6 – ring Hubbard model

6 – Hubbard model ring

Basis for the sector with Sz sector (s1,s2)

```
n = 6;
u = 1.23;
occ = 6;
base =.;
start = {};
end = {};
sectors = {};
j = 0;
For[s1 = 0, s1 < occ + 1, s1++, s2 = occ - s1; k = 0; AppendTo[start, j + 1]
    For[i = 0, i < 4^n, i++, vec = IntegerDigits[i, 2, 2 n];
     n1 = Total[Take[vec, {1, n}]];
     n2 = Total[Take[vec, {n + 1, 2 n}]];
     If [n2 == s2 && n1 == s1, j++;
      k++;
      base[j] = vec]];
  AppendTo[end, j]; AppendTo[sectors, k]];
size = j;
```

Basis size

```
size
sectors
start
end
```

924

{1, 36, 225, 400, 225, 36, 1}

{1, 2, 38, 263, 663, 888, 924}

{1, 37, 262, 662, 887, 923, 924}

Some diagonal operators: double occupancy in site i, Sz in site i, ...

```
up[x_] := Take[x, {1, n}];
dn[x_] := Take[x, {n + 1, 2 n}];
nn[x_] := Total[up[x] * dn[x]];
norm[x_] := Total[Abs[x]];
Double[m_, i_] :=
  DiagonalMatrix[Table[base[k][[i]] * base[k][[i + n]], {k, start[[m]], end[[m]]}]];
DoubleSiteAvg[n_] := Total[Table[Double[n, i], {i, 1, n}]] / n;
OpSz[m_, i_] :=
  DiagonalMatrix[Table[base[k][[i]] - base[k][[i + n]], {k, start[[m]], end[[m]]}]];
SzTot[m_] := Sum[OpSz[m, i], {i, 1, 6}];
OpSzSz12[m_] := OpSz[m, 1].OpSz[m, 2];
OpSzSz13[m_] := OpSz[m, 1].OpSz[m, 3];
OpSzSz14[m_] := OpSz[m, 1].OpSz[m, 4];
SzTot2[m_] := SzTot[m].SzTot[m];
```

Hopping matrix

```
hop = Join[Table[i + j, {i, 1, n - 1}, {j, 0, 1}],
    Table[i - j, {i, 2, n}, {j, 0, 1}], {{n, 1}, {1, n}},
    Table[i + j, {i, n + 1, 2 n - 1}, {j, 0, 1}],
    Table[i - j, {i, n + 2, 2 n}, {j, 0, 1}], {{2 n, n + 1}, {n + 1, 2 n}}];
Length[hop]
hop
```

```
24
```

```
{{1, 2}, {2, 3}, {3, 4}, {4, 5}, {5, 6}, {2, 1}, {3, 2}, {4, 3},
 {5, 4}, {6, 5}, {6, 1}, {1, 6}, {7, 8}, {8, 9}, {9, 10}, {10, 11},
 {11, 12}, {8, 7}, {9, 8}, {10, 9}, {11, 10}, {12, 11}, {12, 7}, {7, 12}}
```

Hopping Hamiltonian in many-body basis

```
HopTest[i_, j_, cre_, anh_] := norm[base[i] - base[j]] == 2 && base[i][[cre]] == 1 &&
   base[i][[anh]] == 0 && base[j][[cre]] == 0 && base[j][[anh]] == 1;
HopSign[i_, anh_] := (-1)^Total[Take[base[i], {anh + 1, 2 n}]];
H1[m_] :=
  Module[{str = start[[m]], sz = sectors[[m]]}, tmp = ConstantArray[0, {sz, sz}];
   For[i = 1, i <= Length[hop], i++, cre = hop[[i]][[1]];
    anh = hop[[i]][[2]];
    For[bra = 0, bra < sz, bra++,
     For[ket = 0, ket < sz, ket++,
      If[HopTest[str + bra, str + ket, cre, anh],
       tmp[[1 + bra]][[1 + ket]] =
        tmp[[1 + bra]][[1 + ket]] + HopSign[str + bra, cre] * HopSign[str + ket, anh]
      ]]]];
   tmp];
```

