

Solutions to Exercises 1. Physics 603. The SSH Model (Oct 7, 2020)

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

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

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

$$\rho(E) = \frac{1}{N} \sum_{\lambda} \delta(E - E_{\lambda}) = \frac{1}{\pi} \frac{dk}{dE} = \frac{1}{\pi} \frac{|E|}{\sqrt{((2t)^2 - E^2)(E^2 - \Delta_g^2)}} \quad (2)$$

where $\Delta_g = 4\alpha u_0$.

Solution: The density of states is given by

$$\begin{aligned} \rho(E) &= \sum_{\pm} \int_0^{\pi} \frac{dk}{2\pi} \delta(E - E_k^{\pm}) \\ &= \sum_{\pm} \int_{-2t}^{2t} \frac{dE}{2\pi} \left| \frac{dk}{dE_k^{\pm}} \right| \delta(E - E_k^{\pm}) = \sum_{\pm} \frac{1}{2\pi} \left| \frac{dk}{dE_k^{\pm}} \right|, \end{aligned} \quad (3)$$

where $E_k^{\pm} = \pm 2t \sqrt{1 - (1 - z^2) \sin^2 k}$. Now the derivative

$$\frac{dE_k^{\pm}}{dk} = \mp \frac{2t(1 - z^2) \sin k \cos k}{\sqrt{1 - (1 - z^2) \sin^2 k}}. \quad (4)$$

However, from the dispersion, we can identify

$$\sin^2(k) = \frac{(4t^2 - E^2)}{(2t)^2(1 - z^2)}, \quad \cos^2(k) = \frac{(E^2 - \Delta_g^2)}{(2t)^2(1 - z^2)}, \quad (5)$$

so that

$$\left| \frac{dk}{dE_k^{\pm}} \right| = \frac{|E|}{\sqrt{(2t)^2 - E^2} \sqrt{E^2 - \Delta_g^2}}. \quad (6)$$

Adding the contribution of both branches of the energy,

$$\rho(E) = \frac{1}{\pi} \frac{|E|}{\sqrt{((2t)^2 - E^2)(E^2 - \Delta_g^2)}}. \quad (7)$$

It is actually useful to write the density of states as $Re[\rho(E - i\delta)]$, where $-i\delta$ is a small imaginary part, and

$$\rho(z) = \sqrt{\frac{z^2}{((2t)^2 - z^2)(z^2 - \Delta_g^2)}}, \quad (8)$$

as this analytic function has branch-cuts outside the conduction and valence bands, giving zero in these regions.

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,

$$H = \sum_j \left[-t_{j+1,j} (c_{j+1\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + \frac{K}{2} (u_{j+1} - u_j)^2 \right] \quad (9)$$

in which the hopping matrix element is $t_{j+1,j} = -t - \alpha(u_{j+1} - u_j)$, 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.

Solution:

Important to check for small size that you have the matrix you are seeking.

```

In[3]:= Clear[H1, H2];
md[i_, j_] := Mod[i - 1, Np] + 1;
Np = 6;
e = 0.03;
H1[t_, d_] := Module[{hh}, hh = Table[0, {i, 1, Np}, {j, 1, Np}];
Do[hh[[md[j + 1, Np], md[j, Np]]] = -t - d (-1)^j, {j, 1, Np}];
hh = hh + Transpose[hh];
MatrixForm[H1[t, d]]
Out[3]/MatrixForm=

```

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

FIG. 1: Mathematica Code for setting up matrix

- (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?

