Quantum Field Theory Computations for Spin Systems

The QFT computations give a series approximation of the Quantum statistics partition function and time ordered correlation functions

(1) $Z = \mathrm{Tr}\left[e^{-\beta H}\right]$

(2) $\left\langle T\, S^{j_1}(v_1,\ t_1)\, S^{j_2}(v_2,\ t_2)\, S^{j_n}(v_n,\ t_n)\right\rangle = \mathrm{Tr}\left[T\, S^{j_1}(v_1,\ t_1)\, S^{j_2}(v_2,\ t_2)\, S^{j_n}(v_n,\ t_n)\, e^{-\beta H}\right] / \mathrm{Tr}\left[e^{-\beta H}\right]$

where $\beta = \frac{1}{k\,T}$ and $S_j(v,\ t) = e^{t\,H}\, S_j(v)\, e^{-t\,H}$ for t∈[0, β].

The input of the QFT computations is

Λ - a lattice,
V - an interaction tensor, and
h - an external magnetic field h.

These inputs encode the Hamiltonian of the system

(3) $H = -(2\ \Sigma_{v \in \Lambda}\ h(v) \cdot S(v)\ + \Sigma_{v, w \in \Lambda}\, S(v) \cdot V(v,\ w) \cdot S(w))$

In particular, we have

(4) $S(v) = (S_+(v),\ S_-(v),\ S_z(v))$ with $S_\pm(v) = S_x(v) \pm i\, S_y(v)$

and

(5) $V(v, w) = \left(V_{i,j}(v, w)\right)_{i,\, j = +, -, z}$

QFT Series Expansion Code

The time ordered correlation functions are obtained from functional derivatives of the partition function for a deformed Hamiltonian with auxiliary external magnetic fields. We introduce the Hamiltonian

(6) $H[p] = H + \Sigma_{v\in\Lambda}\, p(v)\cdot S(v)$,

and we set

(7) $Z[p] = \exp(-\beta\, H[p])$.

Then, the time order correlation functions are given as follows

(8) $\langle T\, S^{j_1}(v_1,\ t_1)\, S^{j_2}(v_2,\ t_2)\, S^{j_n}(v_n,\ t_n)\rangle = \frac{1}{Z}\lim_{p\to 0}\frac{\delta^n Z[p]}{\delta p_{j_1}(v_1, t_1)\cdots\delta p_{j_n}(v_n, t_n)}$

We compute the time correlation functions as a perturbative expansion centered on the partition function the Hamiltonian without any interactions. Take the Hamiltonian with no interactions

(9) $H_{\text{free}}[p] = \Sigma_{v\in\Lambda}\, p(v)\cdot S(v) - 2\,\Sigma_{v\in\Lambda}\ h(v)\cdot S(v)$,

and we set

(10) $W[p] = \exp(-\beta\, H_{\text{free}}[p])$.

Then, the partition function for the Hamiltonian with interactions is given by

(11) $Z[p] = \exp(\Phi)\, W[p]$

where F is a functional operator given as follows

(12) $\Phi :\ W[p] \mapsto \int_{[0,\beta]} V_{j_1, j_2}(v_1,\ v_2)\,\frac{\delta^2 W[p]}{\delta p_{j_1}(v_1, t)\,\delta p_{j_2}(v_2, t)}\, dt$.

We expand the functional above to obtain the

(13) $\exp(\Phi) = \Sigma_{k\geq 0}\,\frac{1}{k!}\,\Phi^{\circ k}$.

Additionally, we express each term in series above as a sum of functionals indexed by directed labelled graphs

(14) $\Gamma(k) = \{(\Lambda, E) :\ |E| = k,\ E\subset(\Lambda\times\{+, -, z\})^2\}$ - the set of directed labelled graphs with k edges.

Each edge $e\in(\Lambda\times\{+, -, z\})^2$ is a quadruple $e = (v_1(e),\ j_1(e);\ v_2(e),\ j_2(e))$ where $v_1,\ v_2\in\Lambda$ are the vertices of the graph and $j_1,\ j_2 \in \{+,\ -,\ z\}$ are the labels of the edge. We introduce the following operators indexed by a graph G∈ Γ(k)

$$(15)\quad \Phi_G : W[p] \mapsto \int_{[0,\beta]^k} \left(\Pi_{n=1,\dots,k} V_{j_1(e_n),\, j_2(e_n)}(v_1(e_n),\ v_2(e_n)) \frac{\delta^2}{\delta p_{j_1(e_n)}(v_1(e_n), t_n)\, \delta p_{j_2(e_n)}(v_2(e_n), t_n)} \right) W[p]\ \mathrm{d}t_1 \cdots \mathrm{d}t_k$$

where $E(G) = \{e_1,\ \dots,\ e_n\}$. Then,

$$(16)\quad \exp(\Phi) = \Sigma_{k \geq 0} \frac{1}{k!} \Sigma_{G \in \Gamma(k)} \Phi_G.$$

Thus, we compute the correlation function given in (2) as a series expansion using (8), (11), and (16).

Spin-1/2 Operators

We define the spin-1/2 operators where
$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $S_y = \frac{1}{2}\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$, $S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
and
$S_+ = S_x + I\, S_y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $S_- = S_x - I\, S_y = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$.
These operators are the basic building blocks of all the operators we treat.

In[142]:=

```
Sp = {{0, 0}, {1, 0}};
Sm = {{0, 1}, {0, 0}};
Sz = {{1 / 2, 0}, {0 , -1 / 2}};
Ops = {Sp, Sm, Sz, IdentityMatrix[2]};
```

Non-interacting Fields

We compute the partition function and the correlation functions for a Hamiltonian with external magnetic filed and no other interactions.

External Magnetic Field

In[146]:=

```
hm = 0;
hp = 0;
hz = 1;
HbExp[β_] :=
```

$$\left\{\left\{\mathrm{Cosh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]+\frac{\mathrm{hz\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}},\ \frac{\mathrm{hm\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}}\right\},\right.$$
$$\left.\left\{\frac{\mathrm{hp\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}},\ \mathrm{Cosh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]-\frac{\mathrm{hz\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}}\right\}\right\};$$

Correlations

In[150]:=

```
Corr[OpsList_, β_] := Module[{op, n, i},
  op = IdentityMatrix[2];
  n = Length[OpsList];
  For[i = 1, i ≤ n, i++,
   op = op.HbExp[OpsList〚i〛〚2〛].Ops〚OpsList〚i〛〚1〛〛.HbExp[-OpsList〚i〛〚2〛]];
  op = op.HbExp[β];
  Return[Tr[op]];
 ]
```

Interaction Paths

In[151]:=

```
Interactions[λ_, len_] := Module[{int, Paths, SpinLabels, i, j},
  Paths = Tuples[Range[λ], 2 len];
  SpinLabels = Tuples[{1, 2, 3}, 2 len];
  int = {};
  For[i = 1, i ≤ Length[Paths], i++,
   For[j = 1, j ≤ Length[SpinLabels],
    j++, If[Product[V[Λ〚Paths〚i〛〚2 k - 1〛〛, Λ〚Paths〚i〛〚2 k〛〛 ,
        SpinLabels〚j〛〚2 k - 1〛, SpinLabels〚j〛〚2 k〛], {k, 1, len}] ≠ 0,
     AppendTo[int, {Paths〚i〛, SpinLabels〚j〛}]] ]
  ];
  Return[int];
 ]
```

Interaction Contribution

In[154]:=

```
InteractionContribution[λ_, path_, β_] :=
 Module[{OpsLists, i, τ, InterTerm, InterCoupling, k, n},
  n = Length[path[[1]]] / 2;
  OpsLists = Table[{}, {i, 1, λ}];
  If[n == 0, Return[Product[Corr[OpsLists[[i]], β], {i, 1, Length[OpsLists]}]]];
  For[i = 1, i ≤ 2 n, i++,
   AppendTo[OpsLists[[path[[1]][[i]]]], {path[[2]][[i]], τ[Floor[(i + 1) / 2]]}]];
  InterTerm = Product[Corr[OpsLists[[i]], β], {i, 1, Length[OpsLists]}];
  InterCoupling = Product[V[Λ[[path[[1]][[2 i - 1]]]], Λ[[path[[1]][[2 i]]]],
     path[[2]][[2 i - 1]], path[[2]][[2 i]]], {i, 1, Length[path[[1]]] / 2}];
  Return[(1/n!) Integrate[InterCoupling * InterTerm,
     Sequence @@ Table[{τ[k], 0, β}, {k, 1, n}]]];
 ]
NInteractionContribution[λ_, path_, β_] :=
 Module[{OpsLists, i, τ, InterTerm, InterCoupling, k, n},
  n = Length[path[[1]]] / 2;
  OpsLists = Table[{}, {i, 1, λ}];
  If[n == 0, Return[Product[Corr[OpsLists[[i]], β], {i, 1, Length[OpsLists]}]]];
  For[i = 1, i ≤ 2 n, i++,
   AppendTo[OpsLists[[path[[1]][[i]]]], {path[[2]][[i]], τ[Floor[(i + 1) / 2]]}]];
  InterTerm = Product[Corr[OpsLists[[i]], β], {i, 1, Length[OpsLists]}];
  InterCoupling = Product[V[path[[1]][[2 i - 1]], path[[1]][[2 i]],
     path[[2]][[2 i - 1]], path[[2]][[2 i]]], {i, 1, Length[path[[1]]] / 2}];
  Return[(1/n!) NIntegrate[InterCoupling * InterTerm,
     Table[τ[k], {k, 1, n}] ∈ Cuboid[Table[0, {k, 1, n}], Table[β, {k, 1, n}]]]];
 ]
```