Other non-diagonal operators

Local interaction (sum over all sites):

```
H2[m_] := DiagonalMatrix[Table[nn[base[i]], {i, start[[m]], end[[m]]}]];
Shift[m_] := DiagonalMatrix[Table[2 n, {i, start[[m]], end[[m]]}]];
```

Hubbard Hamitonian as a function of local interaction U

```
H[m_] := N[H1[m] + u * H2[m] + Shift[m]];
```

Eigenenergies as a function of U

```
Eng = {};
For[l = 1, l ≤ occ + 1, l++, Eng = Join[Eng, Eigenvalues[H[l]]]];
E0 = Min[Eng];
Eng = Eng - E0;
Eng
```

```
{6.30838, 11.3829, 10.5384, 10.5384, 10.204, 10.204, 9.53838, 9.41512, 9.41512, 9.15305,
 8.53838, 8.53838, 8.18909, 8.18909, 7.53838, 7.53838, 7.53838, 7.53838, 7.53838,
 7.53838, 7.53838, 7.14289, 7.14289, 6.53838, 6.53838, 6.30838, 6.16375, 6.16375,
 5.53838, 5.15558, 5.15558, 5.12994, 4.53838, 4.53838, 4.03825, 4.03825, 3.25764,
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```

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6.66017, 6.53838, 6.53838, 6.45801, 6.45801, 6.30838, 6.24125, 6.24125, 6.16375,
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7.53838, 7.14289, 7.14289, 6.53838, 6.53838, 6.30838, 6.16375, 6.16375, 5.53838,
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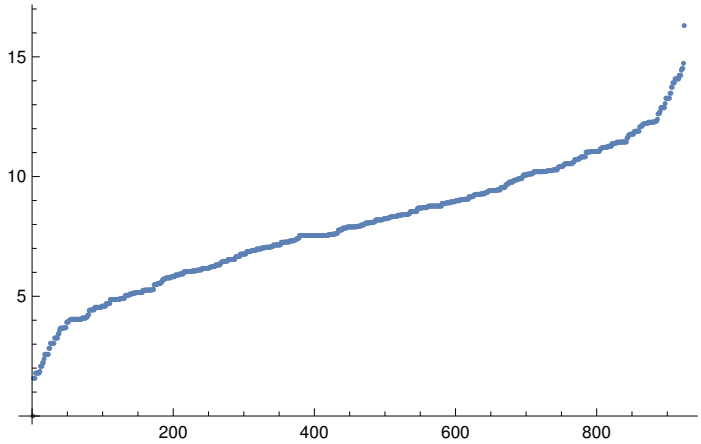
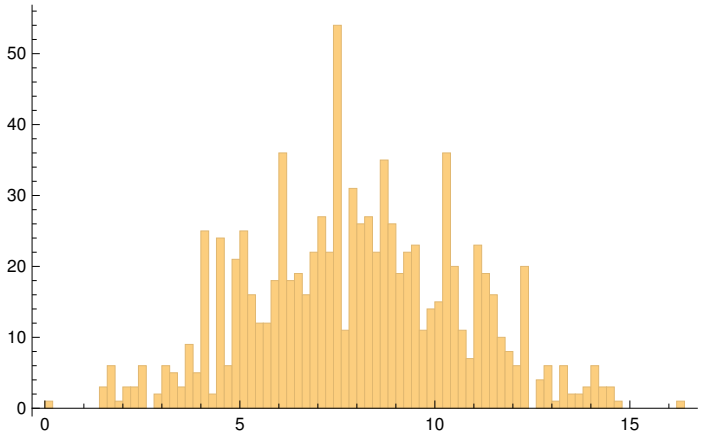
```
ListPlot[Sort[Eng]]
```

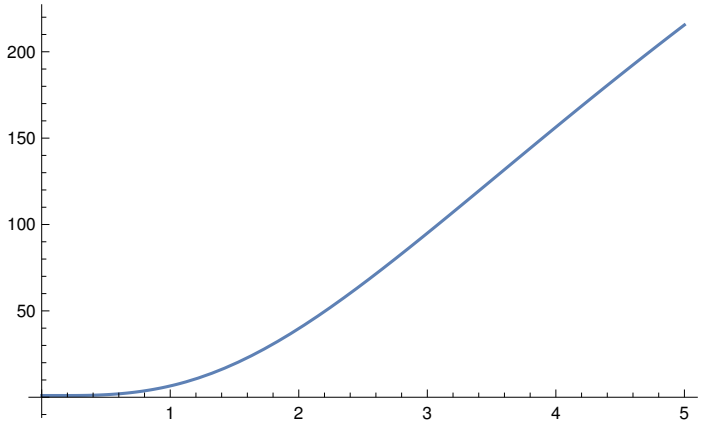


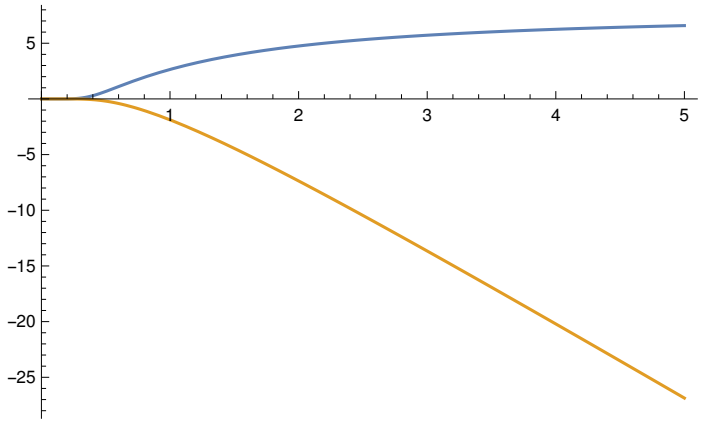

