

XXZ model with NNN interaction

- Parameters of the Hamiltonian

- *) L = number of sites.
- *) 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 1111100000000000
- *) 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.

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(*PARAMETERS OF THE HAMILTONIAN*)
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Clear[L, upspins, downspins, dim, Jxy, Jz,  $\epsilon$ , defectsite, alpha, JJxy, JJz];
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L = 12;
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```
upspins = L / 2;
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downspins = L - upspins;
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```
dim = L! / (upspins! downspins!);
```

```
(*Impurity*)
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```
 $\epsilon$  = 0.0;
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```
defectsite = Floor[L / 2];
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```
(*Parameters for nearest-neighbor couplings*)
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Jxy = 1.0;
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```
Jz = 0;
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```
(*Parameters for next-nearest-neighbor couplings*)
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(*Set alpha=0 if NNN couplings do not exist*)
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```
alpha = 0.5;
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```
JJxy = 1.0;
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```
JJz = 0;
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(*BASIS*)
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```
Clear[onebasisvector, basis];
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```
onebasisvector =
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Flatten[{Table[1, {k, 1, upspins}], Table[0, {k, 1, downspins}]}];
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```
basis = Permutations[onebasisvector];
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(* 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] +  $\epsilon$  / 2., HH[i, i] = HH[i, i] -  $\epsilon$  / 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}];
  (* 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[
    (* 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}];

(*ELEMENTS OF THE HAMILTONIAN WITH NNN COUPLINGS*)
If[alpha > 0,
  (*Diagonal elements*)
  Do[
    (*Ising interaction*)

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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];

(*Choose an initial state*)
(*Do[
  If[basis[[i, 1]] * basis[[i, 2]] == 1 &&
    basis[[i, 2]] * basis[[i, 3]] == 1, initialstate = i];
, {i, 1, dim}]; *)
initialstate = 1;

(*DYNAMICS*)
Clear[endtime, PSI, increment, Magsite];
endtime = 51;
increment = .2;
Do[PSI[t] = Sum[Vector[[j, initialstate]]
  Vector[[j]] Exp[-I Energy[[j]] (t - 1) increment], {j, 1, dim}];
(*Magnetization*)
Do[Magsite[j, t] = 0.5 Sum[Abs[PSI[t] [[i]]]^2 (-1.)^(1 + basis[[i, j]]), {i, dim}];
, {j, 1, L}];
(*Print[{(t-1)increment, Magsite[1, t]}]; *)
, {t, 1, endtime}];

```

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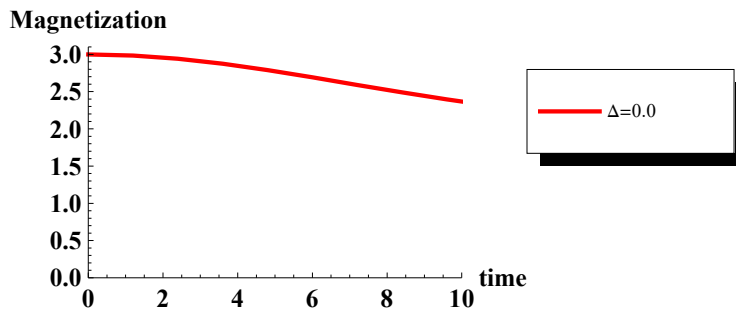
(*Call Package for Legends*)
<< PlotLegends`
Clear[magT];

Do[magT[j] = Table[{(t - 1) increment, Magsite[j, t]}, {t, 1, endtime}], {j, 1, L / 2}];
delta00 = Sum[magT[j], {j, 1, L / 2}];

Print[];
Print["Magnetization of each site"];
ListPlot[delta00, PlotRange -> {{0, 10}, {0, 3.1}},
  Joined -> True, PlotStyle -> {{Thick, Red}},
  LabelStyle -> Directive[Black, Bold, Medium], PlotLegend -> {" $\Delta=0.0$ "},
  LegendPosition -> {1, 0}, AxesLabel -> {"time", "Magnetization"}]

```

Magnetization of each site



Plot three figure together

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ListPlot[{delta00, delta05, delta10}, PlotRange -> {{0, 30}, {0, 3.1}},
  Joined -> True, PlotStyle -> {{Thick, Black}, {Thick, Red}, {Thick, Green}},
  LabelStyle -> Directive[Black, Bold, Medium],
  PlotLegend -> {" $\Delta=0.0$ ", " $\Delta=0.5$ ", " $\Delta=1.0$ "},
  LegendPosition -> {1, 0}, AxesLabel -> {"time", "Magnetization"}]

```

