
EXERCISE 6: Quantum phase transition in the XXZ Hamiltonian

■ Code

```
Clear[L, dim, basis, Jxy];
L = 6;
dim = 2^L;
Jxy = 1.0;

(* BASIS *)
Do[
  basis[i] = IntegerDigits[i - 1, 2, L];
  , {i, 1, dim}];

Clear[Jztot];
(* LOOP FOR THE VALUES OF Jz *)
(* how many time in the loop*)
Jztot = 61;
Do[
  Jz = -1.5 + (kj - 1) 0.05;
  (* ELEMENTS OF THE HAMILTONIAN *)
  Clear[HH];
  (* Initialization *)
  Do[Do[HH[i, j] = 0., {i, 1, dim}], {j, 1, dim}];

  (* Diagonal elements *)
  Do[
    (* 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}];
    (* CLOSED chain *)
    If[basis[i][[1]] == basis[i][[L]],
      HH[i, i] = HH[i, i] + Jz / 4., HH[i, i] = HH[i, i] - Jz / 4.];
      , {i, 1, dim}];

  (* Off-diagonal elements *)
  Clear[howmany, site];
  Do[
    Do[
      (* To guarantee that coupling between subspaces are not added*)
      If[Sum[basis[i][[k]], {k, 1, L}] == Sum[basis[j][[k]], {k, 1, L}],
        (* 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.}]];
        (* CLOSED chain *)
        If[howmany == 2,
          If[site[2] - site[1] == L - 1, {HH[i, j] = Jxy / 2., HH[j, i] = Jxy / 2.}]];
        ];
      , {j, i + 1, dim}];
      , {i, 1, dim - 1}];
```

```

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

(* EIGENVALUES IN INCREASING ORDER *)
Clear[Energy, Vector];
aux = Sort[Table[{Ene[[k]], k}, {k, 1, dim}]];
Energy = Sort[Ene];
Vector = Table[Vec[[aux[[k, 2]]]], {k, 1, dim}];

(* STORE EIGENVALUES OF THE FIRST 5 STATES *)
Do[
  EnergyJz[k, kj] = Energy[[k]];
  , {k, 1, 5}];

(* MAGNETIZATION OF THE FIRST 5 STATES *)
Do[
  Mz[k, kj] =
    Sum[0.5 Vector[[k, kk]]^2 Sum[(-1)^(basis[kk][[j]] + 1), {j, 1, L}], {kk, 1, dim}];
  , {k, 1, 5}];

(* FOR THE FIDELITY *)
GS[kj] = Vector[[1]];

, {kj, 1, Jztot}];

```

■ Plots

```

<< PlotLegends` ;

Clear[TabEnergy, TabMag, TabFidel];
Do[
  TabEnergy[k] = Table[{-1.5 + (kj - 1) 0.05, EnergyJz[k, kj]}, {kj, 1, Jztot}];
  , {k, 1, 5}];
TabMag = Table[{-1.5 + (kj - 1) 0.05, Mz[1, kj]}, {kj, 1, Jztot}];
TabFidel = Table[{-1.5 + (kj - 1) 0.05, Abs[GS[kj - 1].GS[kj]]^2}, {kj, 2, 30}];

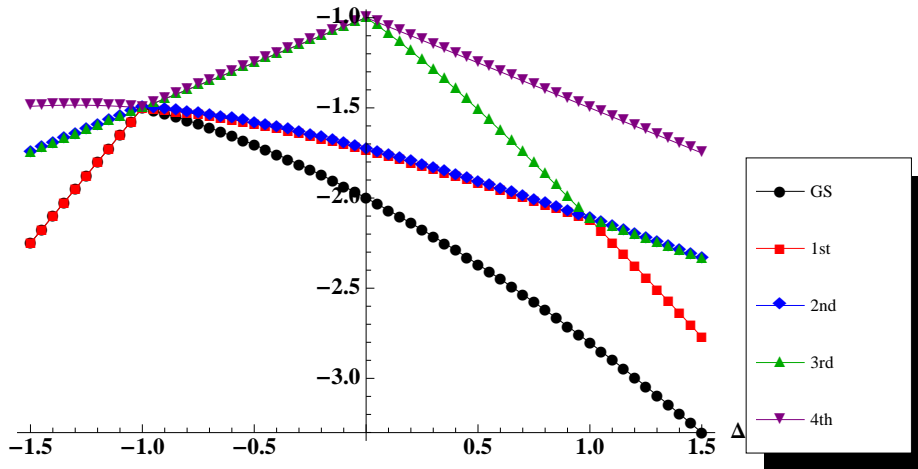
Print[];
Print["Energies of the 5 lowest levels for L=6"];
ListPlot[Table[TabEnergy[k], {k, 1, 5}], PlotMarkers → Automatic,
  Joined → True, PlotLegend → {"GS", "1st", "2nd", "3rd", "4th"},
  LegendPosition → {1, -0.6}, PlotStyle → {Black, Red, Blue, Darker[Green], Purple},
  LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"Δ"}, ImageSize → 500]

Print["Magnetization the GS for L=6"];
ListPlot[Table[TabMag, {k, 1, 2}], PlotMarkers → Automatic, Joined → True,
  PlotLegend → {"GS"}, LegendPosition → {1, -0.6}, PlotStyle → {Black},
  LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"Δ"}, ImageSize → 500]

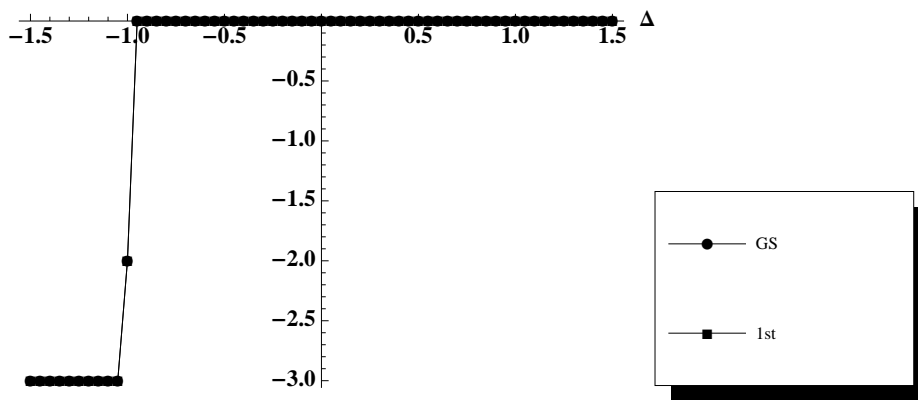
Print["Fidelity for L=6"];
ListPlot[TabFidel, PlotMarkers → Automatic, Joined → True,
  PlotLegend → {"GS", "1st"}, LegendPosition → {1, -0.6}, PlotStyle → {Black},
  LabelStyle → Directive[Black, Bold, Medium], AxesLabel → {"Δ"}, ImageSize → 500]

```

Energies of the 5 lowest levels for L=6



Magnetization the GS for L=6



Fidelity for L=6