```
Histogram[Eng, 100]
```

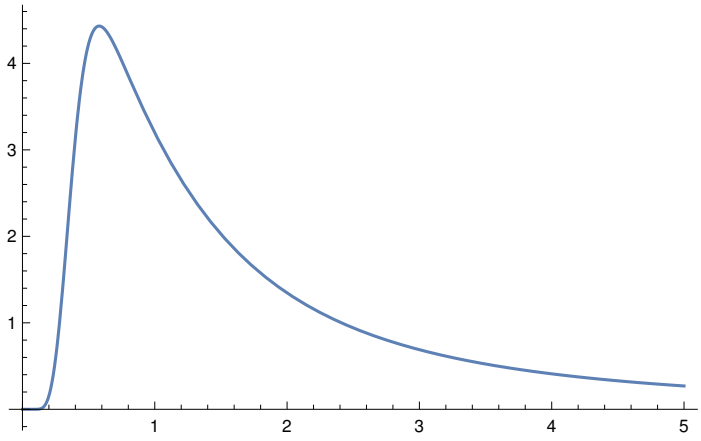


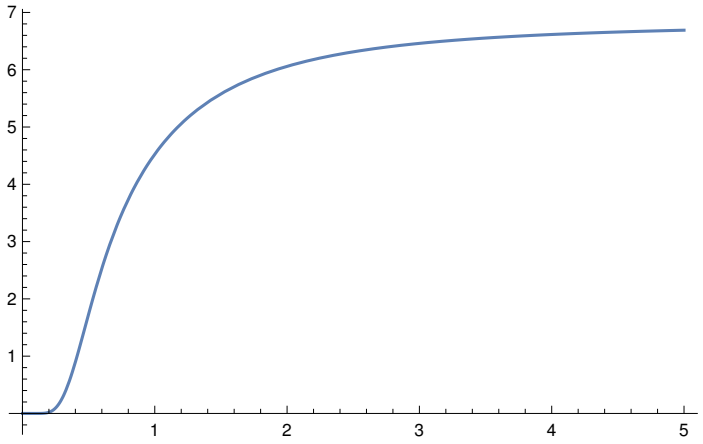

