

This is an example session showing the interactive use of the WaveBlocks simulation packet.

```
In [2]: from WaveBlocks import *
```

Some simulation parameters:

```
In [3]: params = {"eps":0.1, "ncomponents":1, "potential":"quadratic", "dt":0.1, "matrix_exponential":"pade"}
```

Create a Hagedorn wavepacket Ψ

```
In [4]: Phi = HagedornWavepacket(params)
```

Assign the parameter set Π with position 1.0 and momentum 0.5

```
In [5]: Pi = Phi.get_parameters()  
Pi
```

```
Out[5]: (1j, 1.0, 0.0, 0.0, 0.0)
```

```
In [6]: Pi = list(Pi)  
Pi[3] = 0.5  
Pi[4] = 1.0  
Pi
```

```
Out[6]: [1j, 1.0, 0.0, 0.5, 1.0]
```

```
In [7]: Phi.set_parameters(Pi)
```

Set the coefficients such that we start with a ϕ_1 packet

```
In [8]: Phi.set_coefficient(0,1,1)
```

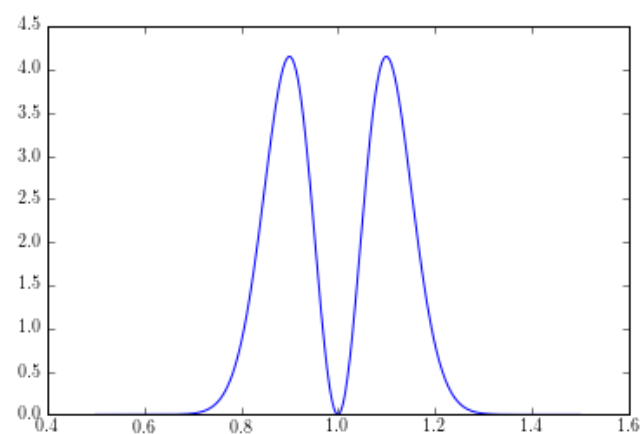
Plot the initial configuration

```
In [9]: x = linspace(0.5,1.5,1000)
```

```
In [10]: y = Phi.evaluate_at(x, prefactor=True)[0]
```

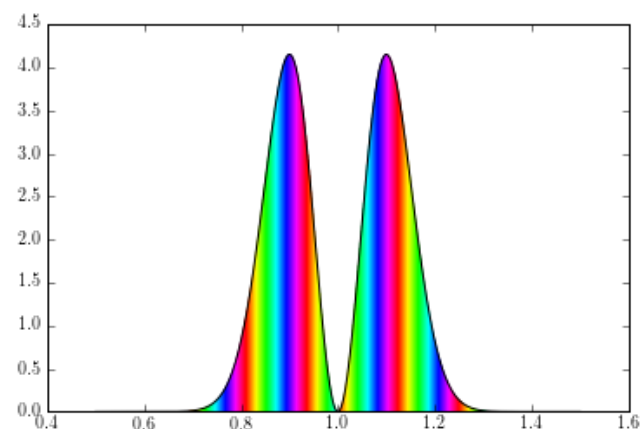
```
In [11]: plot(x, abs(y)**2)
```

```
Out[11]: [Line2D(_line0)]
```



```
In [12]: from WaveBlocks.Plot import plotcf, stemcf
```

```
In [13]: plotcf(x, angle(y), abs(y)**2)
```

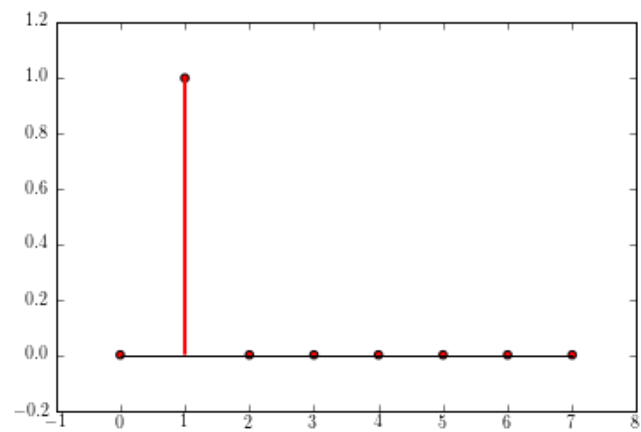


```
In [14]: c = Phi.get_coefficients(component=0)  
c = squeeze(c)
```

```
In [15]: c.shape
```

```
Out[15]: (8,)
```

```
In [16]: figure(figsize(6,4))
stemcf(arange(c.shape[0]), angle(c), abs(c)**2)
```



