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 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.

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(*PARAMETERS OF THE HAMILTONIAN*)
Clear[L, upspins, downspins, dim, Jxy, Jz, ϵ, defectsite, alpha, JJxy, JJz];
L = 12;
upspins = L / 2;
downspins = L - upspins;
dim = L! / (upspins! downspins!);
(*Impurity*)
ϵ = 0.0;
defectsite = Floor[L / 2];

(*Parameters for nearest-neighbor couplings*)
Jxy = 1.0;
 Jz = 1.0;
(*Parameters for next-nearest-neighbor couplings*)
(*Set alpha=0 if NNN couplings do not exist*)
alpha = 0;
JJxy = 1.0;
JJz = 1.0;

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

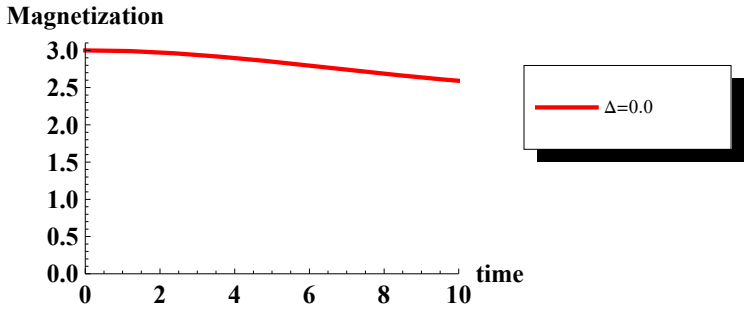
(*DYNAMICS*)
Clear[endtime, PSI, increment, Magsite];
endtime = 51;
increment = .2;
Do[PSI[t] = Sum[Vector[[j, initialstate]]
     Vector[[j]] Exp[-I Energy[[j]] (t - 1) increment], {j, 1, dim}];
(*Magnetization*)
Do[Magsite[j, t] = 0.5 Sum[Abs[PSI[t][[i]]]^2 (-1.)^(1 + basis[[i, j]]), {i, dim}];
, {j,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

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

Do[magT[j] = Table[{(t - 1) increment, Magsite[j, t]}, {t, 1, endtime}], {j, 1, L / 2}];
delta10 = Sum[magT[j], {j, 1, L / 2}];

Print[];
Print["Magnetization of each site"];
ListPlot[delta10, PlotRange → {{0, 10}, {0, 3.1}},
 Joined → True, PlotStyle → {{Thick, Red} },
 LabelStyle → Directive[Black, Bold, Medium], PlotLegend → {"Δ=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, 20}, {0, 3.1}},
 Joined → True, PlotStyle → {{Thick, Black}, {Thick, Red}, {Thick, Green}},
 LabelStyle → Directive[Black, Bold, Medium],
 PlotLegend → {"Δ=0.0", "Δ=0.5", "Δ=1.0"},
 LegendPosition → {1, 0}, AxesLabel → {"time", "Magnetization"}]
```

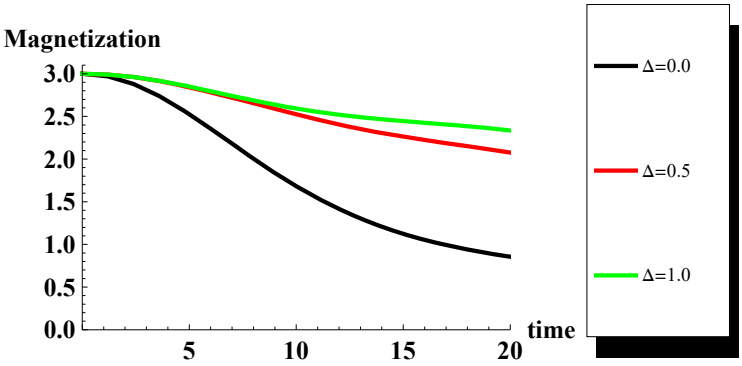
Magnetization
3.0
2.5
2.0
1.5
1.0
0.5
0.0
5
10
15
20
time
Δ=0.0
Δ=0.5
Δ=1.0