6 – ring Hubbard model

6 – Hubbard model ring

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

```
n = 6;
E0 = 10;
s1 = 3;
s2 = 3;
base =.;
j = 0;
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++;
   base[j] = vec]];
size = j;
```

Basis size

```
size
base[224]
```

```
400
```

```
{1, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1, 0}
```

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[i_] := DiagonalMatrix[Table[base[k][[i]] * base[k][[i + n]], {k, 1, size}]];
DoubleSiteAvg := Total[Table[Double[i], {i, 1, n}]] / n;
OpSz[i_] := DiagonalMatrix[Table[base[k][[i]] - base[k][[i + n]], {k, 1, size}]];
OpSzSz[i_, j_] := OpSz[i].OpSz[j];
```

```
nn[base[234]]
```

```
2
```

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[x_, y_, cre_, anh_] :=
  norm[x - y] == 2 && x[[cre]] == 1 && x[[anh]] == 0 && y[[cre]] == 0 && y[[anh]] == 1;
HopSign[x_, anh_] := (-1) ^Total[Take[x, {anh + 1, 2 n}]];
H1 = Table[0, {i, 1, size}, {j, 1, size}];
For[i = 1, i <= Length[hop], i++, cre = hop[[i]][[1]];
  anh = hop[[i]][[2]];
  For[bra = 1, bra <= size, bra++,
   For[ket = 1, ket <= size, ket++, If[HopTest[base[bra], base[ket], cre, anh],
     H1[[bra]][[ket]] = H1[[bra]][[ket]] +
       HopSign[base[bra], cre] * HopSign[base[ket], anh]]]]];
```

Other non-diagonal operators

Local interaction (sum over all sites):

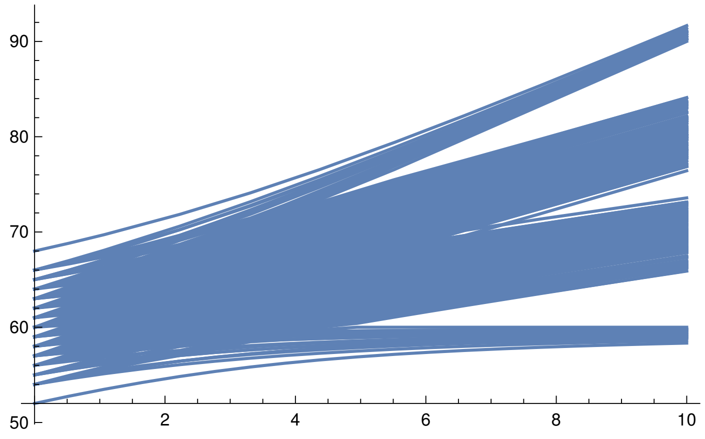
```
H2 = DiagonalMatrix[Table[nn[base[i]], {i, 1, size}]];
Shift = DiagonalMatrix[Table[E0 * (s1 + s2) , {i, 1, size}]];
```

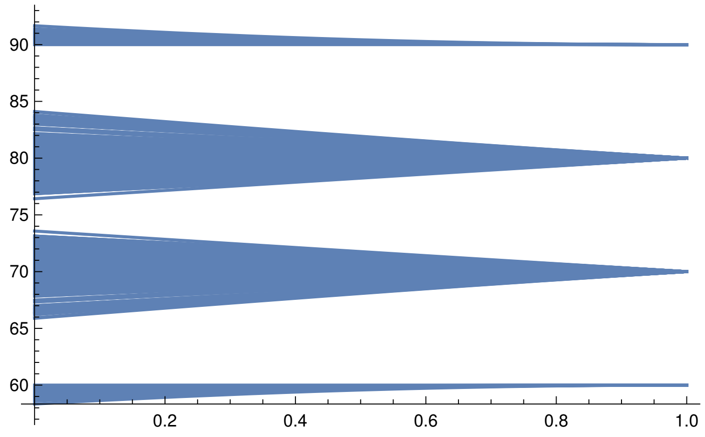
Hubbard Hamitonian as a function of local interaction U

```
H[u_] := N[H1 + u * H2 + Shift];
Egs[u_] := Eigenvalues[H[u], -1][[1]];
gs[u_] := Eigenvectors[H[u], -1][[1]];
Hpom[t_] := N[t * H1 + 10 * H2 + Shift];
```