```
Z[T_] := Total[Exp[-1 / T * Eng]];
F[T_] := -T * Log[Z[T]];
Ene[T_] := Total[Eng * Exp[-1 / T * Eng]] / Z[T];
Ene2[T_] := Total[Eng^2 * Exp[-1 / T * Eng]] / Z[T];
Cv[T_] := -1 / T^2 * (Ene[T]^2 - Ene2[T]);
entropy[T_] := (Ene[T] - F[T]) / T;
Z[0.001]
Plot[Z[T], {T, 0.001, 5}]
Plot[{Ene[T], F[T]}, {T, 0.001, 5}]
Plot[Cv[T], {T, 0.001, 5}]
Plot[entropy[T], {T, 0.001, 5}]
```

1.

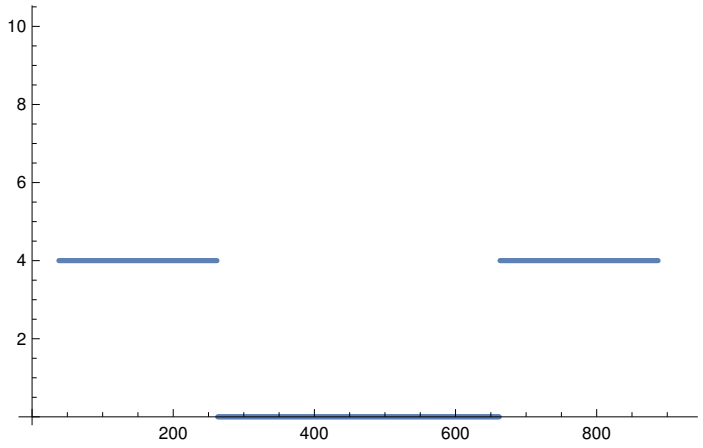

200
150
100
50
1
2
3
4
5


5
−5
−10
−15
−20
−25
1
2
3
4
5

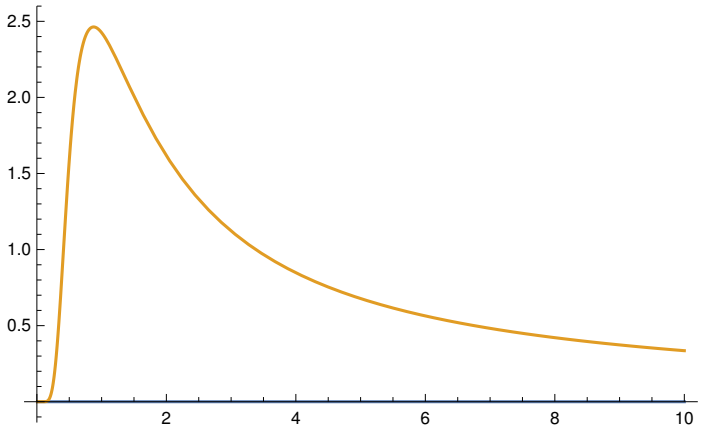

4
3
2
1
1
2
3
4
5



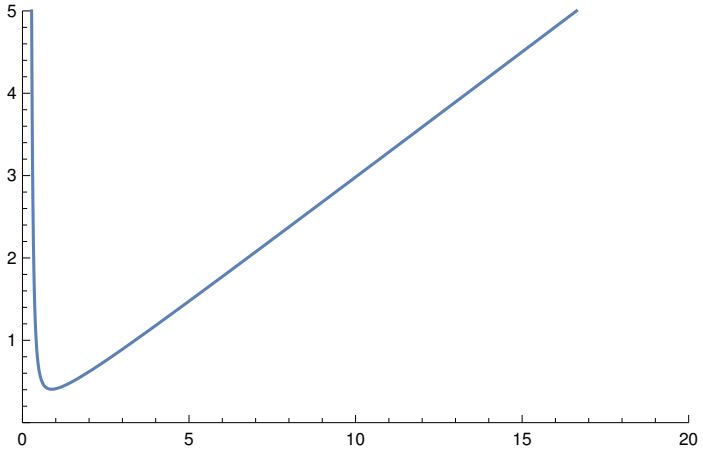

