Chain of interacting spins-1/2

Below we give codes for finding:
(1) the Hamiltonian in the site-basis, as well as its eigenvalues and eigenstates;
(2) the density of states;
(3) the number of principal components (NPC) of each eigenstate in the site-basis;
(4) the number of principal components (NPC) of each eigenstate in the mf-basis;
(5) the level spacing distribution when parity does not need to be taken into account (when we have a defect);
(6) the level spacing distribution when parity needs to be taken into account (when we deal with a clean chain);

(1) Hamiltonian in the site-basis

Parameters of the Hamiltonian

*) L = number of sites.
In Figs. 1 and 3 [panels (b), (c), (d) and (e)] we consider L=15 and L/3 spins up; dimension=3003.
Figure 3 (a) uses L=14 and L/2 spins up; dimension=3432.
Figure 2 has L=18 and L/3 spins up; dimension=18564. The data was obtained using Fortran 77. *Mathematica* can deal with L=15, but has memory problems with larger systems. The fact that NPC becomes a smooth function of energy in the chaotic regime is more evident for L=18 than L=15, which explains why we resorted to Fortran. However, the *Mathematica* codes to compute NPC when L=15, which are provided below, can still give an idea of the general trend.

*) upspins = number of spins pointing up in the z direction.
*) downspins = number of spins pointing down in the z direction.
*) dim = dimension of the Sz-subspace considered.
*) ϵ = value of the defect (all other Zeeman splittings are assumed = 0).
*) defectsite = site where the defect is placed.

*) Jxy = strength of the flip-flop term between nearest-neighbors (NNs).
*) Jz = strength of the Ising interaction between NNs.
*) alpha different from zero indicates the presence of next-nearest-neighbor (NNN) couplings.
*) JJxy = strength of the flip-flop term between NNNs.
*) JJz = strength of the Ising interaction between NNNs.

*) onebasisvector is the site-basis vector 111110000000000
*) its permutations generate all basis vectors for that particular subspace

*) HH are the elements of the Hamiltonian. In the site-basis, the on-site defect and the Ising interaction contribute to the diagonal elements. The flip-flop term contributes to the off-diagonal elements.

The code

```
(* PARAMETERS OF THE HAMILTONIAN *)
Clear[L, upspins, downspins, dim, Jxy, Jz, ϵ, defectsite, alpha, JJxy, JJz];
L = 15;
upspins = L / 3;
downspins = L - upspins;
```