Solution: If $\delta > 0$ is positive, the ground-state and forms edge states at each end of the strip. This is most easily seen by setting $\delta = t$, whereupon the first and last sites in the strip are decoupled from the bulk. The ground-state is actually topological.

```

gap = eig[[(Np / 2) + 1]] - eig[[(Np / 2)]];
gaptheory = 4  $\delta$ ;
Print["Matrix Dimension = ", Np, ", 2 $\Delta$  (numerical)=", gap, ", 2 $\Delta$  =4 $\delta$ = ", gaptheory]
Esum = (2 / Np) Sum[eig[[i]], {i, 1, Np / 2}];
Dens[x_] := (1 / ( $\pi$  Np)) Im[Tr[1 / (x - eig -  $\epsilon$  I)]];
pa = Plot[Dens[x], {x, -5, 5}, PlotRange -> {0, 1}, PlotStyle -> Green, AxesLabel -> {"E/t", " $\rho(E)$ "},
  AxesStyle -> Medium];
 $\epsilon$  = 0.02;
eig2 = Sort[Eigenvalues[H2[t,  $\delta$ ]]];
Dens2[x_] := (1 / ( $\pi$  Np)) Im[Tr[1 / (x - eig2 -  $\epsilon$  I)]];
pb = Plot[Dens2[x], {x, -5, 5}, PlotRange -> {0, 1}, PlotStyle -> Blue, AxesLabel -> {"E/t", " $\rho(E)$ "},
  AxesStyle -> Medium];
GraphicsRow[{pa, pb}, ImageSize -> Full]

```

Matrix Dimension = 200, 2 Δ (numerical)=0.4, 2 Δ =4 δ = 0.4

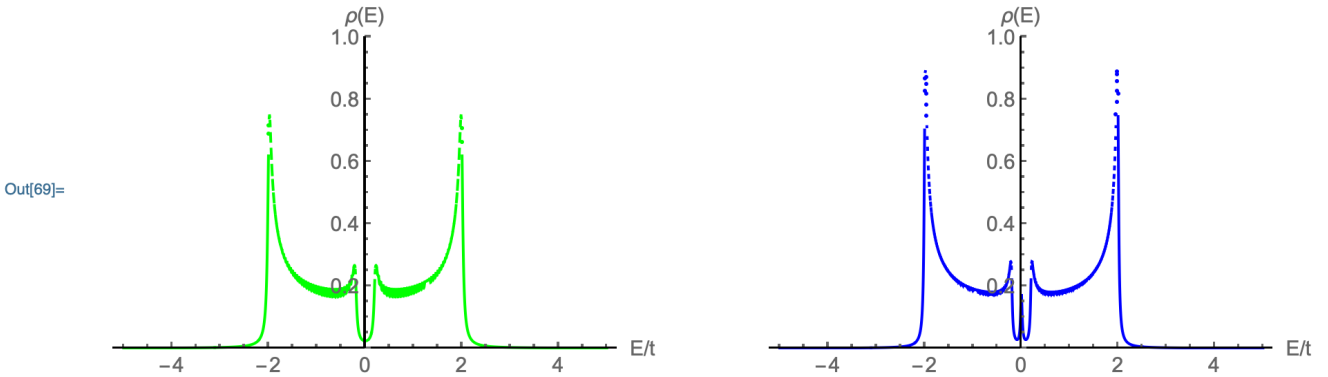


FIG. 2: Mathematica Code for evaluating the density of states for periodic (H1) and open (H2) boundary conditions, showing the formation of zero energy states in the latter case.

(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

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

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

Solution: Here is a comparison of the numerical and analytic density of states.

```

In[201]:= dos[E_] := (1/π) Re[Sqrt[E^2 / ((-E^2 + (2 t)^2) (E^2 - (2 δ)^2))]];
p2 = ListPlot[Table[{x, dos[x - I ε / 10]}, {x, -2.5, 2.5, 0.01}],
  PlotStyle → Red, Filling → Axis, Joined → True];
Show[pa, pb, p2, ImageSize → Full]