Partition Function

In[156]:=

```
Z[deg_, β_] := Module[{paths, i, len},
  paths = Flatten[Table[Interactions[λ, len], {len, 0, deg}], 1];
  Return[Sum[InteractionContribution[λ, paths〚i〛, β], {i, 1, Length[paths]}]]
   ]
NZ[deg_, β_] := Module[{paths, i, len},
  paths = Flatten[Table[Interactions[λ, len], {len, 0, deg}], 1];
  Return[Sum[NInteractionContribution[λ, paths〚i〛, β], {i, 1, Length[paths]}]]
  ]
```

One-point Correlation Function

Contributions

In[160]:=

```
OnePointContribution[λ_, path_, β_, vertexIndex_, spinIndex_, t_] :=
 Module[{OpsLists, i, τ, InterTerm, InterCoupling, k, n},
  n = Length[path〚1〛] / 2;
  OpsLists = Table[{}, {i, 1, λ}];
  For[i = 1, i ≤ 2 n, i++,
   AppendTo[OpsLists〚path〚1〛〚i〛〛, {path〚2〛〚i〛, τ[Floor[(i + 1) / 2]]}]];
  AppendTo[OpsLists〚vertexIndex〛, {spinIndex, t}];
  InterTerm = Product[Corr[OpsLists〚i〛, β], {i, 1, Length[OpsLists]}];
  If[n == 0, Return[InterTerm]];
  InterCoupling = Product[V[Λ〚path〚1〛〚2 i - 1〛〛, Λ〚path〚1〛〚2 i〛〛,
     path〚2〛〚2 i - 1〛, path〚2〛〚2 i〛], {i, 1, Length[path〚1〛] / 2}];
  Return[(1/n!) Integrate[InterCoupling * InterTerm,
     Sequence @@ Table[{τ[k], 0, β}, {k, 1, n}]]];
 ]
NOnePointContribution[λ_, path_, β_, vertexIndex_, spinIndex_, t_] :=
 Module[{OpsLists, i, τ, InterTerm, InterCoupling, k, n},
  n = Length[path〚1〛] / 2;
  OpsLists = Table[{}, {i, 1, λ}];
  For[i = 1, i ≤ 2 n, i++,
   AppendTo[OpsLists〚path〚1〛〚i〛〛, {path〚2〛〚i〛, τ[Floor[(i + 1) / 2]]}]];
  AppendTo[OpsLists〚vertexIndex〛, {spinIndex, t}];
  InterTerm = Product[Corr[OpsLists〚i〛, β], {i, 1, Length[OpsLists]}];
  If[n == 0, Return[InterTerm]];
  InterCoupling = Product[V[path〚1〛〚2 i - 1〛, path〚1〛〚2 i〛,
     path〚2〛〚2 i - 1〛, path〚2〛〚2 i〛], {i, 1, Length[path〚1〛] / 2}];
  Return[(1/n!) NIntegrate[InterCoupling * InterTerm,
     Table[τ[k], {k, 1, n}] ∈ Cuboid[Table[0, {k, 1, n}], Table[β, {k, 1, n}]]]];
 ]
```

Expansion

In[164]:=

```
OnePoint[deg_, β_, vertexIndex_, spinIndex_, t_] := Module[{paths, i, len},
  paths = Flatten[Table[Interactions[λ, len], {len, 0, deg}], 1];
  Return[Sum[OnePointContribution[λ, paths⟦i⟧,
     β, vertexIndex, spinIndex, t], {i, 1, Length[paths]}]]
  ]
NOnePoint[deg_, β_, vertexIndex_, spinIndex_, t_] := Module[{paths, i, len},
  paths = Flatten[Table[Interactions[λ, len], {len, 0, deg}], 1];
  Return[Sum[NOnePointContribution[λ, paths⟦i⟧,
     β, vertexIndex, spinIndex, t], {i, 1, Length[paths]}]]
 ]
```

Correlation Function for 3x3x2 Lattice

Set up

Lattice

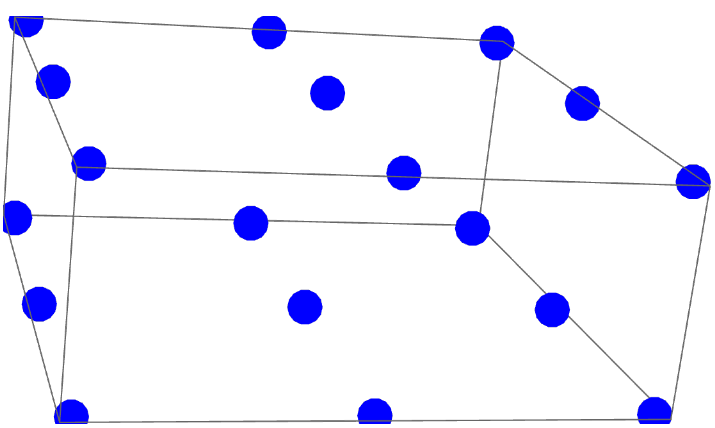
In[166]:=

```
L = 1;
Λ1 = Flatten[Table[{i, j, 0}, {i, -L, L}, {j, -L,  L}], 1];
Λ2 = Flatten[Table[{i, j, 1}, {i, -L, L}, {j, -L,  L}], 1];
Λ = Union[Λ1, Λ2];
λ = Length[Λ];
```

In[8]:=

```
ListPointPlot3D[Λ, PlotStyle → {Blue, PointSize[0.05]},
 Axes → False, PlotRange → Full]
```

Out[8]=



External Magnetic Field

In[171]:=

```
hm = 0;
hp = 0;
hz = 0.005;
HbExp[β_] :=
```

$$\left\{\left\{\mathrm{Cosh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]+\frac{\mathrm{hz\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}},\ \frac{\mathrm{hm\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}}\right\},\right.$$
$$\left.\left\{\frac{\mathrm{hp\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}},\ \mathrm{Cosh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]-\frac{\mathrm{hz\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}}\right\}\right\};$$

Interaction Tensors

Constants

In[175]:=

```
a = 1;
b = 1;
c = 2.2688141391106043`;
LS = {{a, 0, 0}, {0, b, 0}, {0, 0, c}};
Ja = -29.196403937649`;
Jb = -29.196403937649`;
Jc = 0.43189946653326927`;
Ds = 0.5399190454220628`;
βscaling = 1.3434276312661886`;
```

Spin-Spin exchange Interaction

In[184]:=

```
V1[v1_, v2_, s1_, s2_] := Module[{r, dx, dy, dz},
  r = Norm[(v1 - v2)];
  If[r ≠ 1, Return[0] ];
  dx = Norm[(v1 - v2)⟦1⟧];
  If[dx == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Ja / 4], If[s1 == 3 && s2 == 3, Return[Ja / 2]]]];
  dy = Norm[(v1 - v2)⟦2⟧];
  If[dy == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jb / 4], If[s1 == 3 && s2 == 3, Return[Jb / 2]]]];
  dz = Norm[(v1 - v2)⟦3⟧];
  If[dz == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jc / 4], If[s1 == 3 && s2 == 3, Return[Jc / 2]]]];
  Return[0];
 ]
```

Dipole Interaction

In[185]:=

```
V2[v1_, v2_, s1_, s2_] := Module[{r, dx, dy, dz},
  If[v1 == v2, Return[0]];
  r = Norm[LS.(v1 - v2)];
  dx = (LS. v1 - v2)[[1]];
  dy = (LS. v1 - v2)[[2]];
  dz = (LS. v1 - v2)[[3]];
  If[s1 == 1 && s2 == 1, Return[-3/8 Ds (dx - ⅈ dy)^2 / r^5]];
  If[s1 == 1 && s2 == 2, Return[-1/8 Ds (3 dx^2 + 3 dy^2 - 2 r^2) / r^5]];
  If[s1 == 1 && s2 == 3, Return[-3/4 Ds (dx - ⅈ dy) dz / r^5]];
  If[s1 == 2 && s2 == 1, Return[-1/8 Ds (3 dx^2 + 3 dy^2 - 2 r^2) / r^5]];
  If[s1 == 2 && s2 == 2, Return[-3/8 Ds (dx + ⅈ dy)^2 / r^5]];
  If[s1 == 2 && s2 == 3, Return[-3/4 Ds (dx + ⅈ dy) dz / r^5]];
  If[s1 == 3 && s2 == 1, Return[-3/4 Ds (dx - ⅈ dy) dz / r^5]];
  If[s1 == 3 && s2 == 2, Return[-3/4 Ds (dx + ⅈ dy) dz / r^5]];
  If[s1 == 3 && s2 == 3, Return[-1/2 Ds (3 dz^2 - r^2) / r^5]];
  Return[0];
 ]
V[v1_, v2_, s1_, s2_] := V1[v1, v2, s1, s2] + V2[v1, v2, s1, s2];
```

Correlation Function: dipole, Sz

In[187]:=

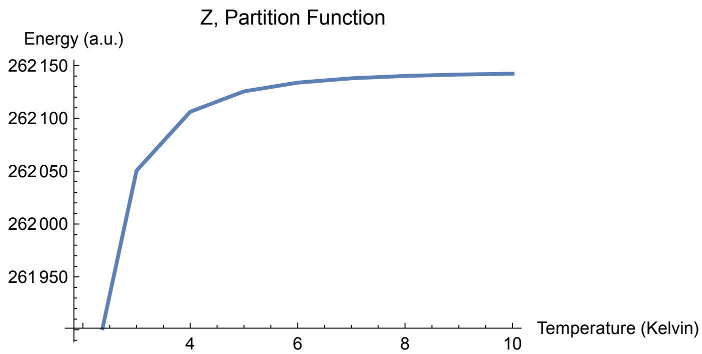
```
acc = 1;
vIndex = 9;
sIndex = 3;(*3→Sz spin operator*)
t = 0;(*One-point correlations are independent of time b/c traces of linear
  operators are invariant under cyclic permutation of operators.*)
Tmin = 2;
Tmax = 10;
Tdelta = 1;
```

