In [1]:
```
from numpy import *
from matplotlib.pyplot import *
```

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]:
```
Psi = HagedornWavepacket(params)
```

Assign the parameter set Π with position 1.0 and momentum 0.5

In [5]:
```
Pi = Psi.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]:
```
Psi.set_parameters(Pi)
```

Set the coefficients such that we start with a ϕ_1 packet

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

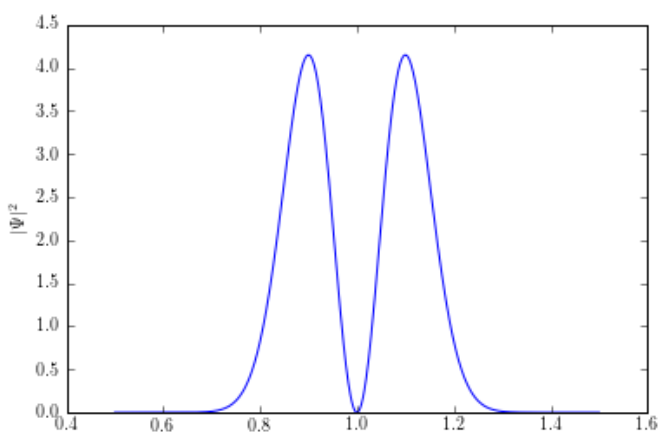
Plot the initial configuration

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

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

In [11]:
```
plot(x, abs(y)**2)
xlabel(r"$x$")
ylabel(r"$|\Psi|^2$")
```

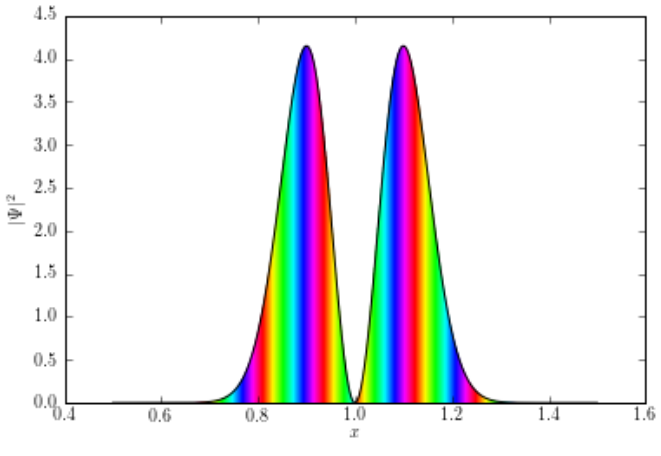
Out[11]:
```