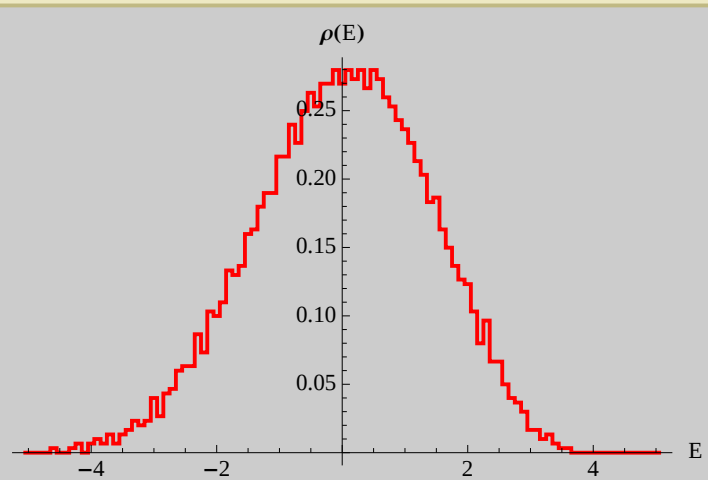
```
dim = L! / (upspins! downspins!);
(* Impurity *)
ϵ = 0.5;
defectsite = Floor[L / 2];
(* Parameters for nearest-neighbor couplings *)
Jxy = 1.0;
Jz = 0.5;
(* Parameters for next-nearest-neighbor couplings *)
(* Set alpha=0 if NNN couplings do not exist *)
alpha = 0.0;
JJxy = 1.0;
JJz = 0.5;

(* BASIS *)
Clear[onebasisvector, basis];
onebasisvector =
  Flatten[{Table[1, {k, 1, upspins}], Table[0, {k, 1, downspins}]}];
basis = Permutations[onebasisvector];

(* ELEMENTS OF THE HAMILTONIAN *)
(* Impurity and NN couplings *)
Clear[HH];
(* Initialization *)
Do[Do[HH[i, j] = 0., {i, 1, dim}], {j, 1, dim}];

(* Diagonal elements *)
Do[
  (* Impurity *)
  If[basis[[i, defectsite]] == 1,
   HH[i, i] = HH[i, i] + ϵ / 2.,  HH[i, i] = HH[i, i] - ϵ / 2.];
  (* Ising interaction *)
  Do[If[basis[[i, j]] == basis[[i, j + 1]],
     HH[i, i] = HH[i, i] + Jz / 4., HH[i, i] = HH[i, i] - Jz / 4.];
   , {j, 1, L - 1}];
  , {i, 1, dim}];

(* Off-diagonal elements *)
Clear[howmany, site];
Do[
  Do[
    (* Initialization *)
    howmany = 0;
    Do[site[kk] = 0, {kk, 1, L}];
    (* Sites where states i and j differ *)
    Do[
     If[basis[[i, k]] ≠ basis[[j, k]], {howmany = howmany + 1, site[howmany] = k}];
     , {k, 1, L}];
    (* If only two neighbor sites differ,
    there is a coupling matrix element *)
    If[howmany == 2,
     If[site[2] - site[1] == 1, {HH[i, j] = Jxy / 2., HH[j, i] = Jxy / 2.}]];
    , {j, i + 1, dim}];
  , {i, 1, dim - 1}];

(* ELEMENTS OF THE HAMILTONIAN WITH NNN COUPLINGS *)
```

```
If[alpha > 0,

(* Diagonal elements *)
  Do[
   (* Ising interaction *)
   Do[If[basis[[i, j]] == basis[[i, j + 2]],
       HH[i, i] = HH[i, i] + alpha JJz / 4., HH[i, i] = HH[i, i] - alpha JJz / 4.];
     , {j, 1, L - 2}];
   , {i, 1, dim}];

  (* Off-diagonal elements *)
  Clear[howmany, site];
  Do[
   Do[
     (* Initialization *)
     howmany = 0;
     Do[site[kk] = 0, {kk, 1, L}];
     (* Sites where states i and j differ *)
     Do[ If[basis[[i, k]] ≠ basis[[j, k]],
         {howmany = howmany + 1, site[howmany] = k}];
      , {k, 1, L}];
     (* If only two next-neighbor sites differ,
     there is a coupling matrix element *)
     If[howmany == 2,
      If[site[2] - site[1] == 2,
        {HH[i, j] = alpha JJxy / 2., HH[j, i] = alpha JJxy / 2.}]];
     , {j, i + 1, dim}];
   , {i, 1, dim - 1}];

 ];

(* TOTAL HAMILTONIAN AND DIAGONALIZATION *)
Clear[Hamiltonian, Energy, Vector];
Hamiltonian = Table[Table[HH[i, j], {j, 1, dim}], {i, dim}];
Energy = Eigenvalues[Hamiltonian];
Vector = Eigenvectors[Hamiltonian];
```

(2) Density of states

```
Clear[bin, Nbin, Eint, NinWindow, hisden, hisdenPlot];

bin = 0.1;
Nbin = ((5 + bin) - (-5)) / bin;
Eint = Table[(-5 - bin - bin / 2) + bin k, {k, 1, Nbin + 1}];

Do[
  NinWindow[k] = 0;
  , {k, 1, Nbin}];

Do[
  Do[
    If[Eint[[k]] ≤ Energy[[j]] < Eint[[k + 1]], { NinWindow[k] = NinWindow[k] + 1}];
    , {k, 1, Nbin}];
  , {j, 1, dim}];

(* density of states NORMALIZED: hisden *)
hisden = Flatten[Table[{{Eint[[k]], NinWindow[k] / (bin dim)},
     {Eint[[k + 1]], NinWindow[k] / (bin dim)}}, {k, 1, Nbin}], 1];

hisdenPlot =
 ListPlot[hisden, Joined → True, PlotRange → All, PlotStyle → {Thick, Red},
  LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"E", "ρ(E)"}]
```

Below : density of states for L = 15, 5 up spins,
Jxy = 1.0, Jz = 0.5, ϵ = 0.5, alpha = 0.0



(3) NPC in the site-basis

```
Clear[NPC];
Do[
  NPC[j] = 1 / Sum[Abs[Vector[[j, k]] ]^4, {k, 1, dim}];
  , {j, 1, dim}];

(* Data and plot NPC vs energy *)
Clear[tabEnNPC];
tabEnNPC = Table[{Energy[[j]], NPC[j]}, {j, 1, dim}];
ListPlot[tabEnNPC, PlotRange → All,
 LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"E", "NPC"}]
```