In[∘]:=

```
ZT = Table[{T, Z[acc, βscaling / T]}, {T, Tmin , Tmax, Tdelta}];
```

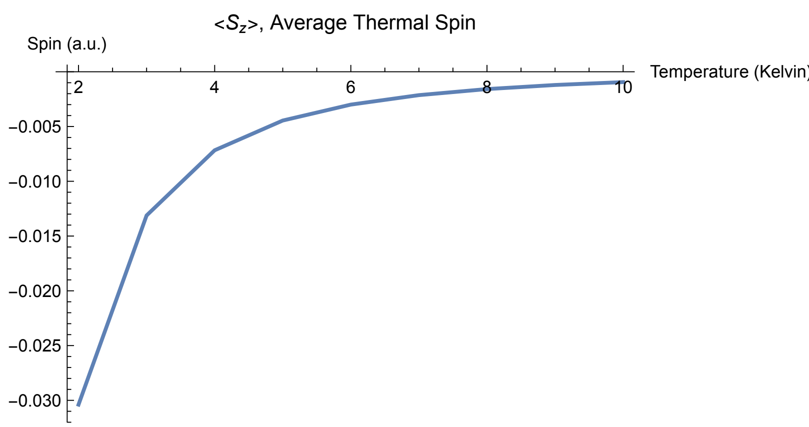
```
In[ ]:= OzTun =
          Table[OnePoint[acc, βscaling / T, vIndex, sIndex, t], {T, Tmin, Tmax, Tdelta}];

In[ ]:= OzT = Table[{ZT⟦k⟧⟦1⟧, OzTun⟦k⟧ / ZT⟦k⟧⟦2⟧}, {k, 1, Length[ZT]}];

In[ ]:= ListPlot[ZT, Joined → True, AxesLabel → {"Temperature (Kelvin)", "Energy (a.u.)"},
         PlotLabel → "Z, Partition Function"]
```

Out[ ]=




```
In[ ]:= P1 = ListPlot[OzT, Joined → True,
          AxesLabel → {"Temperature (Kelvin)", "Spin (a.u.)"},
          PlotLabel → "<Sz>, Average Thermal Spin"]
```

Out[ ]=



Dispersion relations and low relaxation of spin waves in thin magnetic films

Constants

In[338]:=

```
(*Plank's constant*)
ℏ = 6.582119569 * 10^-16 ;(*eV sec*)
ℏSI = 1.054571817 × 10^-34;(*Joules seconds*)
(*Bohr magneton*)
μb = 5.7883818060 × 10^-5; (*eV per Tesla*)
μbSI = 9.2740100657 × 10^-24;(*Joules per Tesla*)
(*Vacuum permeability*)
μ0 = 1.256637 × 10^-6; (*Newton per Ampere squared*)
(*Spin*)
S = 1 / 2;
(*Lande factor*)
g = 2; (*from google*)
(*The gyromagnetic ratio*)
γ = g μb / ℏ;
γSI = g μbSI / ℏ;
(*Inverse temperature*)
k = 8.617333262 × 10^-5;(*eV per Kelvin*)(*Boltzman constant*)
T = 100;(*Kelvin*)(*Temperature*)
β = 1/(k T);
(*Lattice distance*)
a = 3.508 × 10^-10;(*meters*)
(*Ref:"CrSBr: an air-stable, two-dimensional magnetic semiconductor"*)
Sa = a^2; (*See Equation (17)*)
(*Distance between layers*)
d = 7.959 × 10^-10;(*meters*)
(*Ref:"CrSBr: an air-stable, two-dimensional magnetic semiconductor"*)
(*Inter-layer coupling, i.e. coupling in the same layer.*)
I0 = - 3.38 × 10^-3; (*eV*)
(*Ref: "Spin Waves and Magnetic Exchange Hamiltonian for CrSBr"*)
(*Intra-layer coupling, i.e. coupling between diferent layers.*)
Id = 0.05 × 10^-3; (*eV*)
(*External magetic field*)
H = 0.01;(*Tesla*)
(*z-Spin, Thermal Average*)
SzAvg = -0.003;(*arbitrary units*)
(*We obtain this quantity from QFT computation in the
 previous computation block "Correlation for 3x3x2 lattice".*)
```

Scaling

In[ ]:=
```
(*magnetic energy*)
{ g μbSI, (g μbSI) / (g μbSI) }
(*spin-spin exchange, same layer*)
{I0 (1.602176 × 10^-19), I0 (1.602176 × 10^-19) / (g μbSI) }
(*spin-spin exchange, different layer*)
{Id (1.602176 × 10^-19), Id (1.602176 × 10^-19) / (g μbSI)}
(*Dipole energy*)
{μ0 (g μbSI)^2 / a^3, μ0 (g μbSI)^2 / (a^3 (g μbSI))}
(*lattice spacing: in layer, out of layer*)
{a, d, a / a, d / a}
(*Boltzman weight*)
{1 / k, (g μb) / (k)}
```

Out[ ]= $\{1.8548 \times 10^{-23}, 1.\}$

Out[ ]= $\{-5.41535 \times 10^{-22}, -29.1964\}$

Out[ ]= $\{8.01088 \times 10^{-24}, 0.431899\}$

Out[ ]= $\{1.00144 \times 10^{-23}, 0.539919\}$

Out[ ]= $\{3.508 \times 10^{-10}, 7.959 \times 10^{-10}, 1., 2.26881\}$

Out[ ]= $\{11\,604.5, 1.34343\}$

Spin waves in magnetic bilayer

Demagnetization Fields

In[358]:=

$$\text{Dstrength} = \text{NSum}\left[\frac{4}{\left(x^2+y^2\right)^{3/2}}, \{x, 0, \infty\}, \{y, 1, \infty\}\right] + \text{NSum}\left[\frac{1-3\left(\frac{d}{a}\right)^2}{\left(\left(\frac{d}{a}\right)^2+x^2+y^2\right)^{3/2}}, \{x, -\infty, \infty\}, \{y, -\infty, \infty\}\right]$$

(*Multiplicative factor for the dipole interactions for two parallel infinite 2D lattices*)

NSum : Summand (or its derivative) $-\frac{12.\,x\,\sqrt{x^2+y^2}}{\left(\left(x^2+y^2\right)^{1.5}\right)^2}$ is not numerical at point y = 1.`.

NSum : Summand (or its derivative) $-\frac{3.\,(1.-1.\,(3.\,5.14752))\,x\,\sqrt{5.14752+x^2+y^2}}{\left(\left(5.14752+x^2+y^2\right)^{1.5}\right)^2}$ is not numerical at point y = 0.

NSum : Summand (or its derivative) $-\frac{3.\,(1.-1.\,(3.\,5.14752))\,x\,\sqrt{5.14752+x^2+y^2}}{\left(\left(5.14752+x^2+y^2\right)^{1.5}\right)^2}$ is not numerical at point y = 0.

General : Further output of NSum::nsnum will be suppressed during this calculation.

Out[358]=

-30.9633

In[359]:=

$$\text{Dstrength} = \text{NSum}\left[\frac{4}{\left(x^2+y^2\right)^{3/2}}, \{x, 0, 1\}, \{y, 1, 1\}\right] + \text{NSum}\left[\frac{1-3\left(\frac{d}{a}\right)^2}{\left(\left(\frac{d}{a}\right)^2+x^2+y^2\right)^{3/2}}, \{x, -1, 1\}, \{y, -1, 1\}\right]$$

(*Multiplicative factor for the dipole interactions for two parallel 3x3 2D lattices*)

Out[359]=

-2.6358

In[360]:=

```
(*He is the exchange field given by Equation (10)*)
```

$$He = \left(\frac{4\,I0 + Id}{g\,\mu b}\right) SzAvg$$

```
(*Hm is the depolarizing magnetic field given by Equation (10)*)
```

$$Hm = \left(\frac{4\,\pi\,g\,\mu bSI\,\mu 0\,Dstrength}{a^3}\right) SzAvg$$

Out[360]=

0.349061

Out[361]=

0.0536503

Normal magnetized films

In[362]:=

```
S = 1 / 2;
(*Hc is the self-consistent field*)
Hc = Hm + He;
(*Brillouin function B_S[p] and B[p] = S B_S[S p]*)
```

$$B[p\_] := \left(S + \frac{1}{2}\right) Coth\left[\left(S + \frac{1}{2}\right) p\right] - \frac{1}{2} Coth\left[\frac{p}{2}\right];$$

```
p = β g μb Abs[H + Hc];
(*σm is the surface magnetic moment density*)
σm = g μb B[p] / Sa;
```

$$q = \sqrt{qx^2 + qy^2};$$

```
(*Equation (21)*)
```

$$\Omega[qx\_, qy\_, qz\_] := \gamma\,(H + Hm) + \frac{2\,B[p]\,I0}{\hbar}\,(2 - Cos[qx\,a] - Cos[qy\,a])$$