```
Evec = {};
For[l = 1, l ≤ occ + 1, l++, AppendTo[Evec, Eigenvectors[H[l]]]];


Elements[O_] := Module[{elem = {}}, For[s = 1, s ≤ Length[sectors],
    s++, For[i = 1, i ≤ sectors[[s]], i++, x = Evec[[s]][[i]];
     AppendTo[elem, x.O[s].x]]]; elem];
SzElements = Elements[SzTot];
Sz2Elements = Elements[SzTot2];

SzSz12Elements = Elements[OpSzSz12];
SzSz13Elements = Elements[OpSzSz13];
SzSz14Elements = Elements[OpSzSz14];

ListPlot[Sz2Elements]
```



```
Sz[T_] := Total[SzElements * Exp[-1 / T * Eng]] / Z[T];
Sz2[T_] := Total[Sz2Elements * Exp[-1 / T * Eng]] / Z[T];
Plot[{Sz[T], Sz2[T] / T}, {T, 0.01, 10}]
SzSz12[T_] := Total[SzSz12Elements * Exp[-1 / T * Eng]] / Z[T];
SzSz13[T_] := Total[SzSz13Elements * Exp[-1 / T * Eng]] / Z[T];
SzSz14[T_] := Total[SzSz14Elements * Exp[-1 / T * Eng]] / Z[T];
```

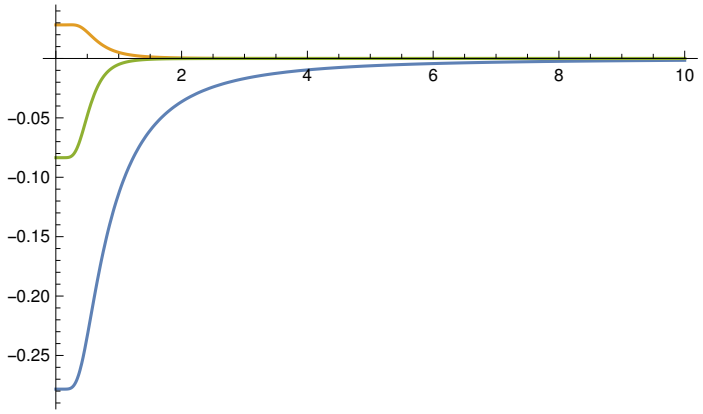



```
Plot[T / Sz2[T], {T, 0.1, 20}, PlotRange → {{0, 20}, {0, 5}}]
```



Average double occupancy

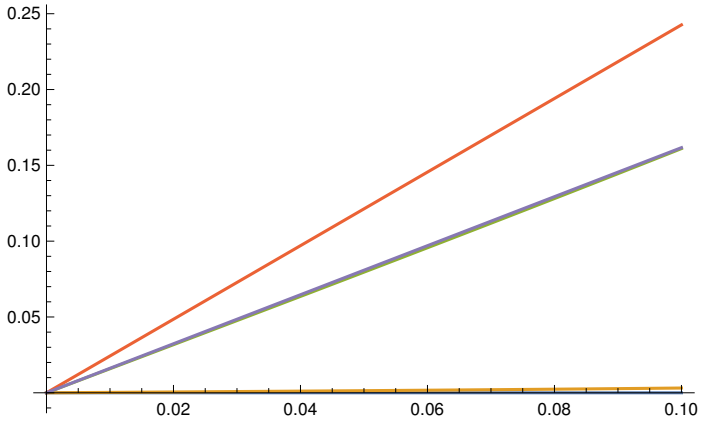
```
Plot[{SzSz12[T], SzSz13[T], SzSz14[T]}, {T, 0.001, 10}, PlotRange → Full]
```



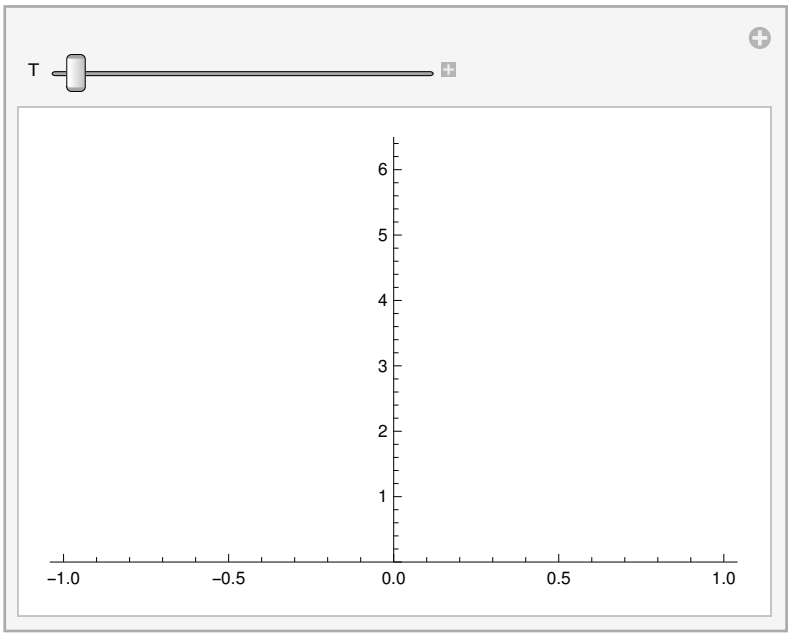