(4) NPC in the mean-field basis

```
(* FIRST WE FIND THE MEAN-FIELD BASIS *)
(* Here the mean-field basis corresponds to the eigenstates
  of the Hamiltonian with the defect + the NN flip-flop term *)
Clear[HH];
(* Initialization *)
Do[Do[HH[i, j] = 0., {i, 1, dim}], {j, 1, dim}];
(* Diagonal elements *)
Do[
  (* Impurity *)
  If[basis[[i, defectsite]] == 1,
    HH[i, i] = HH[i, i] + ϵ / 2.,  HH[i, i] = HH[i, i] - ϵ / 2.];
  , {i, 1, dim}];
(* Off-diagonal elements *)
Clear[howmany, site];
Do[
  Do[
    (* Initialization *)
    howmany = 0;
    Do[site[kk] = 0, {kk, 1, L}];
    (* Sites where states i and j differ *)
    Do[
     If[basis[[i, k]] ≠ basis[[j, k]], {howmany = howmany + 1, site[howmany] = k}];
     , {k, 1, L}];
    (* If only two neighbor sites differ,
    there is a coupling matrix element *)
    If[howmany == 2,
     If[site[2] - site[1] == 1, {HH[i, j] = Jxy / 2., HH[j, i] = Jxy / 2.}]];
    , {j, i + 1, dim}];
  , {i, 1, dim - 1}];

(* Vmf is the mean-field basis written in the site-basis *)
Clear[Hmf, Vmf];
Hmf = Table[Table[HH[i, j], {j, 1, dim}], {i, dim}];
Vmf = Eigenvectors[Hmf];
(* Now we can compute NPC IN THE MEAN-FIELD BASIS *)
Clear[NPCmf];
Do[
  NPCmf[j] =
   1 / Sum[Abs[Sum[Vector[[j, kk]] Vmf[[k, kk]], {kk, 1, dim}] ]^4, {k, 1, dim}];
  If[Mod[j, 100] == 0, Print[{j, Energy[[j]], NPCmf[j]}]];
  , {j, 1, dim}];

(* Data and plot NPCmf vs energy *)
Clear[tabEnNPCmf];
tabEnNPCmf = Table[{Energy[[j]], NPCmf[j]}, {j, 1, dim}];
ListPlot[tabEnNPCmf, PlotRange → All,
 LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"E", "NPCmf"}]
```

(5) Level spacing distribution for NN+defect (parity is not taken into account)

```
(* LEVEL SPACINGS OF THE UNFOLDED SPECTRUM *)
(* Order the eigenvalues from lowest to highest values *)
```

```
Clear[Ener];
Ener = Sort[Table[Energy[[k]], {k, 1, dim}]];

(* Discard ~10% of the eigenvalues located at the borders of the spectrum *)
Clear[percentage, half, spacing];
percentage = 0.1 dim;
half = Floor[percentage / 2.];
Do[
  Clear[average];
  (* Compute the neighboring level spacings
   for the remaining eigenvalues after unfolding them *)
  (* Unfolding here means that the average of each
    group of 10 level spacings = 1 *)
  average = (Ener[[half + 10 j]] - Ener[[half + 10 (j - 1)]]) / 10.;
  Do[spacing[i] = (Ener[[half + i]] - Ener[[(half - 1) + i]]) / average;
   , {i, 1 + 10 (j - 1), 10 j}];
  , {j, 1, Floor[(dim - percentage) / 10]}];

(* HISTOGRAM *)
Clear[spcmin, spcmax, bin, Nofbins];
spcmin = 0.;
spcmax = 8.;
bin = 0.1;
Nofbins = IntegerPart[(spcmax - spcmin) / bin];

Clear[SPChist, Nhist];
SPChist[1] = spcmin;
Do[SPChist[i + 1] = SPChist[i] + bin, {i, 1, Nofbins}];
Do[Nhist[j] = 0., {j, 1, Nofbins}];

(* Nhist[j] gives how many spacings we have
 in the interval SPChist[j+1] and SPChist[j] *)
Do[
  Do[
    If[SPChist[j] ≤ spacing[k] < SPChist[j + 1], Nhist[j] = Nhist[j] + 1];
    , {j, 1, Nofbins}];
  , {k, 1, 10 Floor[(dim - percentage) / 10]}];

(* Normalization *)
Clear[Norma];
Norma = Sum[bin Nhist[j], {j, 1, Nofbins}];
Do[Nhist[j] = Nhist[j] / Norma, {j, 1, Nofbins}];

(* ListPlot with the obtained data *)
Clear[jj, nl];
jj = 0;
nl = {};
Do[jj += 1;
  nl = Append[nl, {SPChist[jj], Nhist[jj]}];
  nl = Append[nl, {SPChist[jj + 1], Nhist[jj]}];
  , {j, 1, Nofbins - 1}];
DataPlot = ListPlot[nl, Joined → True,
   PlotRange → {{0, 8}, {0, 1}}, PlotStyle → {Black, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
(* Theoretical curves *)
```

```
WignerDyson = Plot[Pi s / 2. Exp[-Pi s^2 / 4.],
   {s, 0, 8}, PlotRange → {0, 1}, PlotStyle → {Red, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
Poisson = Plot[Exp[-s], {s, 0, 8}, PlotRange → {0, 1}, PlotStyle → {Blue, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
(* The three curves together *)
Show[{DataPlot, WignerDyson, Poisson}, PlotRange → {{0, 4}, {0, 1.1}}]
```