In[369]:=

```
(*Dispersion relation given by Equation (23)*)
(*Ref:"Dispersion relations and low
   relaxation of spin waves in thin magnetic films"*)
```

$$\omega 1[qx\_, qy\_, qz\_] := \left(\Omega[qx, qy, qz]\left(\Omega[qx, qy, qz] + 2\,\pi\left(\frac{g^2\,\mu bSI^2\,B[p]\,\mu 0}{Sa\,\hbar SI}\right)\sqrt{qx^2 + qy^2}\left(1 + Exp\left[-\sqrt{qx^2 + qy^2}\,d\right]\right)\right)\right)^{1/2}$$

$$\omega 2[qx\_, qy\_, qz\_] := \left(\left(\Omega[qx, qy, qz] + \frac{2\,B[p]\,Id}{\hbar}\right)\left(\Omega[qx, qy, qz] + \frac{2\,B[p]\,Id}{\hbar} + 2\,\pi\left(\frac{g^2\,\mu bSI^2\,B[p]\,\mu 0}{Sa\,\hbar SI}\right)\sqrt{qx^2 + qy^2}\left(1 - Exp\left[-\sqrt{qx^2 + qy^2}\,d\right]\right)\right)\right)^{1/2}$$

In[371]:=

```
Ω[0, 0, 0] / 10^9
ω1[0, 0, 10] / 10^9
ω2[10^3, -10^3, 10] / 10^9
```

Out[371]=

11.1949

Out[372]=

11.1949

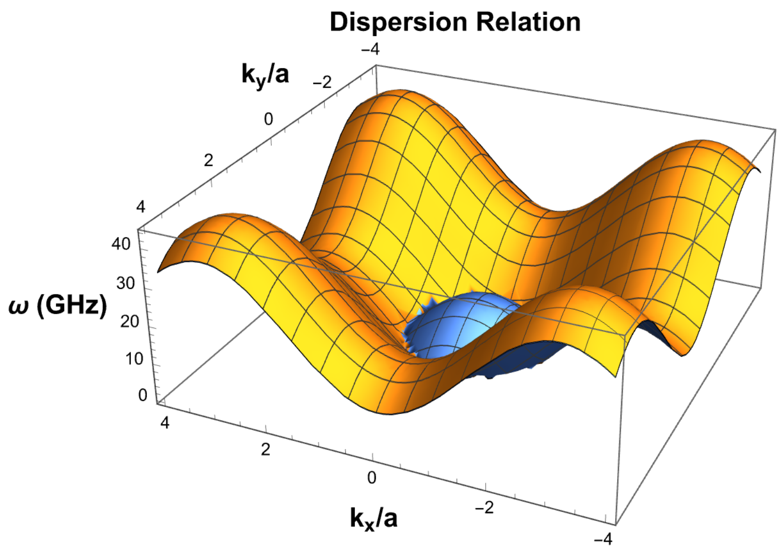
Out[373]=

11.4055

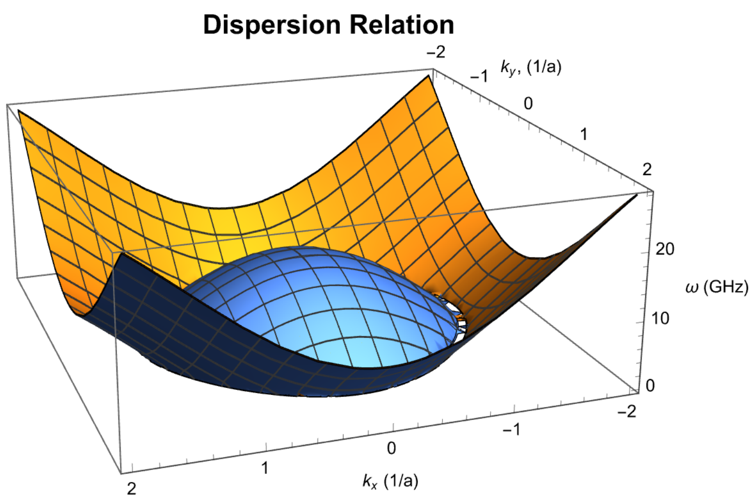
In[374]:=

```
WNscale = 1 / a;(*Wave number scaling, 1/lattice spacing*)
Fscale = 10^9;(*Frequency scaling, GHz*)
Plot3D[
 {ω1[qx WNscale, qy WNscale, 0] / Fscale, ω2[qx WNscale, qy WNscale, 0] / Fscale},
 {qx, -4, 4}, {qy, -4 , 4 }, PlotRange → Full, AxesLabel →
  {Text[Style["kx/a", Bold, Black, 14]], Text[Style["ky/a", Bold, Black, 14]],
   Text[Style["ω (GHz)", Bold, Black, 14]]},
 PlotLabel → Text[Style["Dispersion Relation", Bold, Black, 14]]]
Plot3D[{ω1[qx WNscale, qy WNscale, 0] / Fscale,
  ω2[qx WNscale, qy WNscale, 0] / Fscale}, {qx, -4 / 2, 4 / 2}, {qy, -4 / 2 , 4 / 2 },
 PlotRange → Full, AxesLabel → {"kx (1/a)", "ky, (1/a)", "ω (GHz)"},
 PlotLabel → Text[Style["Dispersion Relation", Bold, Black, 14]]]
```

Out[376]=



Out[377]=



Comparing QFT and exact computations

We check that the QFT computations give us the right computations. We perform the QFT computations and the exact computations and compare.

The input of the QFT computations is a lattice Λ, an interaction tensor V, and an external magnetic field h. These inputs encode the Hamiltonian of the system

$$H = -(2 \Sigma_{v\in\Lambda} \; h(v)\cdot S(v) + \Sigma_{v,w\in\Lambda} S(v)\cdot V(v, w)\cdot S(w))$$

In particular, we have

$$S(v) = (S_+(v), S_-(v), S_z(v)) \text{ with } S_\pm(v) = S_x(v) \pm i\, S_y(v)$$

and

$$V(v, w) = \left(V_{i,j}(v, w)\right)_{i,\, j = +, -, z}$$

We compare with the Hamiltonian for the XXX spin-1/2 chain. We take the lattice

$$\Lambda = \{1, 2, \ldots, \lambda\}$$
$$H = -\Sigma_{k=1,\ldots,\lambda} \; 2\; h(k)\cdot S(k) - J\; \Sigma_{k=1,\ldots,\lambda-1} S(k)\cdot S(k+1)$$

The corresponding interaction tensor in this case is

$$V(k, k\pm 1) = \begin{pmatrix} 0 & J/4 & 0 \\ J/4 & 0 & 0 \\ 0 & 0 & J/2 \end{pmatrix} \text{ and } V(k, j) = 0 \text{ for } j\neq k\pm 1$$

The QFT computations give a series approximation of the Quantum statistics partition function and correlation functions

$$Z[\beta] = \mathrm{Tr}\left[e^{-\beta H}\right]$$
$$\langle S(v)\rangle = \mathrm{Tr}\left[S(v)\, e^{-\beta H}\right]$$

where $\beta = \frac{1}{k\,T}$.

○ Example: L=2 XXZ line

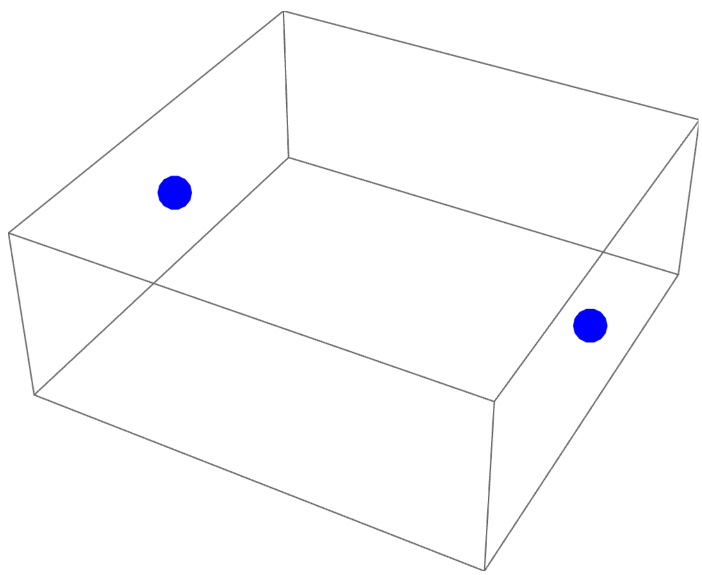
QFT computations

Lattice

In[194]:=

```
L = 2;
Λ = Table[{i, 0, 0}, {i, 1, L}];
λ = Length[Λ];
ListPointPlot3D[Λ, PlotStyle → {Blue, PointSize[0.05]},
 Axes → False, PlotRange → Full]
```

Out[197]=



External Magnetic Field

In[198]:=

```
hm = 0;
hp = 0;
hz = 0.01;
HbExp[β_] :=
```

$$\left\{\left\{\mathrm{Cosh}\left[\sqrt{hm\,hp + hz^2}\;\beta\right] + \frac{hz\,\mathrm{Sinh}\left[\sqrt{hm\,hp + hz^2}\;\beta\right]}{\sqrt{hm\,hp + hz^2}}, \frac{hm\,\mathrm{Sinh}\left[\sqrt{hm\,hp + hz^2}\;\beta\right]}{\sqrt{hm\,hp + hz^2}}\right\},\right.$$
$$\left.\left\{\frac{hp\,\mathrm{Sinh}\left[\sqrt{hm\,hp + hz^2}\;\beta\right]}{\sqrt{hm\,hp + hz^2}}, \mathrm{Cosh}\left[\sqrt{hm\,hp + hz^2}\;\beta\right] - \frac{hz\,\mathrm{Sinh}\left[\sqrt{hm\,hp + hz^2}\;\beta\right]}{\sqrt{hm\,hp + hz^2}}\right\}\right\};$$

Interaction Tensors

Constants

In[202]:=

```
a = 1;
b = 1;
c = 1;
LS = {{a, 0, 0}, {0, b, 0}, {0, 0, c}};
Ja = 1;
Jb = 1;
Jc = 1;
Ds = 1;
βscaling = 1;
```