Set up the potential $V(x)$ for our simulation. We use a simple harmonic oscillator.

```
In [17]: V = PotentialFactory.create_potential(params)
```

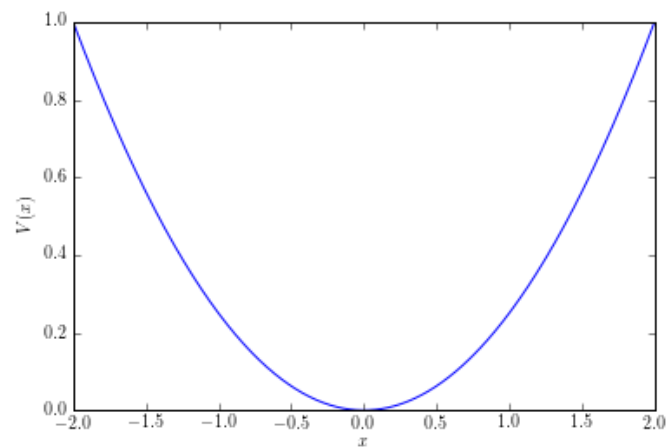
```
In [18]: V.potential
```

```
Out[18]:  $\frac{1}{4}x^2$ 
```

```
In [19]: u = linspace(-2,2,1000)
v = V.evaluate_at(u)[0]
```

```
In [20]: plot(u,v)
xlabel(r"$x$")
ylabel(r"$V(x)$")
```

```
Out[20]: Text(0,0.5, '$V(x)$')
```



Don't forget to set up the quadratur rule (γ, ω)

```
In [21]: Phi.set_quadrature(None)
```

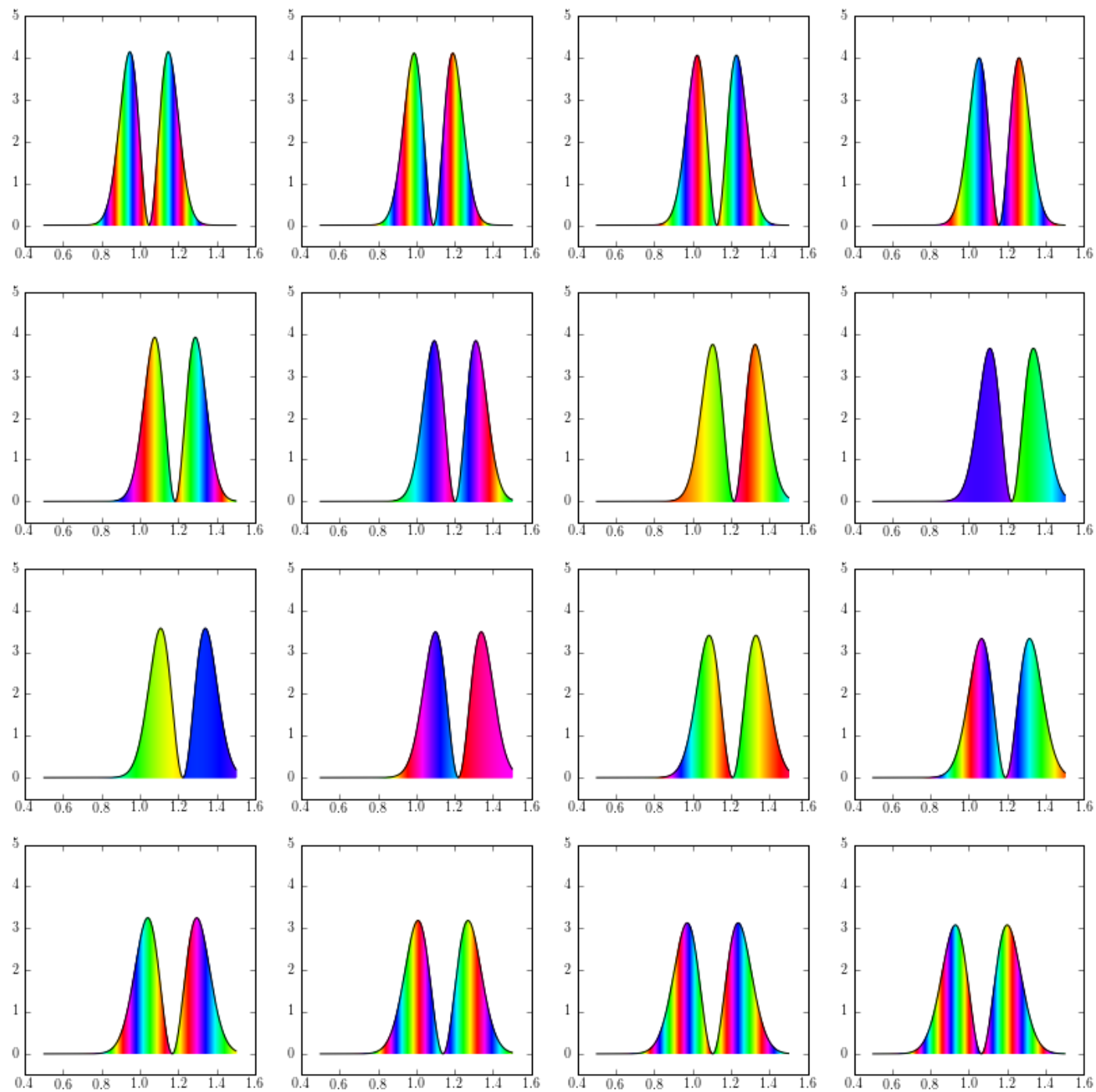
Now construct the time propagator

```
In [22]: P = HagedornPropagator(V, Phi, 0, params)
```