- **(6) Level spacing distribution for NN+NNN (parity is taken into account)**

```
(* PARITY *)
(* First we find all pairs of equivalent basis vectors *)
(* Example: state 1100 pairs with state 0011 *)
Clear[i, j, k, pair];
Do[
  Do[Clear[mirror];
    mirror = 0;
    Do[mirror = mirror + Mod[basis[[i, k]] + basis[[j, L + 1 - k]], 2];
     , {k, 1, L}];
    If[mirror == 0, pair[i] = j];
    , {j, 1, dim}];
  , {i, 1, dim}];

(* Now we separate the eigenstates according to their parity, even or odd *)
Clear[Neven, Nodd];
(* Neven is the number of states with even parity *)
(* Nodd is the number of states with odd parity *)
Neven = 0;
Nodd = 0;
Do[
  Clear[project];
  project = 0;
  Do[ project = project + (1 / 4.) (Vector[[i]][[j]] + Vector[[i]][[pair[j]]])^2;
   , {j, 1, dim}];
  (* project will be very close to 1 if the parity is even *)
  (* project will be very close to 0 if the parity is odd *)
  If[1. - project < 0.001,
   {Neven = Neven + 1, even[Neven] = i}, {Nodd = Nodd + 1, odd[Nodd] = i}];
  , {i, 1, dim}];

(* FOR THE HISTOGRAM *)
Clear[spcmin, spcmax, bin, Nofbins];
spcmin = 0.;
spcmax = 8.;
bin = 0.1;
Nofbins = IntegerPart[(spcmax - spcmin) / bin];
(* Theoretical curves *)
Clear[WignerDyson, Poisson];
WignerDyson = Plot[Pi s / 2. Exp[-Pi s^2 / 4.],
   {s, 0, 8}, PlotRange → {0, 1}, PlotStyle → {Red, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
Poisson = Plot[Exp[-s], {s, 0, 8}, PlotRange → {0, 1}, PlotStyle → {Blue, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
```

```
(* EVEN EIGENSTATES *)
(* LEVEL SPACINGS OF THE UNFOLDED SPECTRUM *)
(* Order the eigenvalues *)
Clear[Ener];
Ener = Sort[Table[Energy[[even[k]]], {k, 1, Neven}]];
(* Discard ~10% of the eigenvalues located at the borders of the spectrum *)
Clear[percentage, half, spacing];
percentage = 0.1 Neven;
half = Floor[percentage / 2.];
(* Compute the level spacings for the
 remaining eigenvalues after unfolding them *)
(* Unfolding here means that the average of
  each group of 10 level spacings = 1 *)
Do[
  Clear[average];
  average = (Ener[[half + 10 j]] - Ener[[half + 10 (j - 1)]]) / 10.;
  Do[spacing[i] = (Ener[[half + i]] - Ener[[(half - 1) + i]]) / average;
   , {i, 1 + 10 (j - 1), 10 j}];
  , {j, 1, Floor[(Neven - percentage) / 10]}];
(* ... *)
(* HISTOGRAM -- EVEN *)
Clear[SPChist, Nhist];
SPChist[1] = spcmin;
Do[SPChist[i + 1] = SPChist[i] + bin, {i, 1, Nofbins}];
Do[Nhist[j] = 0., {j, 1, Nofbins}];
(* ... *)
Do[
  Do[
    If[SPChist[j] ≤ spacing[k] < SPChist[j + 1], Nhist[j] = Nhist[j] + 1];
    , {j, 1, Nofbins}];
  , {k, 1, 10 Floor[(Neven - percentage) / 10]}];
(* Normalization *)
Clear[Norma];
Norma = Sum[bin Nhist[j], {j, 1, Nofbins}];
Do[Nhist[j] = Nhist[j] / Norma, {j, 1, Nofbins}];
(* ... *)