Spin-Spin exchange Interaction

In[211]:=

```
V[v1_, v2_, s1_, s2_] := Module[{r, dx, dy, dz},
  r = Norm[(v1 - v2)];
  If[r ≠ 1, Return[0] ];
  dx = Norm[(v1 - v2)〚1〛];
  If[dx == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Ja / 4], If[s1 == 3 && s2 == 3, Return[Ja / 2]]]];
  dy = Norm[(v1 - v2)〚2〛];
  If[dy == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jb / 4], If[s1 == 3 && s2 == 3, Return[Jb / 2]]]];
  dz = Norm[(v1 - v2)〚3〛];
  If[dz == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jc / 4], If[s1 == 3 && s2 == 3, Return[Jc / 2]]]];
  Return[0];
 ]
```

In[∘]:=

```
Table[V[Λ〚1〛, Λ〚2〛, s1, s2], {s1, 1, 3}, {s2, 1, 3}] // MatrixForm
```

Out[∘]//MatrixForm=

$$\begin{pmatrix} 0 & \frac{Ja}{4} & 0 \\ \frac{Ja}{4} & 0 & 0 \\ 0 & 0 & \frac{Ja}{2} \end{pmatrix}$$

Correlation Function: Sz

In[212]:=

```
acc = 2;
vIndex = 1;
sIndex = 3;(*3→Sz spin operator*)
t = 0;(*One-point correlations are independent of time b/c traces of linear
  operators are invariant under cyclic permutation of operators.*)
Tmin = 2;
Tmax = 10;
Tdelta = 1;
```

In[219]:=

```
ZT = Table[{T, Z[acc, βscaling / T]}, {T, Tmin , Tmax, Tdelta}];
```

In[220]:=

```
OzTun =
  Table[OnePoint[acc, βscaling / T, vIndex, sIndex, t], {T, Tmin, Tmax, Tdelta}];
```

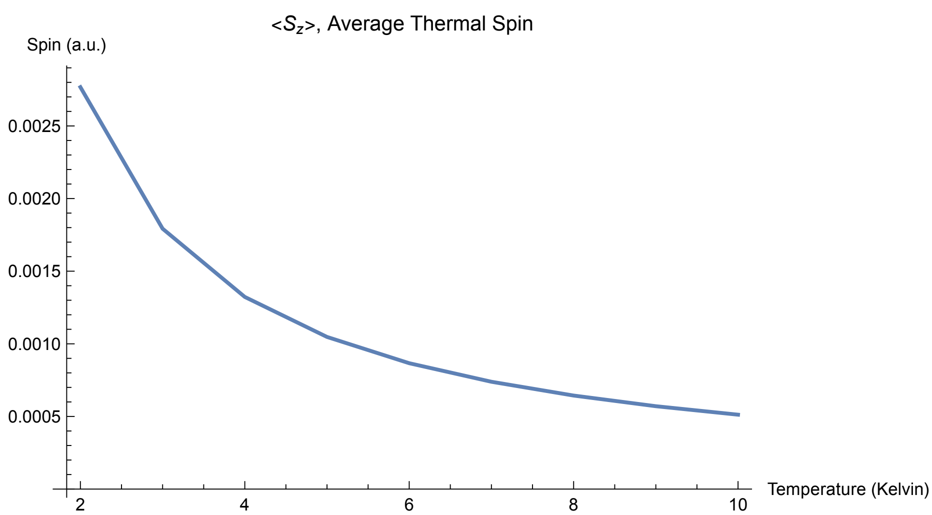
In[221]:=

```
OzT = Table[{ZT〚k〛〚1〛, OzTun〚k〛 / ZT〚k〛〚2〛}, {k, 1, Length[ZT]}];
```

In[222]:=

```
P1 = ListPlot[OzT, Joined → True,
  AxesLabel → {"Temperature (Kelvin)", "Spin (a.u.)"},
  PlotLabel → "<Sz>, Average Thermal Spin"]
```

Out[222]=



Exact Computations

Local Hamiltonians

In[223]:=

```
h = (Ja / 2) (KroneckerProduct[Sp, Sm] + KroneckerProduct[Sm, Sp]) +
    Ja (KroneckerProduct[Sz, Sz]);
Sz = {{1 / 2, 0}, {0 , -1 / 2}};
```

Hamiltonian

In[225]:=

```
H = - (Sum[KroneckerProduct[IdentityMatrix[2^(k-1)], h, IdentityMatrix[2^(λ-k-1)] ],
        {k, 1, λ - 1}] + 2 Sum[KroneckerProduct[IdentityMatrix[2^(k-1)],
          hz Sz, IdentityMatrix[2^(λ-k)]], {k, 1, λ}]);
```

In[ ]:= MatrixForm[H]

Out[ ]//MatrixForm=

$$\begin{pmatrix} -0.02 - \frac{Ja}{4} & 0. & 0. & 0. \\ 0. & 0. + \frac{Ja}{4} & 0. - \frac{Ja}{2} & 0. \\ 0. & 0. - \frac{Ja}{2} & 0. + \frac{Ja}{4} & 0. \\ 0. & 0. & 0. & 0.02 - \frac{Ja}{4} \end{pmatrix}$$

Expected Values

In[226]:=

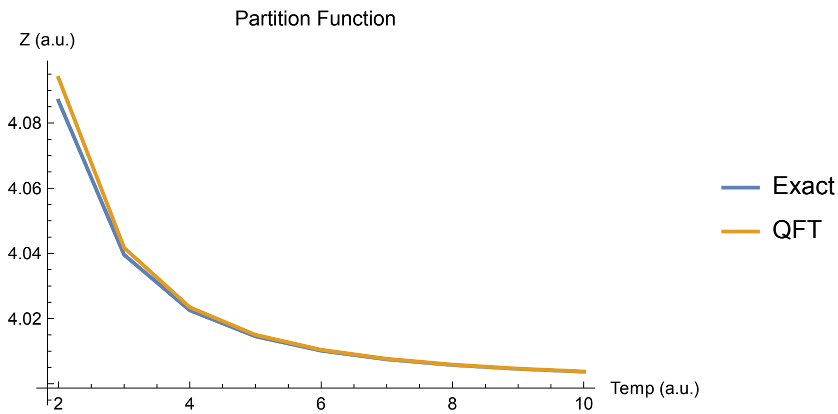
```
Zexact[β_] := Tr[MatrixExp[ -β H]];
Sz1 = KroneckerProduct[Sz, IdentityMatrix[2]];
OzExactUn[β_] := Tr[Sz1.MatrixExp[- β H]];
```

Plots

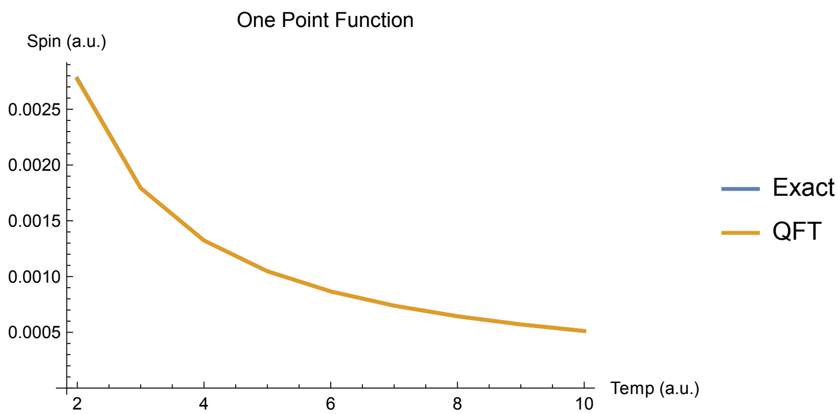
In[229]:=

```
ZexactT = Table[{T, Zexact[βscaling / T]}, {T, Tmin , Tmax, Tdelta}];
OzExactUnT = Table[OzExactUn[βscaling / T], {T, Tmin, Tmax, Tdelta}];
OzExactT = Table[{ZexactT[[k]][[1]], OzExactUnT[[k]] / ZexactT[[k]][[2]]}, {k, 1, Length[ZexactT]}];
ListPlot[{ZexactT, ZT}, PlotLegends → {"Exact", "QFT"}, Joined → True,
 PlotLabel → "Partition Function", AxesLabel → {"Temp (a.u.)", "Z (a.u.)"}]
ListPlot[{OzExactT, OzT}, PlotLegends → {"Exact", "QFT"}, Joined → True,
 PlotLabel → "One Point Function", AxesLabel → {"Temp (a.u.)", "Spin (a.u.)"}]
```

Out[232]=



Out[233]=



○ Example: L=3 XXZ line

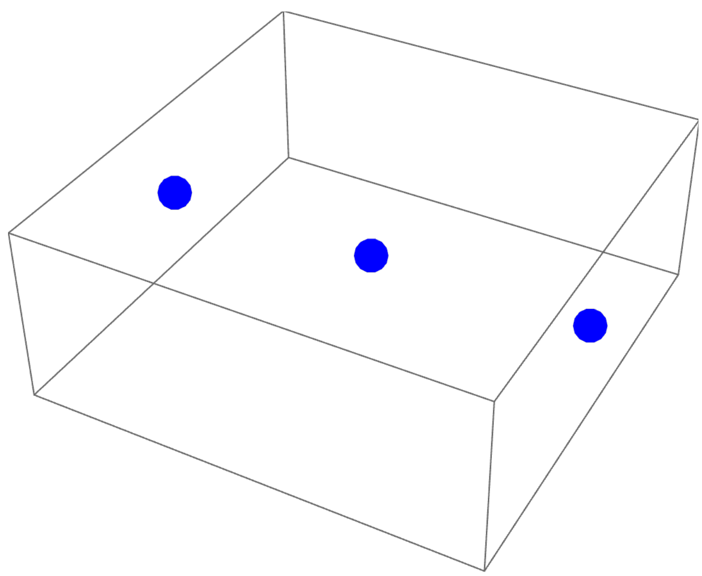
QFT computations

Lattice

In[234]:=

```
L = 3;
Λ = Table[{i, 0, 0}, {i, 1, L}];
λ = Length[Λ];
ListPointPlot3D[Λ, PlotStyle → {Blue, PointSize[0.05]},
 Axes → False, PlotRange → Full]
```

