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In [1]: import matplotlib.pyplot as plt, numpy as np
        from matplotlib import animation as am
        import random as rnd

        # inline plot
        %matplotlib inline
        # inline animation (html5 video)
        from IPython.display import HTML

        class EinsteinSolid:                                # Einstein solid object
        def __init__(self, N=400, q=10):
            self.N = N
            self.cell = [q]*N                                # q units energy per cell

        def __add__(self, other):                            # combine two solids
            self.N += other.N
            self.cell += other.cell
            return self

        def exchange(self, L=20):                            # iterate L times
            for i in range(L):
                take = rnd.randint(0, self.N-1) # random pair
                give = rnd.randint(0, self.N-1)
                while self.cell[take] == 0:      # find a nonzero-energy cell
                    take = rnd.randint(0, self.N-1)
                self.cell[take] -= 1
                self.cell[give] += 1             # exchange energy

        def sample(self):                                    # sample energy distribution
            N, Nt, q = self.N, 0, 0
            pn = []
            while Nt < N:
                n = self.cell.count(q)          # num of oscillators with energy q
                pn.append(n)                    # counts
                Nt += n
                q += 1                          # increase energy
            error = np.sqrt(pn)                 # statistical error
            return q, np.array(pn)/float(N), error/N

        def updateimg(*args):                          # args[0] = frame
            L = 20 if args[0]<100 else 200       # slower initial rate
            solid.exchange(L)
            plot.set_data(np.reshape(solid.cell, (K,K))) # update image
            return [plot]                        # return line object in a list

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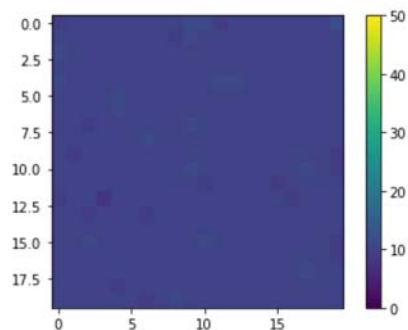
In [2]: # set up solid
        K = 20                                           # grid dimension
        qavg = 10                                       # avg units of energy per oscillator
        solid = EinsteinSolid(N = K*K, q=qavg)
        # analytic Boltzmann dist, qavg = 1/(exp(1/kT)-1), 1/kT=ln(1+1/qavg)
        kT = 1/np.log(1+1./qavg)
        Emax = 4*qavg
        En=np.arange(Emax)

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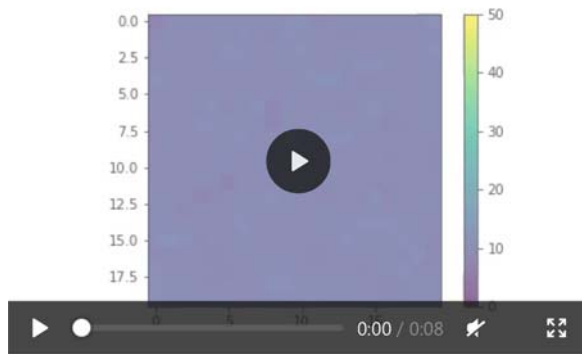
In [3]: fig = plt.figure()
        img = np.reshape(solid.cell, (K,K))           # shape to KxK image
        plot = plt.imshow(img, interpolation='none', vmin=0, vmax=50)
        plt.colorbar(plot)
        anim = am.FuncAnimation(fig, updateimg, frames=400, repeat=True, interval=20, blit=True) # animate

```



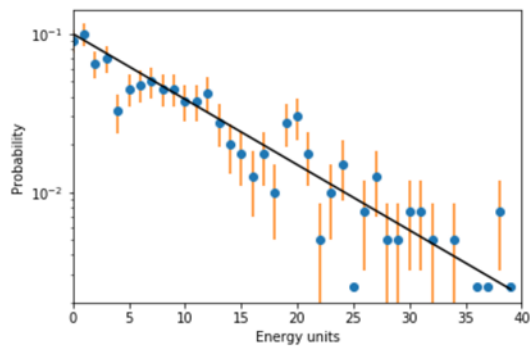
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In [4]: HTML(anim.to_html5_video()) # animate, be patient
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Out[4]:



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In [5]: # plotting results
fig = plt.figure()
solid.exchange(100*solid.N)          # thermalize, 100 interactions per oscillator
qmax, pn, error = solid.sample()
plt.plot(range(qmax), pn, 'o')
plt.errorbar(range(qmax), pn, error, fmt='none')
pmax = max(pn)
plt.plot(En, np.exp(-En/kT)*pmax, '-k') # normalized theoretical result
plt.xlim(0,Emax)
plt.xlabel('Energy units')
plt.ylabel('Probability')
plt.semilogy()                        # semilog scale
```

Out[5]: []



In [ ]: