Exercises 1. Physics 603. The SSH Model (Due Sept 30th)

1. In the SSH model, the dispersion is given by

$$\begin{aligned} E_k &= \pm\sqrt{(2t\cos k)^2 + (2\alpha u_0 \sin k)^2} \\ &= \pm 2t\sqrt{1-(1-z^2\sin^2 k)} \end{aligned} \tag{1}$$

where $z = (2\alpha u_0/t)$. Show that the density of states per spin for a long chain with N sites is given by

$$\rho(E) = \frac{1}{N} = \frac{1}{\pi}\frac{dk}{dE}\frac{|E|}{\sqrt{((2t)^2 - E^2)(E^2 - \Delta_g^2)}} \tag{2}$$

where $\Delta_g = 4\alpha u_0$.

2. Set up in mathematica, Matlab or your favorite notebook code an N (where N is even) dimensional matrix for the one-particle Hamiltonian of the SSH model,

$$H = \sum_j \left[-t_{j+1,j}(c^\dagger_{j+1\sigma} c_{j\sigma} + \text{H.c}) + \frac{K}{2}(u_{j+1} - u_i)^2 \right] \tag{3}$$

in which the hopping matrix element is

$$t_{j+1,j} = -t - \alpha(u_{j+1} - u_j), \tag{4}$$

and in the ground-state $u_j = -u_0(-1)^j$. Your one-particle Hamiltonian will look something like this

$$H = -\begin{pmatrix} & t+\delta & & \dots & & & t-\delta \\ t+\delta & & t-\delta & & & & \\ & t-\delta & & & & & \\ \vdots & & & \ddots & & & \\ & & & & & t-\delta & \\ & & & & t-\delta & & t+\delta \\ t-\delta & & & & & t+\delta & \end{pmatrix}$$

where $\delta = 2\alpha u_0$. Note the corner elements are present for periodic boundary conditions.

(a) Confirm numerically that you obtain a gap $2\Delta_g$ in the one-particle spectrum, where $\Delta_g = 4\alpha u$. What happens to your spectrum when you eliminate the corner matrix elements? Why?

(b) Calculate the density of states numerically, and compare your answer with that obtained in (1). You can do this succinctly in Mathematica by broadening each energy level into a Lorentzian and calculating

$$\rho(E) = \frac{1}{\pi N} \mathrm{Im} \sum_{\lambda} \frac{1}{E - E_\lambda - i\epsilon}$$

where $I\epsilon$ is a smalll imaginary part.

(c) By summing over the energies of the filled states, and adding in the phonon energy $2NKu_0^2$, confirm that the dependence of the energy on the displacement u_0 is a double-well potential. How well does your result compare with the exact result for the ground-state energy?

$$\frac{E_0[u_0]}{N} = -\frac{4t}{\pi} E[1 - (2\alpha u_0/t)^2] + 2Ku_0^2$$

where

$$E[x] = \int_0^{\pi/2} \sqrt{1 - x^2 \sin k^2} dk$$

is the complete elliptic integral of the second kind. Does your result improve as you increase the number of sites N?

(d) Now modify your to include a soliton by using $2N+1$ sites. You can put a soliton at the $N+1$ st site by taking

$$u_j = -u_0(-1)^{j-(N+1)} \tanh\left(\frac{j - (N+1)}{l}\right)$$

Choose the value of u_0 you obtained at the minimum of your calculation in (c). Recompute the one-particle electron spectrum and confirm that it now contains a zero energy mode.

(e) Now recompute the energy for a variety of soliton sizes l and calculate the optimal soliton size.