Out[237]=



External Magnetic Field

In[238]:=

```
hm = 0;
hp = 0;
hz = 0.01;
HbExp[β_] :=
```

$$\left\{\left\{\mathrm{Cosh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]+\frac{\mathrm{hz\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}},\ \frac{\mathrm{hm\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}}\right\},\right.$$
$$\left.\left\{\frac{\mathrm{hp\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}},\ \mathrm{Cosh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]-\frac{\mathrm{hz\,Sinh}\left[\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}\ \beta\right]}{\sqrt{\mathrm{hm\,hp}+\mathrm{hz}^2}}\right\}\right\};$$

Interaction Tensors

Constants

In[242]:=

```
a = 1;
b = 1;
c = 1;
LS = {{a, 0, 0}, {0, b, 0}, {0, 0, c}};
Ja = 1;
Jb = 1;
Jc = 1;
Ds = 1;
βscaling = 1;
```

Spin-Spin exchange Interaction

In[251]:=

```
V[v1_, v2_, s1_, s2_] := Module[{r, dx, dy, dz},
  r = Norm[(v1 - v2)];
  If[r ≠ 1, Return[0] ];
  dx = Norm[(v1 - v2)〚1〛];
  If[dx == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Ja / 4], If[s1 == 3 && s2 == 3, Return[Ja / 2]]]];
  dy = Norm[(v1 - v2)〚2〛];
  If[dy == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jb / 4], If[s1 == 3 && s2 == 3, Return[Jb / 2]]]];
  dz = Norm[(v1 - v2)〚3〛];
  If[dz == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jc / 4], If[s1 == 3 && s2 == 3, Return[Jc / 2]]]];
  Return[0];
 ]
```

Correlation Function: Sz

In[252]:=

```
acc = 2;
vIndex = 1;
sIndex = 3;(*3→Sz spin operator*)
t = 0;(*One-point correlations are independent of time b/c traces of linear
  operators are invariant under cyclic permutation of operators.*)
Tmin = 2;
Tmax = 10;
Tdelta = 1;
```

In[259]:=

```
ZT = Table[{T, Z[acc, βscaling / T]}, {T, Tmin , Tmax, Tdelta}];
```

In[260]:=

```
OzTun =
  Table[OnePoint[acc, βscaling / T, vIndex, sIndex, t], {T, Tmin, Tmax, Tdelta}];
```

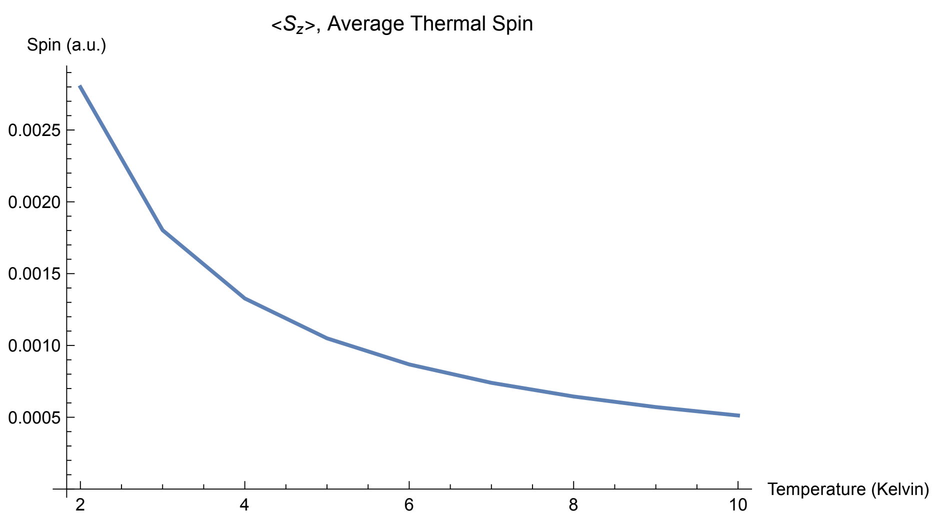
In[261]:=

```
OzT = Table[{ZT[[k]][[1]], OzTun[[k]] / ZT[[k]][[2]]}, {k, 1, Length[ZT]}];
```

In[262]:=

```
P1 = ListPlot[OzT, Joined → True,
  AxesLabel → {"Temperature (Kelvin)", "Spin (a.u.)"},
  PlotLabel → "<Sz>, Average Thermal Spin"]
```

Out[262]=



Exact Computations

Local Hamiltonians

In[263]:=

```
h = ((Ja / 2) (KroneckerProduct[Sp, Sm] + KroneckerProduct[Sm, Sp]) +
     Ja (KroneckerProduct[Sz, Sz]));
Sz = {{1 / 2, 0}, {0 , -1 / 2}};
```

Hamiltonian

In[265]:=

```
H = - (Sum[KroneckerProduct[IdentityMatrix[2^(k-1)], h, IdentityMatrix[2^(λ-k-1)] ],
        {k, 1, λ - 1}] + 2 Sum[KroneckerProduct[IdentityMatrix[2^(k-1)],
          hz Sz, IdentityMatrix[2^(λ-k)]], {k, 1, λ}]);
```

Expected Values

In[266]:=

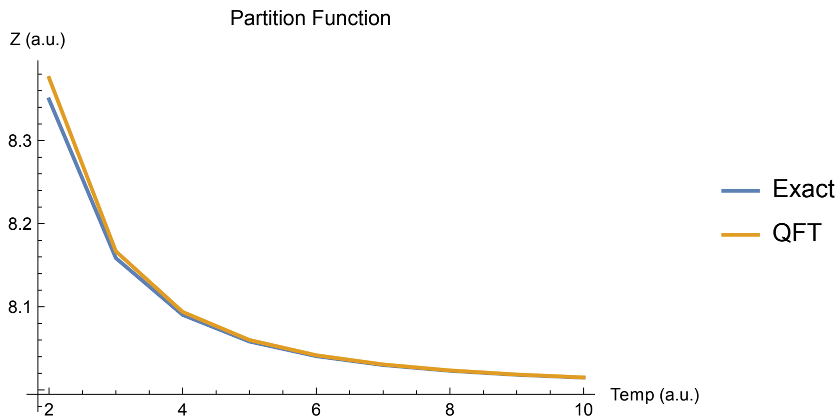
```
Zexact[β_] := Tr[MatrixExp[ - β H]];
Sz1 = KroneckerProduct[Sz, IdentityMatrix[2^(λ-1)]];
OzExactUn[β_] := Tr[Sz1.MatrixExp[- β H]];
```

Plots

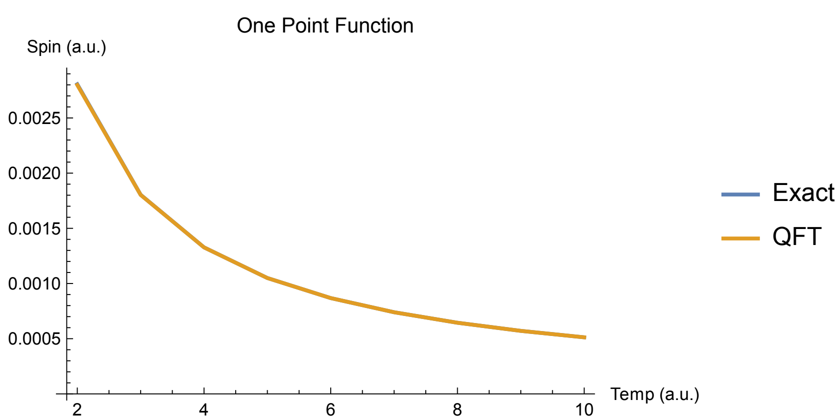
In[269]:=

```
ZexactT = Table[{T, Zexact[βscaling / T]}, {T, Tmin , Tmax, Tdelta}];
OzExactUnT = Table[OzExactUn[βscaling / T], {T, Tmin, Tmax, Tdelta}];
OzExactT = Table[{ZexactT⟦k⟧⟦1⟧, OzExactUnT⟦k⟧ / ZexactT⟦k⟧⟦2⟧}, {k, 1, Length[ZexactT]}];
ListPlot[{ZexactT, ZT}, PlotLegends → {"Exact", "QFT"}, Joined → True,
 PlotLabel → "Partition Function", AxesLabel → {"Temp (a.u.)", "Z (a.u.)"}]
ListPlot[{OzExactT, OzT}, PlotLegends → {"Exact", "QFT"}, Joined → True,
 PlotLabel → "One Point Function", AxesLabel → {"Temp (a.u.)", "Spin (a.u.)"}]
```

