.plot(iteration, h_ev - eigenvalue[0])  # Subtract lowest eigenvalue of H
plt.title('$<H> - <\psi|H|\psi>$ as a function of iterations')
plt.xlabel('iteration')

plt.show()
```




```
In [36]: psi = F_function(5, get_params(5, ini_state=zero_state), ini_state=zero_state)[1]
         psi
```

```
Out[36]:  +(-0.4905+0.4045j) |0> +(0.02767-0.6352j) |1> +(0.3815+0.2145j) |2>
         dim: (4,) <- (1,)
```