```

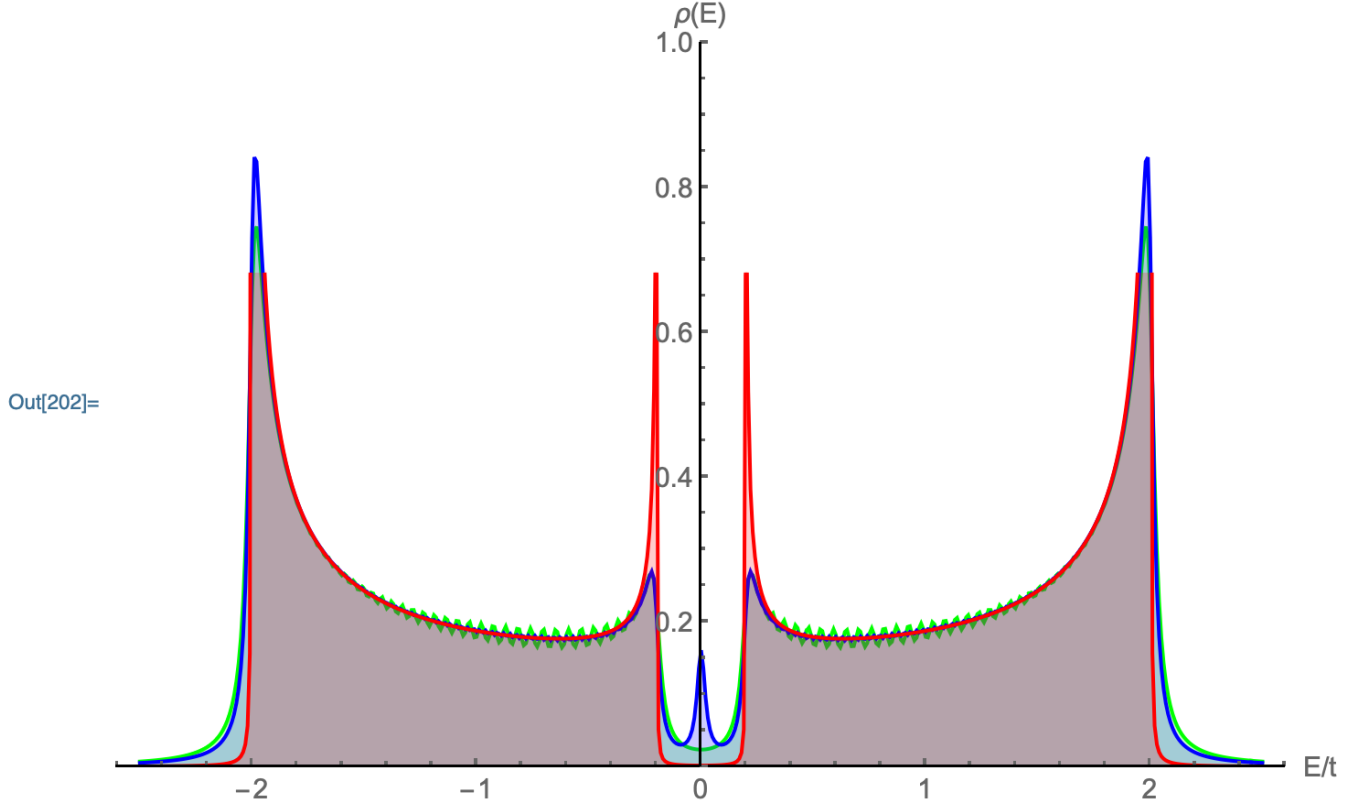


FIG. 3: Comparison of density of states for periodic (green), and open (blue) boundary conditions for $N_s = 200$ sites, with analytical formula (8).