Text(0,0.5,'$|\\Psi|^2$')
```



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

In [13]:
```
plotcf(x, angle(y), abs(y)**2)
xlabel(r"$x$")
ylabel(r"$|\Psi|^2$")
```

Out[13]: Text(0,0.5,'$|\\Psi|^2$')



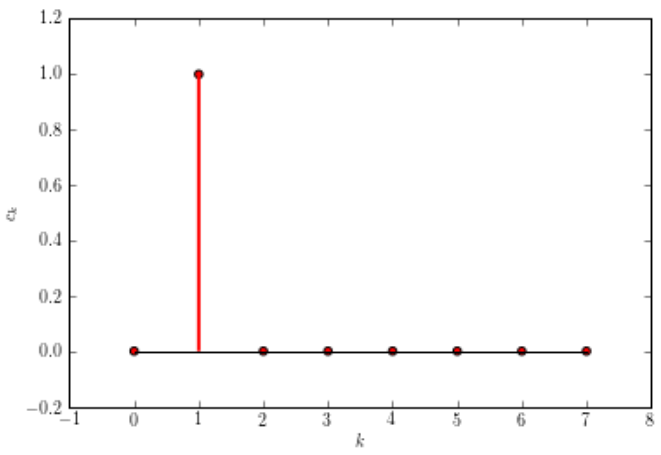
In [14]:
```
c = Psi.get_coefficients(component=0)
c = squeeze(c)
```

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

Out[15]: (8,)

In [16]:
```
figure(figsize=(6,4))
stemcf(arange(c.shape[0]), angle(c), abs(c)**2)
xlabel(r"$k$")
ylabel(r"$c_k$")
```

Out[16]: Text(0,0.5,'c_k')



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

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

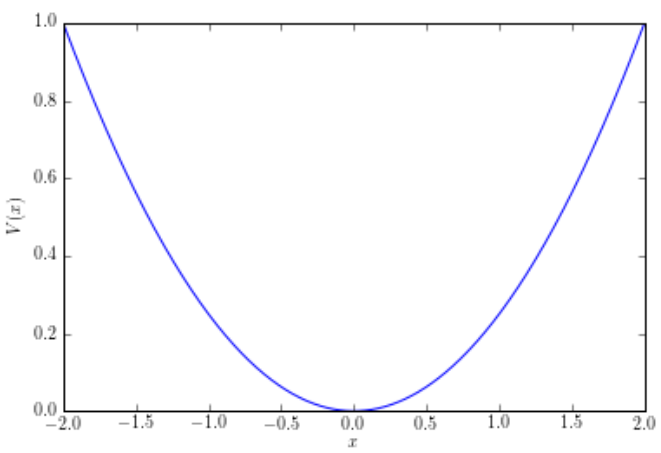
In [18]:
```
V.potential
```

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]:
