Localization

(Sethna, "Entropy, Order Parameters, and Complexity", ex. XXX)

In Section 7.4, we discussed how non-interacting electrons provide a useful model for metals, even though the electron-electron interactions are strong. The Fermi liquid of quasiparticles is a kind of adiabatic continuation of the noninteracting electron system, connected by perturbation theory. Here we shall study how a one-dimensional non-interacting metal responds to disorder. We shall discuss how metals with weak disorder are understood by perturbing around the clean state. We shall discover that strong disorder leads to an insulating system whose eigenstates are not extended, but *localized*. We will describe these localized states explicitly by perturbing about a state of isolated atomic states.

Consider a one--dimensional chain of atoms n, each with one noninteracting electron state $|n\rangle$ of energy U_n, that can be occupied by either zero or one spinless electrons. Electrons can hop between atoms with matrix element t, leading to the Hamiltonian

$$\mathcal{H} = \sum_{n=1}^{N} U_n |n\rangle\langle n| - t \sum_{n=1}^{N-1} (|n\rangle\langle n+1| + |n+1\rangle\langle n|)$$

$$= \begin{pmatrix} U_1 & -t & 0 & \dots & 0 & 0 \\ -t & U_2 & -t & \dots & 0 & 0 \\ 0 & -t & U_3 & \dots & 0 & 0 \\ 0 & 0 & -t & \dots & 0 & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & -t \\ 0 & 0 & 0 & \dots & -t & U_N \end{pmatrix}$$

We shall take the random energies U_n as uniformly distributed between $-W$ and W.

Without disorder ($W = 0$), this is a textbook model used to describe energy bands in crystals. Three dimensional analogs of this 'tight-binding' model are quite realistic models of Fermi surfaces and energy bands in real materials.

(We shall see that even a small disorder changes the metallic behavior of one-dimensional electrons in a qualitative and interesting way. Indeed, one dimensional electrons are unstable in many interesting ways. Adding interactions between electrons, they become *Luttinger liquids*, with emergent scale invariance. Adding interactions with lattice vibrations, they can become topological insulators, with solitons and fractional charges.)

(a) *Write a function that builds the Hamiltonian matrix above with size N, bandwidth $2W$, and hopping matrix element t. Studying zero disorder $W = 0$, find the eigenvectors for $t = 1$, and $N = 100$, sorted by their eigenvalues. Plot the eigenvectors for the four lowest energies. Check numerically that these four are sinusoidal with wavevectors $k_\alpha = \pi\alpha/(N + 1)$ appropriate for a box of size N with hard-wall boundary conditions half a grid spacing to either side. Check that their four eigenvalues are the corresponding $E_{k_\alpha} = -2t \cos(k_\alpha)$*

```
In [ ]:  # Sometimes gives interactive new windows
         # Must show() after plot, figure() before new plot
         # %matplotlib

         # Adds static figures to notebook: good for printing
         %matplotlib inline

         # Interactive windows inside notebook! Must include plt.figure() betwee
         # %matplotlib notebook

         # Better than from numpy import *, but need np.sin(), np.array(), plt.p
         import numpy as np
         import matplotlib.pyplot as plt
         from numpy.linalg import eigh
```

```
In [ ]:  def Ham(W,t,N):
             U = ...*np.random.rand(N) - ...
             ham = np.diag(U)
             for i in range(N-1):
                 ham[i,i+1]=...
                 ...
             return ham

         ham = Ham(0.,1.,100)

         vals, Tvecs = eigh(ham)
         vecs = np.transpose(Tvecs)

         n = np.arange(100)
         for curve in range(...):
             plt.plot(...,vecs[...])

         # The overall sign of the eigenvector is chosen arbitrarily.
         # For my python run, these were the signs for the four curves. Modify a
         sign = [0,1,-1,-1,1]

         # Shift theory curves by eps
         eps = 0.005
         for alpha in range(1,5):
             k = ...
             print("Eigenvalue", vals[alpha-1], "equals", ...)
             plt.plot(sign[alpha]*...+eps,"k")
```

Imagine a 1D metal at zero temperatures with electrons filling the states up to a Fermi surface, here just two points at some $\pm k_{\text{Fermi}}$. Consider a packet of electrons made up of eigenstates near k_{Fermi} traveling to the right. The wavepacket will travel, as usual, at the group velocity $dE_k/dk|_{k_{\text{Fermi}}}$, without dissipation.