(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

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

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

Solution:

```

Etot[t_, α_, K_, u0_, Np_] := Module[{hh, eig, δ}, hh = Table[0, {i, 1, Np}, {j, 1, Np}];
δ = 2 α u0;
Do[hh[[md[j + 1, Np], md[j, Np]]] = -t - δ (-1)^j, {j, 1, Np}];
hh = hh + Transpose[hh];
eig = Sort[Eigenvalues[H1[t, δ]]];
(2 / Np) Sum[eig[[i]], {i, 1, Np / 2}] + 2 K u0^2];
Ean[t_, α_, K_, u0_] := - (4 t / π) EllipticE[1 - (2 α u0 / t)^2] + 2 K u0^2 t;
α = 0.8;
t = 1;
K = 1;
p5s = Plot[Ean[t, α, K, u] + 0.005, {u, -1, 1}, PlotStyle → {Blue, Thick}];
Np = 6;
p6s = Plot[Etot[t, α, K, u, Np], {u, -1, 1}, PlotStyle → Red];
Np = 200;
p6 = Plot[Etot[t, α, K, u, Np], {u, -1, 1}, PlotStyle → Red];
umin = x /. FindMinimum[Ean[t, α, K, x], {x, 0.1}][[2]];
psmall = Show[p5s, p6s, AxesLabel -> {"u", "E[u]/N_s"}, PlotLabel -> "N_s=6"];
pbig = Show[p5s, p6, AxesLabel -> {"u", "E[u]/N_s"}, PlotLabel -> "N_s=200"];
Print["umin = ±", umin]
GraphicsRow[{psmall, pbig}, ImageSize -> Full]

umin = ±0.326378

```

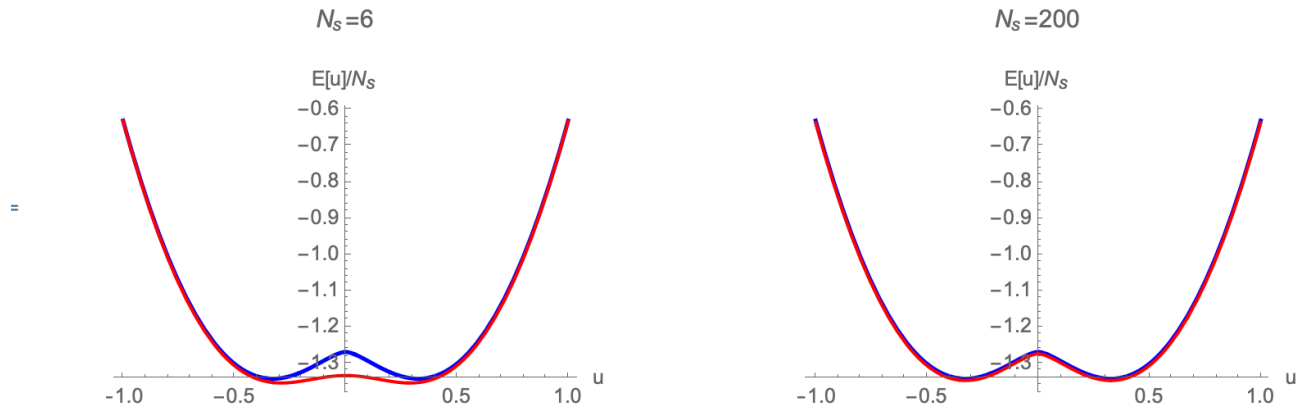


FIG. 4: Comparison of the numerical (red) and analytic (blue) total energy for $N_s = 6$ and $N_s = 200$ sites, showing convergence to the analytic result as N_s increases.

(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). Re-compute the one-particle electron spectrum and confirm that it now contains a zero energy mode.

Solution:

```

Nn = 800; Np = 2 Nn + 1; ε = 0.01; t = 1; α = 0.3; K = 0.3; l = 9;
u = x //. FindMinimum[Ean[t, α, K, x], {x, 0.1}][[2]];
gap = 4 α u;
coherencelength = 2 t / gap;
Print["u0 = ", u, " Δg = ", gap, " ξ(coherence length) = ", coherencelength];
u0 = Table[u (-1) ^ (j - (Nn + 1)) (Tanh[(j - 1) / l]), {j, 1, Np}];
hh = Table[0, {i, 1, Np}, {j, 1, Np}];
Do[hh[[md[j + 1, Np], md[j, Np]]] = -t + α (u0[[md[j + 1, Np]]] - u0[[md[j, Np]]]), {j, 1, Np}];
hh = hh + Transpose[hh];
MatrixForm[hh];
MatrixForm[u0];
eig = Sort[Eigenvalues[hh]];
Dens2[x_] := (1 / (π Np)) Im[Tr[1 / (x - eig)]];
pb = ListPlot[Table[{x, Dens2[x - ε I]}, {x, -4, 4, 0.05}], PlotRange → {0, 1},
  Filling → Axis, PlotStyle → Blue, Joined → True];
pc = Plot[10 Dens2[x - ε I / 10], {x, -gap / 2, gap / 2}, PlotRange → {0, 1}, PlotStyle → Red];
Show[pb, pc]
u0 = 0.182637 Δg = 0.219164 ξ(coherence length) = 9.12557