```
Psi.set_quadrature(None)
```

In [22]:
```
Q = Psi.get_quadrature()
Q
```

Out[22]: <WaveBlocks.HomogeneousQuadrature.HomogeneousQuadrature instance at 0xa124eec>

Now retrieve the bare quadrature rule (γ, ω)

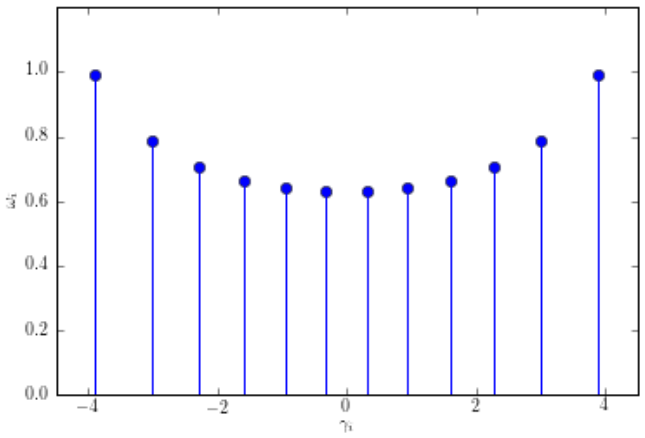
In [23]:
```
QR = Q.get_qr()
```

And extract nodes and weights

In [24]:
```
g = QR.get_nodes()
w = QR.get_weights()
```

In [25]:
```
figure(figsize=(6,4))
stem(squeeze(real(g)),squeeze(real(w)))
xlim(-4.5,4.5)
ylim(0,1.2)
xlabel(r"$\gamma_i$")
ylabel(r"$\omega_i$")
```

Out[25]: Text(0,0.5,'$\\omega_i$')



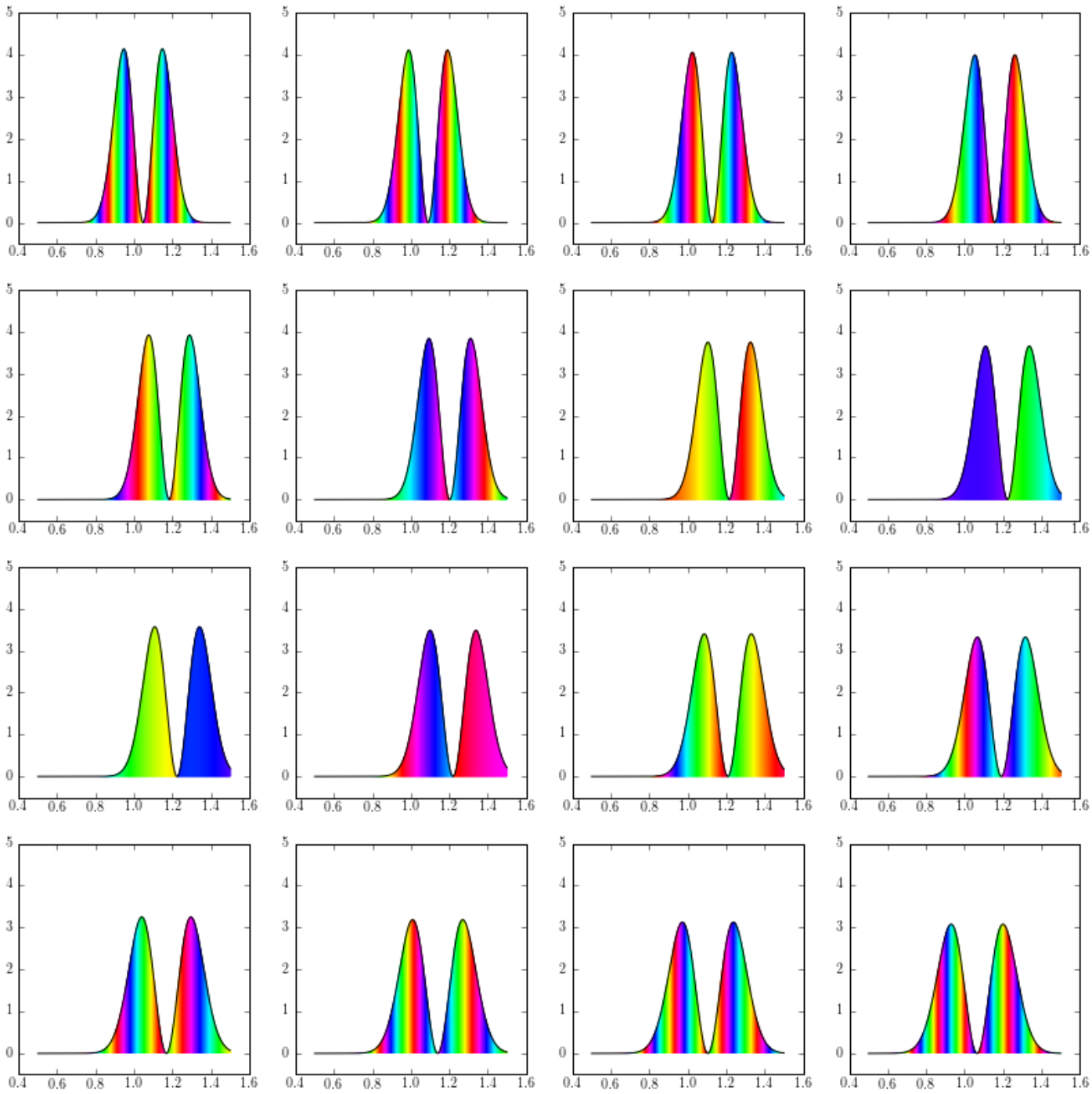
Now construct the time propagator

In [26]:
```
P = HagedornPropagator(V, Psi, 0, params)
```

Propagate for 16 timesteps and plot each state