(Wavepackets are used to connect waves to particle-like motion. In a non-disordered system, one superimposes states with similar momenta to make a spatially localized wavefunction, which then moves with the group velocity of the wave. We discuss wavepackets to motivate the effects of disorder, but no knowledge about them is required to do this exercise.)

Now let us explore what happens when we add a weak disorder.

(b) *Build a Hamiltonian with weak disorder $W = W_{\text{weak}} = 0.04$, $t = 1$, and $N = 100$. Plot the lowest four eigenvectors. Are the eigenstates still extensive (reaching from one side of the box to the other)?*

```
In [ ]: Wweak = ...
        ham = Ham(Wweak,1.,100)

        vals, Tvecs = ...
        ...

        for curve in range(4):
            ...
```

Answer?

At this point, we could use perturbation theory to calculate the disordered eigenstates and energy levels. We could then create wavepackets and see how they evolve. In three dimensions, the scattering off of the disorder changes the electron transport qualitatively. Instead of wavepackets moving forever in one direction (ballistic transport, infinite conductivity), one gets diffusive motion of the electron probability through space (disorder providing an elastic scattering length, and a finite conductivity). In three dimensions, this is a good model for metals with impurities or dopants, illustrating how one can understand complex behavior by perturbing around solvable special cases.

Instead, let us examine what happens at large disorder W, or equivalently, small hopping t. (All of our eigenvectors depend only on W/t, and we will perturb in t to study the localized states.)

(c) *Set $t = t_{\text{Weak}} = 0.1$, $W = 1$, and $N = 100$, plotting the ten eigenvectors with lowest energies. Also do a log-linear plot of the probability density (absolute square of the wavefunctions) for these eigenvectors. Do the eigenstates still look as if the will be extensive (stretching from one end of a macroscopic wire to the other)? What solvable special limit of $\mathcal{H}$ should we use to capture this new behavior?*

```
In [ ]: tWeak = 0.1
        ...

        vals, ...
        ...

        for curve in range(10):
            plt.plot(vecs[curve])

        plt.figure()
        for curve in range(...):
            plt.plot(vecs[curve]**2)
        plt.yscale('log')
        plt.ylim(10**(-4),1)
```

Answer?

Here we find the eigenstates appear *localized* - fixed in space near individual 'atoms'. The probabilities in these states fall exponentially with distance from their centers. A wavepacket formed from localized states like these cannot transport current: for large disorder, our model describes an insulator.

Just as one can use perturbation theory to describe dirty metals in three dimensions from models like ours, we can use perturbation theory to calculate and understand these localized states. You should remember the use of second-order perturbation theory to describe the energies of a Hamiltonian $\mathcal{H} = \mathcal{H}_0 + V$ for small V. You may not remember that the first step was to use first-order perturbation theory to determine the eigenvectors. If $|\Psi_i^{(0)}\rangle$ has unperturbed eigenvalue $E_i^{(0)}$, then to first order

$$|\Psi_i^{(1)}\rangle = |\Psi_i^{(0)}\rangle + \sum_{i \neq j} \frac{\langle \Psi_j^{(0)}|V|\Psi_i^{(0)}\rangle}{E_i^{(0)} - E_j^{(0)}}|\Psi_j^{(0)}\rangle.$$

If the hopping is small compared to the disorder, let us perturb in t.

(d) *What are the eigenenergies for our Hamiltonian $\mathcal{H}_0$ in the equation above with $t = 0$? Argue that, to first order in t, the new eigenstates will be confined to three adjacent sites.*

Answer?