```

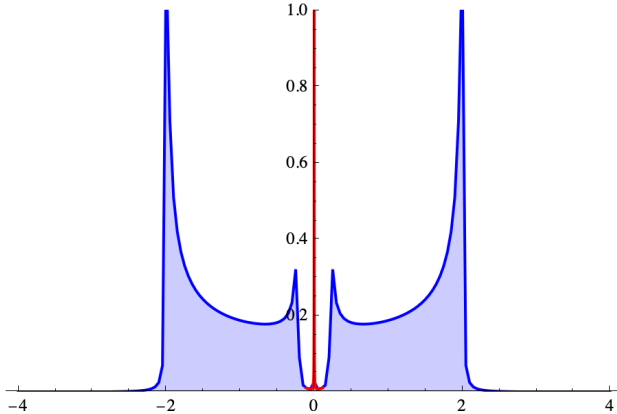


FIG. 5: Density of states for a single soliton in a ring with 1601 sites.

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

Solution:

Here it was important to make sure that the gap size was small enough, so that the coherence length $\xi = v_F/\Delta_g$ of the order was larger than the lattice spacing. This means using a sufficiently weak phonon coupling α and K . I adjusted things to get a coherence length of about $\xi = 9$, and discovered that the optimal soliton came out with the same size.

```
In[387]:= npts = 20; Eg = Ean[t,  $\alpha$ , K, u]; sola = Table[{x, Np (EnS[t,  $\alpha$ , u, K, x] -
      Eg)}, {x, 0.001, 5, 5 / npts}]; solb = Table[{x, Np (EnS[t,  $\alpha$ , u, K, x] -
      Eg)}, {x, 5.05, 20, 15 / npts}];
sol = Join[sola, solb];
solg = Table[{sol[[i, 1]] / coherenceLength, sol[[i, 2]] / gap}, {i, 1, 2 npts - 2}];
pp2 = ListPlot[solg, Joined  $\rightarrow$  True, AxesLabel  $\rightarrow$  {"x/ $\xi$ ", "ES/ $\Delta$ "}, PlotStyle  $\rightarrow$  Red,
      Filling  $\rightarrow$  Axis];
Show[pp2]
```

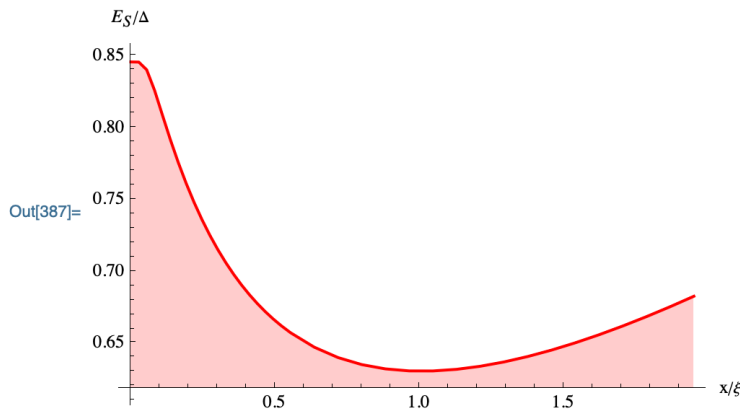


FIG. 6: Energy as a function of Soliton size l , for a ring of 1601 sites, showing that an optimal soliton has $l \sim \xi = v_F/\Delta_g$, the coherence length.