```
Zh[T_, h_] := Total[Exp[-1 / T * (Eng - h * SzElements)]];
Szh[T_, h_] := Total[SzElements * Exp[-1 / T * (Eng - h * SzElements)]] / Zh[T, h];
Szh[1, 1]
```

```
2.44073
```

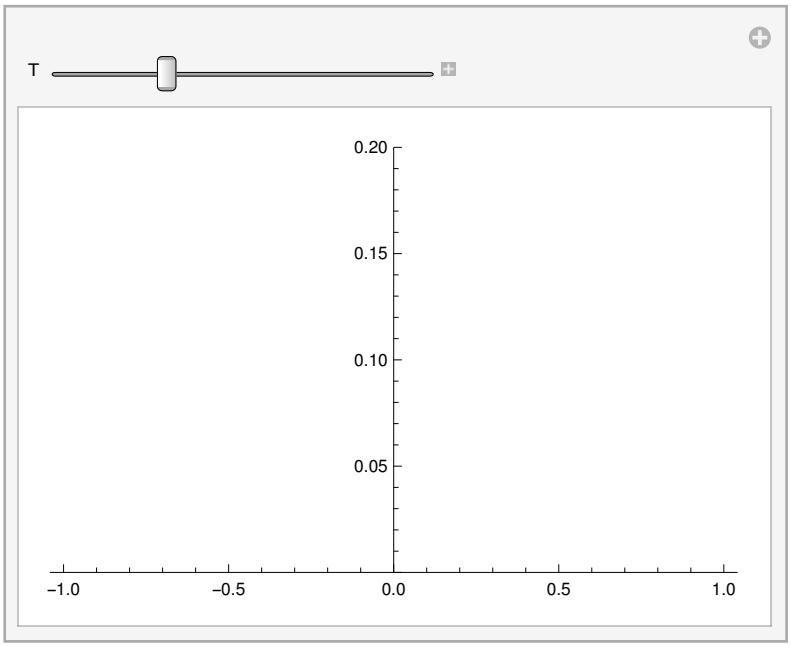
```
Plot[{Szh[0.1, h], Szh[0.2, h], Szh[0.5, h], Szh[1, h], Szh[2, h]}, {h, 0, 0.1}]
```



```
Manipulate[Plot[Szh[T, h], {h, 0, 5}, PlotRange → {0, 6.5}], {T, 0.01, 5}]
```




```
Manipulate[Plot[Szh[T, h], {h, 0, 0.1}, PlotRange → {0, 0.2}], {T, 0.01, 5}]
```



```
Manipulate[Plot[Szh[T, h] / h, {h, 0.001, 0.5}, PlotRange → {0, 2.5}], {T, 0.01, 5}]
```