(e) *Write a function, given $\mathcal{H}$, i, t, and N, that gives the perturbed eigenstate to lowest order in t that is centered at site i. Find the site of the ground state with largest probability. Plot the ground state and your first-order approximation to it.* (Hint: You may be unlucky, and happen to have a neighbor site with a near degenerate energy. Just create a new Hamiltonian and try again.)

```
In [ ]: def PerturbedEigenstate(ham, i, t, N):
            vecPert = np.zeros(N)
            vecPert[i] = ...
            if i!=0:
                vecPert[i-1] = ...
            if i!=N-1:
                vecPert[i+1] = ...
            return vecPert

        iGround = np.argmax(vecs[0]**2)
        print("Ground state centered at", iGround)

        # Again, you may need to adjust the sign of the eigenvector

        plt.plot(vecs[0])
        plt.plot(+PerturbedEigenstate(...))
        plt.xlim(iGround-2,iGround+2)
```

What controls whether our model is a metal or an insulator? For a given W/t, are all the states either extended or all localized? Or could there be some mixture?

We can examine this by defining a rough measure of how spread out the wavefunction is, called the *participation ratio*:

$$P(\psi) = \frac{\left(\sum_n |\psi(n)|^2\right)^2}{\sum_n |\psi(n)|^4} = \frac{1}{\sum_n |\psi(n)|^4}.$$

(f) *Show that a state whose probability is spread uniformly among M sites has $P = M$. At zero disorder, what is the participation ratio for the lowest energy state? For the long-wavelength next few states? What is the ratio for a localized state that decays exponentially, $\psi(j) \propto \exp(-|i - j|/\lambda)$, in an infinite chain, with λ much larger than one?*

Answer?

If the participation ratio $P \ll N$ we can reasonably expect that the eigenstate is localized.

(g) *Calculate the participation ratio for all the eigenstates for intermediate disorder $W_{\text{inter}} = 0.5$, $t = 1$, $N = 100$, and plot them against the energy. Is there a systematic variation? Plot the wavefunction for an energy in the middle of the band (eigenvalue E near zero), and one at the top and bottom of the band. Which are less localized - the states near the edges of the band, or the states in the center?*

```
In [ ]: def ParticipationRatio(vec):
            return ...
```

```
In [ ]: N=100
        ham = ...

        vals, ...

        ratios = [ParticipationRatio(vec) for vec in vecs]

        plt.plot(vals,...,"ko")

        plt.figure()
        plt.plot(vecs[int(N/2)])
        plt.figure()
        plt.plot(...)
        plt.figure()
        plt.plot(vecs[0])
```

Answer?

In experiments, one finds a region of localized states at the edges of a band, and extended states in the middle of the band. Between these is a *mobility edge*, where a metal-insulator transition occurs as more electrons are added.

(Each time we add one order to perturbation theory, we get a wavefunction extending outward by one atom. It appears from the first two terms that each order multiplies the terminal amplitude by a factor $|\psi(i + n)/\psi(i + (n - 1))| = |t/(U_i - U_{i+n})|$. Roughly speaking, if U_i is at the edge of the band, this factor is twice as small as if U_i is in the center, so there is less localization at the center. Notice, though, that this is useful only when $t > |U_i - U_{i+n}|$. Rare, nearly degenerate states can mix strongly, even at long distances, making the arguments subtle.)

Finally, can we find a mobility edge for our model? One thing to check is if the wavefunctions might have decay lengths larger than our system (so they just look extended at $N = 100$).

(h) *Find the eigenvectors and eigenvalues for the same parameters as in part (g), $W = W_{inter} = 0.5$ and $t = 1$, except for a much larger system ($N = 2000$ or 4000 if it is feasible on your system). Plot the participation ratio verses energy, and plot eigenstate in the center of the band and at the two edges. Do the states in the middle of the band now appear localized? Are their participation ratios larger than 100 - the system size in part~(g)? Does it make sense that they looked extended in the smaller system, but clearly in an infinite system are localized?*

```
In [ ]: N = 4000
        ham = ...
```

Answer?

As it happens, disordered electrons in one dimension are always localized, even for tiny disorder. The spinless, noninteracting electrons we study here are also always localized in two dimensions. In two dimensions, they can become extended when interactions, spin, or strong

magnetic fields are added. In particular, 2D electrons in a strong magnetic field exhibit the quantum Hall effect (with extended states around the edges). Even more interesting, interacting electrons in a strong magnetic field exhibit the fractional quantum Hall effect - our first example of an experimental system with fractional charges and fractional statistics.