In [27]:
```
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))
```

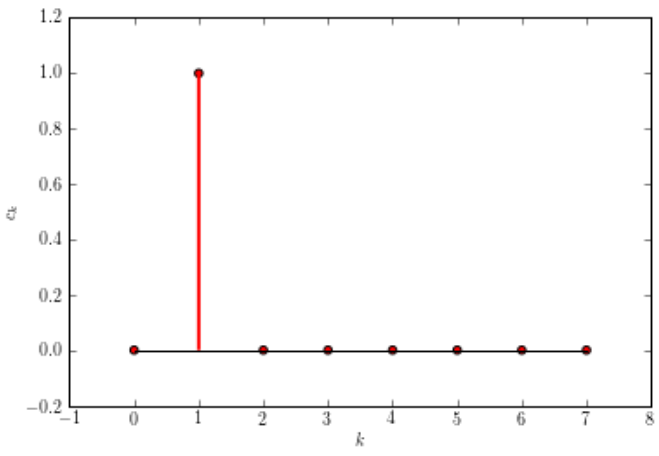


Look at the coefficients c again

In [28]:
```
cnew = Psi.get_coefficients(component=0)
cnew = squeeze(cnew)
```

In [29]:
```
figure(figsize=(6,4))
stemcf(arange(cnew.shape[0]), angle(cnew), abs(cnew)**2)
xlabel(r"$k$")
ylabel(r"$c_k$")
```

Out[29]: Text(0,0.5,'c_k')



We see that the packet Ψ is still a ϕ_1

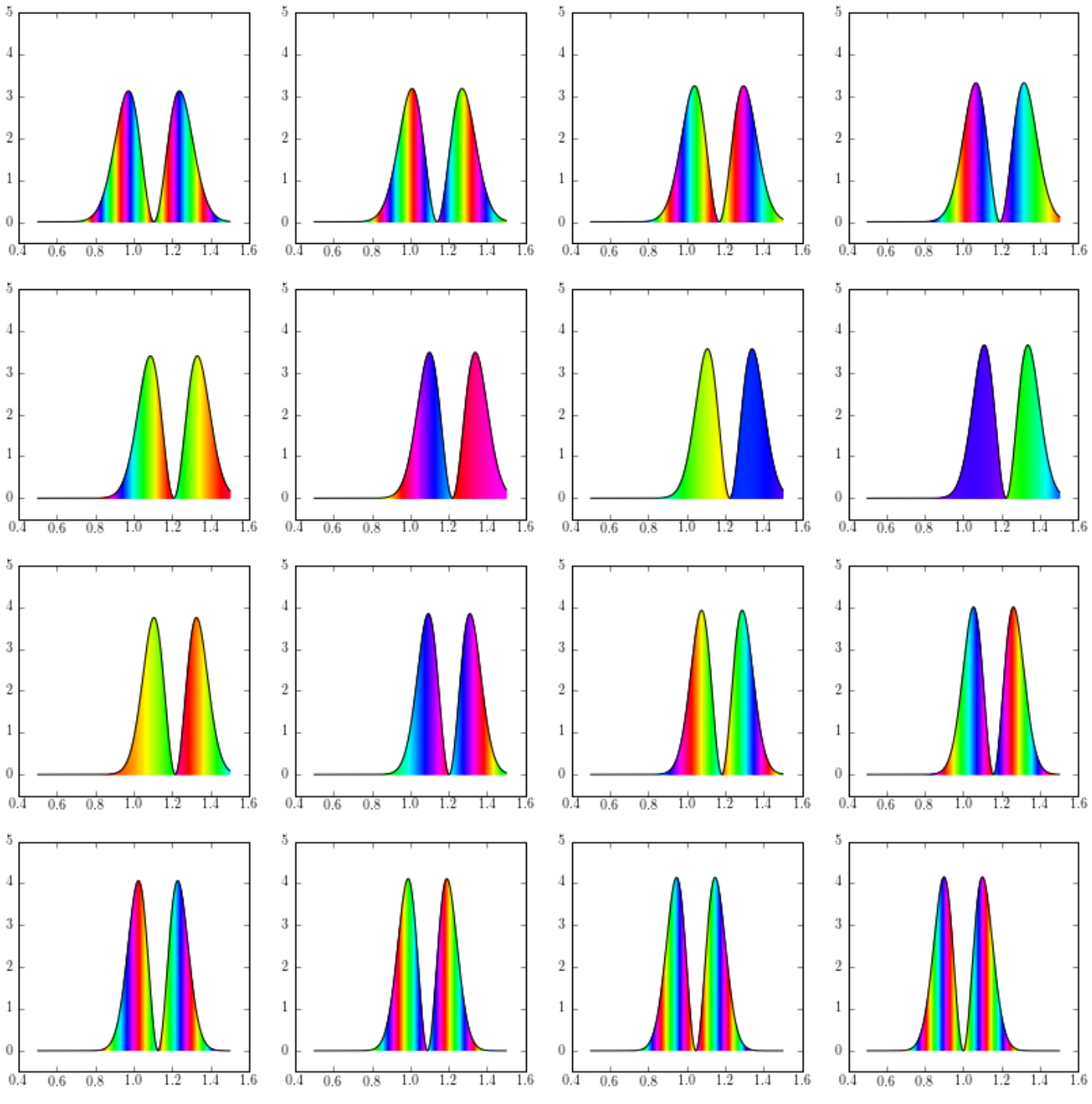
Now we go back in time ...

In [30]:
```
params["dt"] *= -1
```

In [31]:
```
Pinv = HagedornPropagator(V, Psi, 0, params)
```

In [32]:
```
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 [33]:
```
Psi.get_parameters()
```

Out[33]: ((-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!