Out[272]=



Out[273]=



○ Example: L=4 XXZ line

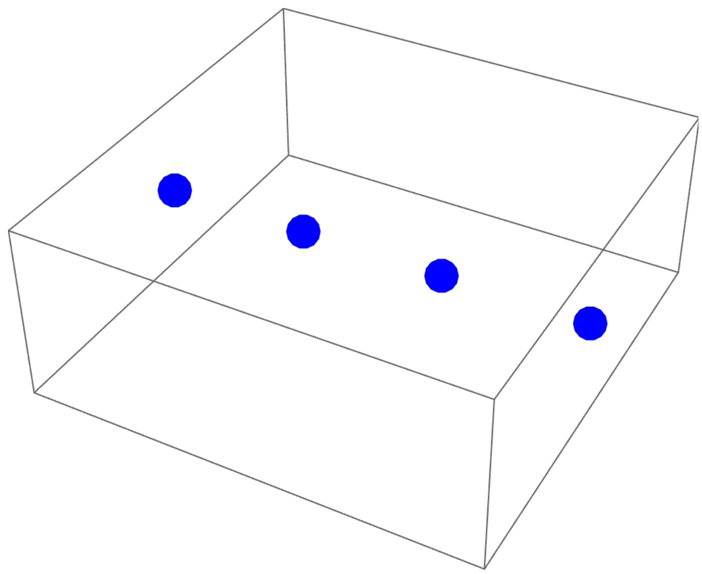
QFT computations

Lattice

In[274]:=

```
L = 4;
Λ = Table[{i, 0, 0}, {i, 1, L}];
λ = Length[Λ];
ListPointPlot3D[Λ, PlotStyle → {Blue, PointSize[0.05]},
 Axes → False, PlotRange → Full]
```

Out[277]=



External Magnetic Field

In[278]:=

```
hm = 0;
hp = 0;
hz = 0.01;
HbExp[β_] :=
```

$$\left\{\left\{\text{Cosh}\left[\sqrt{\text{hm hp}+\text{hz}^2}\ \beta\right]+\frac{\text{hz Sinh}\left[\sqrt{\text{hm hp}+\text{hz}^2}\ \beta\right]}{\sqrt{\text{hm hp}+\text{hz}^2}},\ \frac{\text{hm Sinh}\left[\sqrt{\text{hm hp}+\text{hz}^2}\ \beta\right]}{\sqrt{\text{hm hp}+\text{hz}^2}}\right\},\right.$$

$$\left.\left\{\frac{\text{hp Sinh}\left[\sqrt{\text{hm hp}+\text{hz}^2}\ \beta\right]}{\sqrt{\text{hm hp}+\text{hz}^2}},\ \text{Cosh}\left[\sqrt{\text{hm hp}+\text{hz}^2}\ \beta\right]-\frac{\text{hz Sinh}\left[\sqrt{\text{hm hp}+\text{hz}^2}\ \beta\right]}{\sqrt{\text{hm hp}+\text{hz}^2}}\right\}\right\};$$

Interaction Tensors

Constants

In[282]:=

```
a = 1;
b = 1;
c = 1;
LS = {{a, 0, 0}, {0, b, 0}, {0, 0, c}};
Ja = 1;
Jb = 1;
Jc = 1;
Ds = 1;
βscaling = 1;
```

Spin-Spin exchange Interaction

In[291]:=

```
V[v1_, v2_, s1_, s2_] := Module[{r, dx, dy, dz},
  r = Norm[(v1 - v2)];
  If[r ≠ 1, Return[0] ];
  dx = Norm[(v1 - v2)〚1〛];
  If[dx == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Ja / 4], If[s1 == 3 && s2 == 3, Return[Ja / 2]]]];
  dy = Norm[(v1 - v2)〚2〛];
  If[dy == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jb / 4], If[s1 == 3 && s2 == 3, Return[Jb / 2]]]];
  dz = Norm[(v1 - v2)〚3〛];
  If[dz == 1, If[(s1 == 1 && s2 == 2) || (s1 == 2 && s2 == 1) ,
    Return[Jc / 4], If[s1 == 3 && s2 == 3, Return[Jc / 2]]]];
  Return[0];
 ]
```

Correlation Function: Sz

In[292]:=

```
acc = 2;
vIndex = 2;
sIndex = 3;(*3→Sz spin operator*)
t = 0;(*One-point correlations are independent of time b/c traces of linear
  operators are invariant under cyclic permutation of operators.*)
Tmin = 2;
Tmax = 10;
Tdelta = 1;
```

In[299]:=

```
ZT = Table[{T, Z[acc, βscaling / T]}, {T, Tmin , Tmax, Tdelta}];
```

In[300]:=

```
OzTun =
  Table[OnePoint[acc, βscaling / T, vIndex, sIndex, t], {T, Tmin, Tmax, Tdelta}];
```

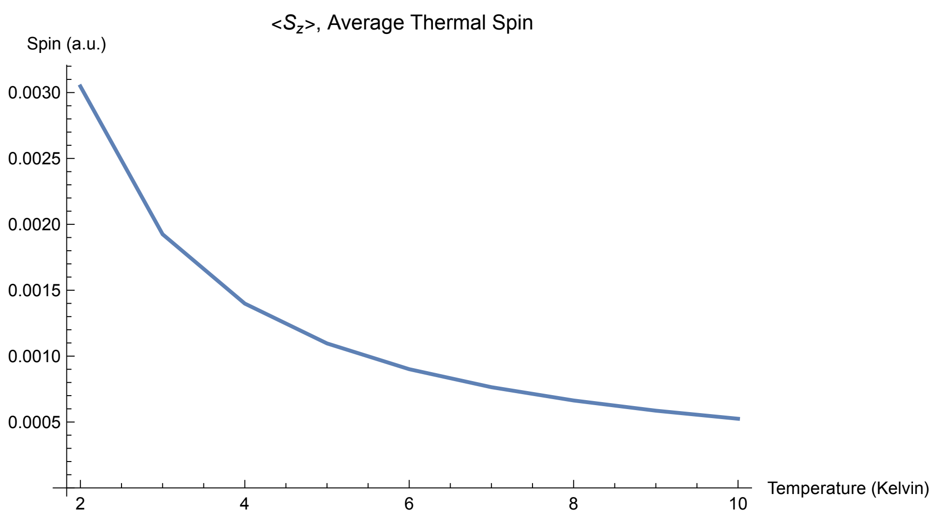
In[301]:=

```
OzT = Table[{ZT⟦k⟧⟦1⟧, OzTun⟦k⟧ / ZT⟦k⟧⟦2⟧}, {k, 1, Length[ZT]}];
```

In[302]:=

```
ListPlot[OzT, Joined → True, AxesLabel → {"Temperature (Kelvin)", "Spin (a.u.)"},
 PlotLabel → "<Sz>, Average Thermal Spin"]
```

Out[302]=



Exact Computations

Local Hamiltonians

In[303]:=

```
h = ((Ja / 2) (KroneckerProduct[Sp, Sm] + KroneckerProduct[Sm, Sp]) +
     Ja (KroneckerProduct[Sz, Sz]));
Sz = {{1 / 2, 0}, {0 , -1 / 2}};
```

Hamiltonian

In[305]:=

```
H = - (Sum[KroneckerProduct[IdentityMatrix[2^(k-1)], h, IdentityMatrix[2^(λ-k-1)] ],
        {k, 1, λ - 1}] + 2 Sum[KroneckerProduct[IdentityMatrix[2^(k-1)],
          hz Sz, IdentityMatrix[2^(λ-k)]], {k, 1, λ}]);
```

Expected Values

In[306]:=

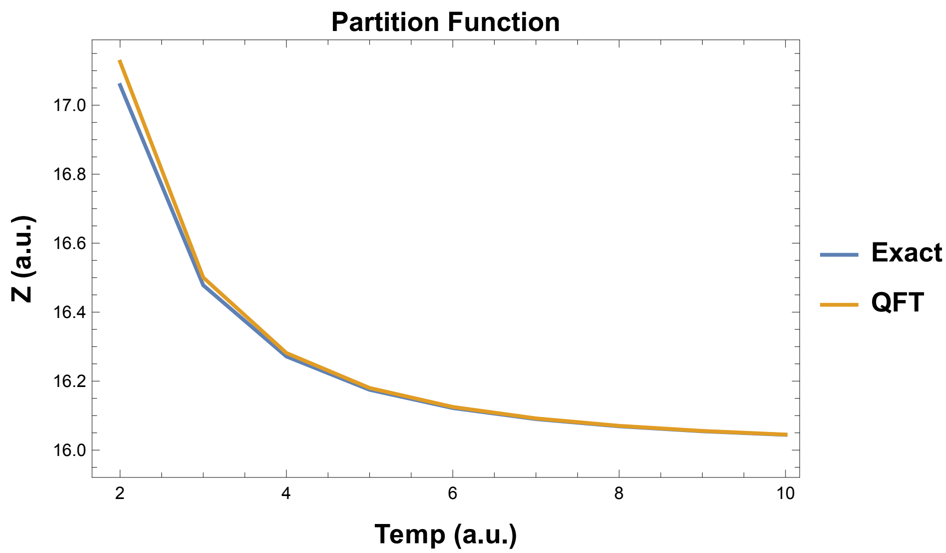
```
Zexact[β_] := Tr[MatrixExp[ - β H]];
Sz1 = KroneckerProduct[Sz, IdentityMatrix[2^(λ-1)]];
OzExactUn[β_] := Tr[Sz1.MatrixExp[- β H]];
```