Eigenenergies as a function of U

```
Plot[Sort[Eigenvalues[H[u]]], {u, 0, 10}, PlotPoints → 10, MaxRecursion → 1]
Plot[Sort[Eigenvalues[Hpom[1 - t]]], {t, 0, 1}, PlotPoints → 10, MaxRecursion → 1]
```



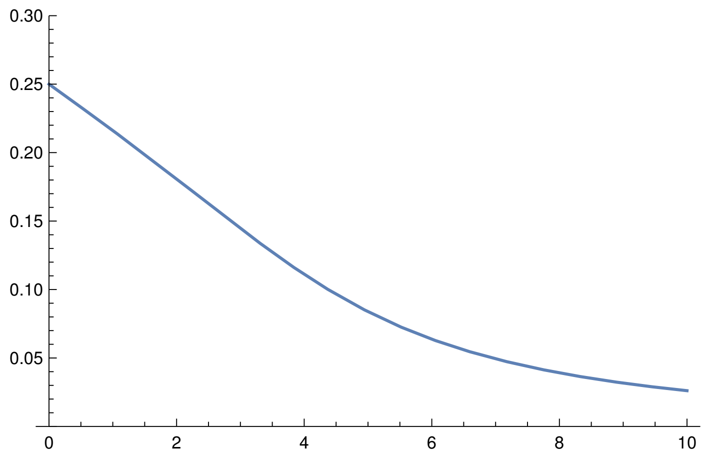


Ground state expectation value of operator A

```
Expect0[A_, u_] := gs[u].A.gs[u];
```

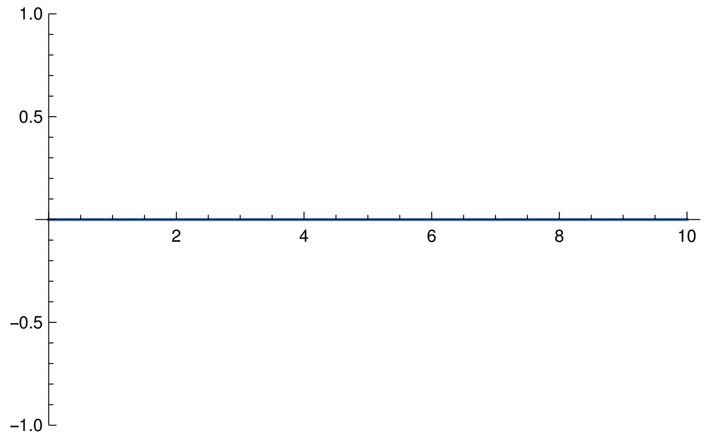
Average double occupancy

```
Plot[Expect0[DoubleSiteAvg, u], {u, 0, 10},
 PlotPoints → 10, MaxRecursion → 1, PlotRange → {0, 0.3}]
```



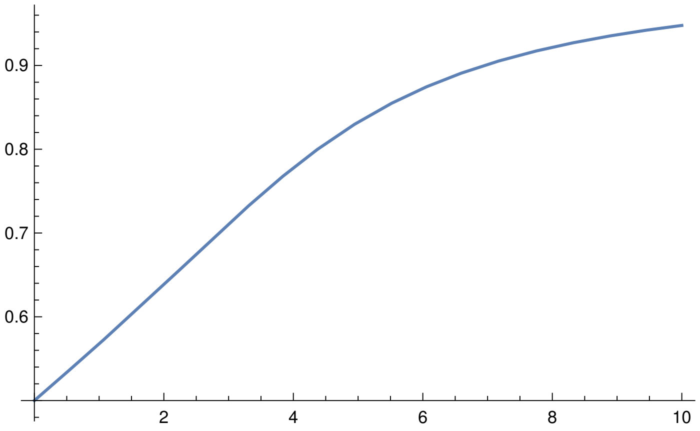
Average ordered spin moment

```
Plot[Expect0[OpSz[1], u], {u, 0, 10},
 PlotPoints → 10, MaxRecursion → 1, PlotRange → {-1, 1}]
```