Propagate for 16 timesteps and plot each state

```
In [23]: fig = figure(figsize(14,14))

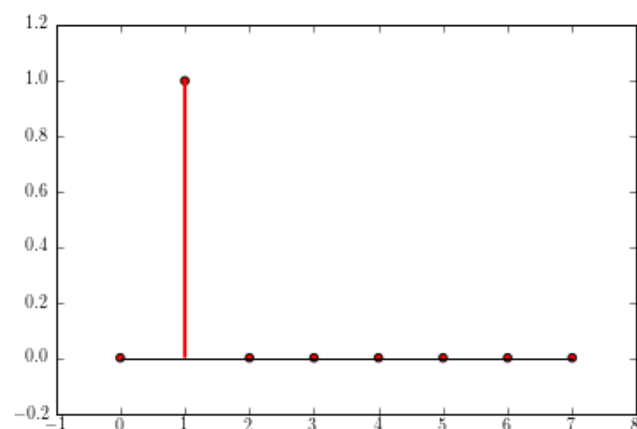
for i in xrange(16):
    P.propagate()
    ynew = P.get_wavepackets().evaluate_at(x, prefactor=True)[0]
    ax = subplot(4,4,i+1)
    plotcf(x, angle(ynew), abs(ynew)**2, axes=ax)
    ax.set_ylim((-0.5, 5))
```



Look at the coefficients C again

```
In [24]: cnew = Phi.get_coefficients(component=0)
cnew = squeeze(cnew)
```

```
In [25]: figure(figsize(6,4))
stemcf(arange(8), angle(cnew), abs(c)**2)
```