(* ListPlot with the obtained data *)
Clear[jj, histEven, PlotEven];
jj = 0;
histEven = {};
Do[jj += 1;
  histEven = Append[histEven, {SPChist[jj], Nhist[jj]}];
  histEven = Append[histEven, {SPChist[jj + 1], Nhist[jj]}];
  , {j, 1, Nofbins - 1}];
PlotEven = ListPlot[histEven, Joined → True,
   PlotRange → {{0, 8}, {0, 1}}, PlotStyle → {Black, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
(* The three curves together *)
Print["Histogram for the even eigenstates"];
Show[{PlotEven, WignerDyson, Poisson}, PlotRange → {{0, 4}, {0, 1.2}}]
```

```
(* ODD EIGENSTATES *)
(* LEVEL SPACINGS OF THE UNFOLDED SPECTRUM *)
(* Order the eigenvalues *)
Clear[Ener];
Ener = Sort[Table[Energy[[odd[k]]], {k, 1, Nodd}]];
(* Discard ~10% of the eigenvalues located at the borders of the spectrum *)
Clear[percentage, half, spacing];
percentage = 0.1 Nodd;
half = Floor[percentage / 2.];
(* Compute the level spacings for the
 remaining eigenvalues after unfolding them *)
(* Unfolding here means that the average of
  each group of 10 level spacings = 1 *)
Do[
  Clear[average];
  average = (Ener[[half + 10 j]] - Ener[[half + 10 (j - 1)]]) / 10.;
  Do[spacing[i] = (Ener[[half + i]] - Ener[[(half - 1) + i]]) / average;
   , {i, 1 + 10 (j - 1), 10 j}];
  , {j, 1, Floor[(Nodd - percentage) / 10]}];
(* ... *)
(* HISTOGRAM -- ODD *)
Clear[SPChist, Nhist];
SPChist[1] = spcmin;
Do[SPChist[i + 1] = SPChist[i] + bin, {i, 1, Nofbins}];
Do[Nhist[j] = 0., {j, 1, Nofbins}];
(* ... *)
Do[
  Do[
    If[SPChist[j] ≤ spacing[k] < SPChist[j + 1], Nhist[j] = Nhist[j] + 1];
    , {j, 1, Nofbins}];
  , {k, 1, 10 Floor[(Nodd - percentage) / 10]}];
(* Normalization *)
Clear[Norma];
Norma = Sum[bin Nhist[j], {j, 1, Nofbins}];
Do[Nhist[j] = Nhist[j] / Norma, {j, 1, Nofbins}];
(* ... *)
(* ListPlot with the obtained data *)
Clear[jj, histOdd, PlotOdd];
jj = 0;
histOdd = {};
Do[jj += 1;
  histOdd = Append[histOdd, {SPChist[jj], Nhist[jj]}];
  histOdd = Append[histOdd, {SPChist[jj + 1], Nhist[jj]}];
  , {j, 1, Nofbins - 1}];
PlotOdd = ListPlot[histOdd, Joined → True,
   PlotRange → {{0, 8}, {0, 1}}, PlotStyle → {Black, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
(* The three curves together *)
Print["Histogram for the odd eigenstates"];
Show[{PlotOdd, WignerDyson, Poisson}, PlotRange → {{0, 4}, {0, 1.2}}]



(* AVERAGE of EVEN and ODD HISTOGRAMS *)
Clear[AveHist];
```

```
AveHist = (histEven + histOdd) / 2.;
PlotAve = ListPlot[AveHist, Joined → True,
   PlotRange → {{0, 8}, {0, 1}}, PlotStyle → {Black, Thick},
   LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"s", "P"}];
(* The three curves together *)
Print["Histogram for the averaged P(s) over even and odd parity"];
Show[{PlotAve, WignerDyson, Poisson}, PlotRange → {{0, 4}, {0, 1.2}}]
```