Plots

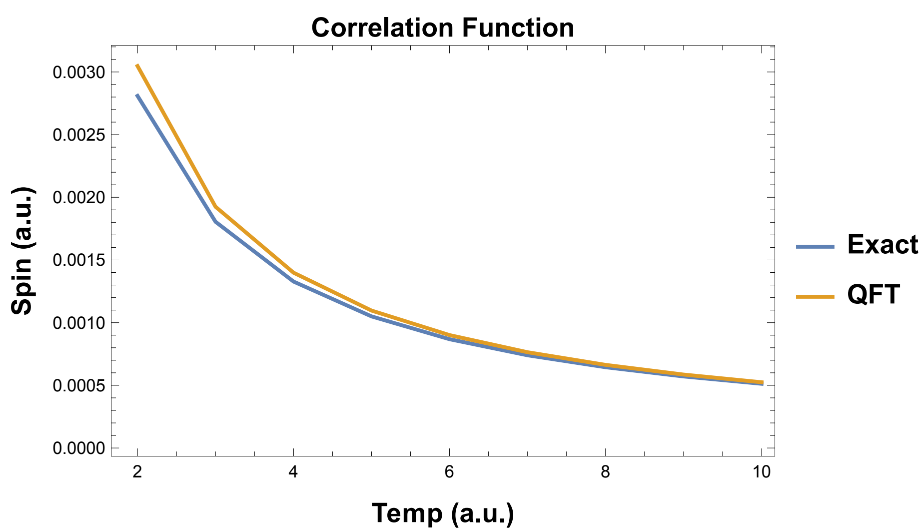
In[309]:=

```
ZexactT = Table[{T, Zexact[βscaling / T]}, {T, Tmin , Tmax, Tdelta}];
OzExactUnT = Table[OzExactUn[βscaling / T], {T, Tmin, Tmax, Tdelta}];
OzExactT = Table[{ZexactT[[k]][[1]], OzExactUnT[[k]] / ZexactT[[k]][[2]]}, {k, 1, Length[ZexactT]}];
ListPlot[{ZexactT, ZT}, Frame → True, PlotLegends →
   {Text[Style["Exact", Bold, Black, 14]], Text[Style["QFT", Bold, Black, 14]]},
  Joined → True, PlotLabel → Text[Style["Partition Function", Bold, Black, 14]],
  FrameLabel → {Text[Style["Temp (a.u.)", Bold, Black, 14]],
    Text[Style["Z (a.u.)", Bold, Black, 14]]}]
ListPlot[{OzExactT, OzT}, Frame → True, PlotLegends →
   {Text[Style["Exact", Bold, Black, 14]], Text[Style["QFT", Bold, Black, 14]]},
  Joined → True, PlotLabel → Text[Style["Correlation Function", Bold, Black, 14]],
  FrameLabel → {Text[Style["Temp (a.u.)", Bold, Black, 14]],
    Text[Style["Spin (a.u.)", Bold, Black, 14]]}]
```

Out[312]=



Out[313]=



Comparing DRG with Exact computations

Example: L=4 XXZ line

We consider a 1D spin chain with L sites.

Exact Computations

In[385]:=

```
λ = 4;
hz = -0.02;
hx = 0;
hy = 0;
Ja = 1;
```

Spin-1/2 Operators

We define the spin-1/2 operators where

$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $S_y = \frac{1}{2}\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$, $S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

and

$S_+ = S_x + I\, S_y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $S_- = S_x - I\, S_y = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$.

In[390]:=

```
Sp = {{0, 0}, {1, 0}};
Sm = {{0, 1}, {0, 0}};
Sz = {{1 / 2, 0}, {0 , -1 / 2}};
Sx = {{0, 1 / 2}, {1 / 2 , 0}};
Sy = {{0, -I}, {I , 0}};
Ops = {Sp, Sm, Sz, IdentityMatrix[2]};
```

Local Hamiltonian

In[396]:=

```
h = ((Ja / 2) (KroneckerProduct[Sp, Sm] + KroneckerProduct[Sm, Sp]) +
     Ja (KroneckerProduct[Sz, Sz]));
```

Hamiltonian

In[397]:=

```
H = -Sum[KroneckerProduct[IdentityMatrix[2^(k-1)], h, IdentityMatrix[2^(λ-k-1)] ],
      {k, 1, λ - 1}] + Sum[KroneckerProduct[IdentityMatrix[2^(k-1)],
      hz Sz, IdentityMatrix[2^(λ-k)]], {k, 1, λ}] +
    Sum[KroneckerProduct[IdentityMatrix[2^(k-1)], hx Sx, IdentityMatrix[2^(λ-k)]],
     {k, 1, λ}] + Sum[KroneckerProduct[IdentityMatrix[2^(k-1)],
      hz Sy, IdentityMatrix[2^(λ-k)]], {k, 1, λ}];
```

Eigenvalues

In[398]:=
```
Evals = Sort[N[Eigensystem[H][[1]]]]
```
Out[398]=
```
{-0.839443, -0.794721, -0.75, -0.705279, -0.660557,
 -0.501828, -0.457107, -0.412385, -0.116025, 0.205279,
 0.25, 0.294721, 0.912385, 0.957107, 1.00183, 1.61603}
```

Partition Function

In[399]:=
```
Zexact[β_] := Sum[Exp[-β Evals[[k]]], {k, 1, Length[Evals]}]
```

Correlation function

In[400]:=
```
Sz1 = KroneckerProduct[IdentityMatrix[2], Sz, IdentityMatrix[2^(λ-2)]];
```
In[401]:=
```
ESz1[β_] := Tr[Sz1.MatrixExp[- β H]] / Zexact[β];
```
In[402]:=
```
Sort[Table[{Eigensystem[H][[1]][[k]],
    ConjugateTranspose[Eigensystem[H][[2]][[k]]].Sz1.Eigensystem[H][[2]][[k]] /
     Norm[Eigensystem[H][[2]][[k]]]^2}, {k, 1, 16}]] // N
```
Out[402]=
```
{{-0.839443, 0.223607 + 0. i}, {-0.794721, 0.111803 + 0. i},
 {-0.75, -8.74301 × 10^-16 + 0. i}, {-0.705279, -0.111803 + 0. i},
 {-0.660557, -0.223607 + 0. i}, {-0.501828, 0.19086 + 0. i},
 {-0.457107, 1.36002 × 10^-15 + 0. i}, {-0.412385, -0.19086 + 0. i},
 {-0.116025, 3.33067 × 10^-16 + 0. i}, {0.205279, 0.111803 + 0. i},
 {0.25, 2.498 × 10^-16 + 0. i}, {0.294721, -0.111803 + 0. i},
 {0.912385, 0.0327465 + 0. i}, {0.957107, 2.03657 × 10^-15 + 0. i},
 {1.00183, -0.0327465 + 0. i}, {1.61603, -4.85723 × 10^-17 + 0. i}}
```

DMRG

Eigenvalues

In[403]:=
```
EvalsDMRG = {-0.789999999999998, -0.7843304055971139,
   -0.7516270709865368, -0.7305694084876648, -0.71388821912133,
   -0.5671646938259722, -0.464543538652116, -0.447588311089416,
   -0.11635448626225058, 0.011099735780816584, 0.23791699845966965};
```

Partition Function

In[404]:=

```
Zdmrg[β_] := Sum[Exp[-β EvalsDMRG[[k]]], {k, 1, Length[EvalsDMRG]}]
```

Correlation Function

In[405]:=

```
Sz1DMRG = {0.49999999999997385, 0.4314327174396475,
   0.022066255129364082, -0.24461424323958045, -0.44205559502745095,
   0.14289853674971467, 0.15243871970344428, -0.21602017234466392,
   0.005253548705354975, -0.057512908025683686, 0.14905220411765358};
```

In[406]:=

```
ESz1DMRG[β_] :=
 Sum[Sz1DMRG[[k]] Exp[-β EvalsDMRG[[k]]], {k, 1, Length[EvalsDMRG]}] / Zdmrg[β]
```

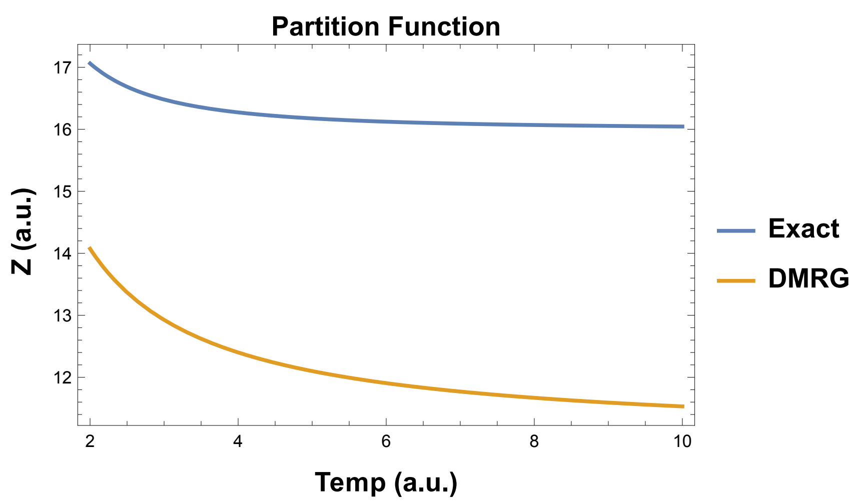
Comparison

Partition Function

In[407]:=

```
Plot[{Zexact[1 / T], Zdmrg[1 / T]}, {T, 2, 10}, Frame → True, PlotLegends →
  {Text[Style["Exact", Bold, Black, 14]], Text[Style["DMRG", Bold, Black, 14]]},
 PlotLabel → Text[Style["Partition Function", Bold, Black, 14]],
 FrameLabel → {Text[Style["Temp (a.u.)", Bold, Black, 14]],
   Text[Style[" Z (a.u.)", Bold, Black, 14]]}]
```

Out[407]=



Partition function don’t match because of the dimensional reduction in DMRG.

Correlation Function

In[408]:=

```
Plot[{ESz1[1 / T], ESz1DMRG[1 / T]}, {T, 2, 10}, Frame → True, PlotLegends →
  {Text[Style["Exact", Bold, Black, 14]], Text[Style["DMRG", Bold, Black, 14]]},
 PlotLabel → Text[Style["Correlation Function", Bold, Black, 14]],
 FrameLabel → {Text[Style["Temp (a.u.)", Bold, Black, 14]],
   Text[Style[" Z (a.u.)", Bold, Black, 14]]}]
```

Out[408]=