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Polyacetylene and solitons: weird quasiparticles

(Sethna, "Entropy, Order Parameters, and Complexity", 2nd edition, ex. XXX.)

This exercise is primarily analytical: only those parts with computational components are included in this file. The exercise will be available at https://sethna.lassp.cornell.edu/StatMech/SethnaExercises.pdf.

... See exercise for long introduction to polyacetylene and the SSH model

(a) Solve for the eigenstates of the $N\times N$ SSH Hamiltonian, with N even (say, 200) and starting with a double-bond connecting the first two carbon atoms for δ>0. (Note that hopping with strength t is represented by Hamiltonian matrix elements $-t$ connecting the two sites, so that hopping prefers neighboring sites to have the same sign.) So, for even N, the matrix should begin and end like this:

$$\begin{pmatrix} 0 & -t-\delta & 0 & 0 & \cdots \\ -t-\delta & 0 & -t+\delta & 0 & \cdots \\ 0 & -t+\delta & 0 & -t-\delta & \cdots \\ 0 & 0 & -t-\delta & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

Use t=2.5 eV and δ=0.35 eV. Plot the eigenstate energies in order from smallest to largest. Which states will be full at zero temperature? An insulator fills an energy band, and has an energy gap. A metal fills only a portion of the band, and has no gap between eigenenergies at the last filled state. Do you find an energy gap between the highest filled state energy and the lowest empty state? Compare it to the predicted gap 4δ for the infinite system. Finally, notice that for every eigenenergy E, there is a partner eigenenergy $-E$.

```
Ham[t_, δ_, N_] :=
  {H[i_, j_] := -(t + δ) /; OddQ[i] && j == i + 1;
   H[j_, i_] := -(t + δ) /; OddQ[i] && j == i + 1;
   H[i_, j_] := ... /; EvenQ[i] && j == i + 1;
   H[j_, i_] := ... /; EvenQ[i] && ...;
   H[i_, j_] := 0; Table[H[i, j], {i, 1, N}, {j, 1, N}]}[[1]]
t = 2.5;
δ = 0.35;
```

```
numSites = 200;
EigSys = Eigensystem[Ham[t, ...]];
(* Need to sort eigenvectors and eigenvalues *)
{vals, vecs} = Transpose[Sort[Transpose[EigSys]]];
ListPlot[vals]
Print[ ..., " =? ", 4 δ]
```

Your answer here (or in a separate writeup).

... Discussion of gaps, particle hole symmetry, and edge states ...

(b) Now take N odd (say 201), again starting with a double bond connecting the first two atoms. Again plot the eigenstate energies. Do you see a state now in the gap? Can you argue from particle-hole symmetry that it must exist?

```
numSites = 201;
EigSys = Eigensystem[Ham[t, δ, numSites]];
{vals, vecs} = ...
ListPlot[vals]
```

Your answer here (or in a separate writeup).

(c) Plot the midgap eigenstate ψ_midgap(n) vs. n. Is it extended or localized? Is it in the center, or on one edge? Which edge? Can you guess why we wanted to start and end with a double bond in part (a)?

```
midgap = ...;
Print["Eigenvalue near zero is number ",
 midgap, " with eigenvalue ", vals[[midgap]]]
ListPlot[vecs[[ ...]], PlotRange → All, Joined → True]
```

Your answer here (or in a separate writeup).

... Discussion of edge states, the quantum Hall effect, domain walls, the spreading of the soliton domain wall to a width of seven atoms, ... and the resulting electronic hopping, which replaces a uniform δ with δsol(n) = –(0.35eV) tanh((n–n0)/ξ), where n0 is the location of the center of the soliton, and the minus sign is chosen so that the chain starts with a double bond.

(d) Modify your Hamiltonian to allow variations in $\delta(n)$, and place the soliton at the center of the chain, using the equation above, and with N=201. (With N odd, you should now have double bonds at both ends of the chain, to avoid midgap states at the edges.) Solve for the eigenstates, and if necessary sort them in order of their eigenvalues. Is there one near zero energy? Plot the wavefunction for the midgap state. Does the midgap electron wavefunction move with the soliton? Does it stay fairly near to the center of the soliton? Should we view it as part of the soliton?

```
ξ = 7.;
δSol[n_, n0_] := -δ Tanh[ ...]
HamSoliton[t_, δSol_, N_, ξ_] :=
 {n0 = (N) / 2;
        H[i_, j_] := - (t + δSol[i, n0]) /; OddQ[i] && j == i + 1;
        ...
       ...
      ...
     H[i_, j_] := 0;
   Table[H[ ...], { ...}, { ...}]][[1]]

numSites = 201;
EigSys = ...;
{vals, vecs} = ...;
vals[[midgap]]

ListPlot[vecs[[ ...]], Joined → True, PlotRange → All]
```

Your answer here (or in a separate writeup).

... Discussion of solitons, weird quantum numbers, and different charge states due to different fillings of the mid-gap state...

When our odd-length chain is neutral, the N=201 carbon atoms each contribute an electron, so there are N=201 electrons to fit into the eigenstates for the system with a soliton. At zero temperature, 200 of these electrons will fill the 100 eigenstates with negative energy. Each of the filled states will have electrons in an antisymmetric singlet state (1/sqrt(2))(↑↓−↓↑) with net spin zero.

(e) At zero temperature, into which eigenstate will the last electron go? Plot the square of the probability density in the midgap state you found. Where along the chain does the last electron mostly reside? If the last electron is spin +1/2 , what is the spin of the system as a whole? Should we attribute that spin to the soliton?

```
ListPlot[ ..., PlotRange → All]
```

Your answer here (or in a separate writeup).

... Discussion of spin quantum numbers of the different charge states of the soliton. Turn to charge quantum numbers...

Let us now carefully consider what the charge of the soliton is in the possible ways to fill this midgap state. We saw in part (e) that the probability density of an electron in the midgap state |ψ_midgap(n)|^2 is localized near the soliton. But all the other eigenstates also change when the Hamiltonian changes due to the soliton. At low temperatures, the negative energy eigenstates will each have two electrons, and the positive energy eigenstates will be empty. Let us label our sorted eigen-

states with
0≤m<N, so ψ_101(n) is the mid-gap state amplitude on carbon n, and the negative energy eigenstates are ψ_m(n) with m<101.

(f) Numerically calculate the net electron probability density due to the doubly occupied negative energy eigenstates, $\rho(n) = 2\sum_{\text{occupied}} |\psi\_m(n)|$^2, and plot it. (This, times the charge $-e$ on the electron and plus the charge $+e$ on the carbon ions, is the net charge distribution for a soliton with an empty mid-gap state.) Is the soliton with an empty midgap state, together with the associated dip in the electron density nearby, neutral? Now plot $\rho(n)$ plus the probability |ψ_midgap(n)|^2 you calculated in part (e), to find the charge density with one electron in the midgap state. Is the soliton with spin ±1/2 positively charged, negatively charged, or neutral? Finally, plot the net charge density when the midgap state is doubly occupied. To summarize, what is the net charge for our soliton quasiparticle in these three cases?

```
(* Two electrons in each valence eigenstate*)
valenceFill = Sum[2 ..., {i, 1, ...}];
ListPlot[valenceFull, PlotRange → All]
midgapProb = ...;
ListPlot[ ... + ..., PlotRange → All]
ListPlot[ ... + ..., PlotRange → All]
```

Your answer here (or in a separate writeup).

Discussion of spin-charge separation, fractional charge, whether the soliton is the lowest energy charge or spin excitation. Parts (g), (h), and (i) to be answered.