We see that the packet Ψ is still a ϕ_1

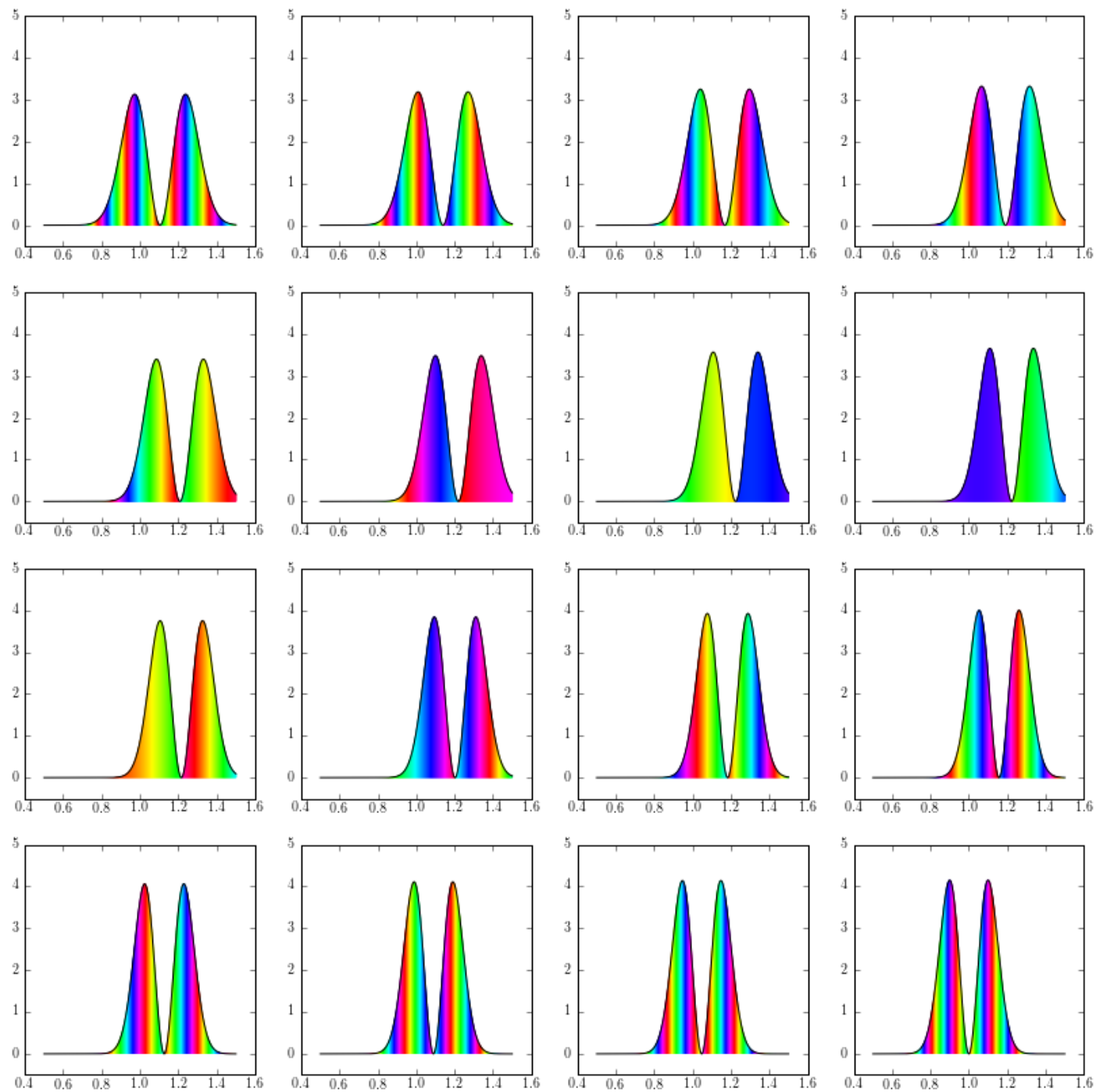
Now we go back in time ...

```
In [26]: params["dt"] *= -1
```

```
In [27]: Pinv = HagedornPropagator(V, Phi, 0, params)
```

```
In [28]: fig = figure(figsize(14,14))

for i in xrange(16):
    Pinv.propagate()
    ynew = Pinv.get_wavepackets().evaluate_at(x, prefactor=True)[0]
    ax = subplot(4,4,i+1)
    plotcf(x, angle(ynew), abs(ynew)**2, axes=ax)
    ax.set_ylim((-0.5,5))
```



```
In [29]: Phi.get_parameters()
```

```
Out[29]: ((-2.08166817117e-17+1j), (1-1.17961196366e-16j), 3.29597460436e-17, 0.5, 1.0)
```

We see that the propagation is reversible up to machine precision!