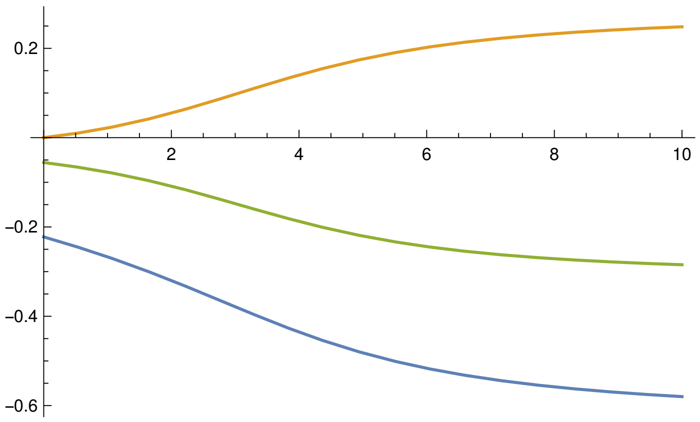
Average amplitude of the spin moment Sz^2

```
Plot[Expect0[OpSzSz[1, 1], u] - Expect0[OpSz[1], u]^2,
 {u, 0, 10}, PlotPoints → 10, MaxRecursion → 1]
```



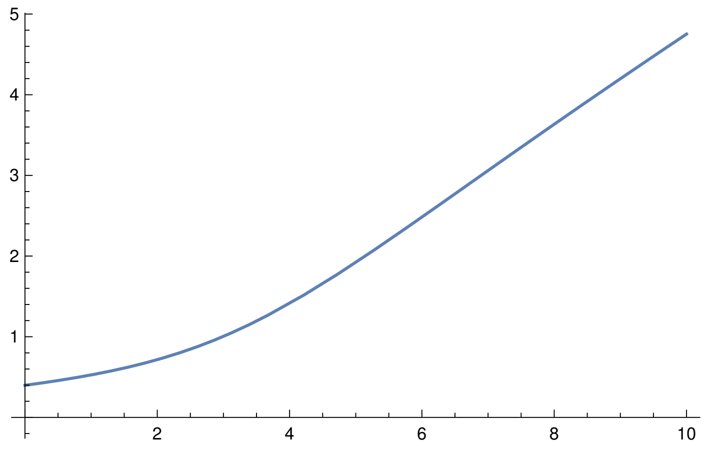
Spin spin correlation function (instantaneous) <Sz(i)Sz(j)>

```
Plot[{Expect0[OpSzSz[1, 2], u], Expect0[OpSzSz[1, 3], u], Expect0[OpSzSz[1, 4], u]},
 {u, 0, 10}, PlotPoints → 10, MaxRecursion → 1]
```



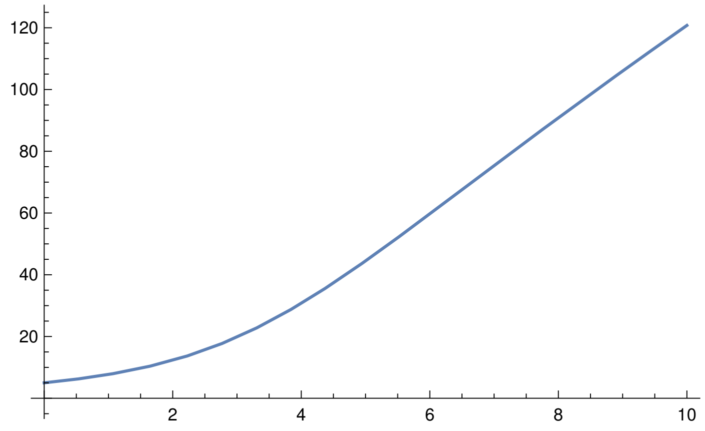
Local susceptibility

```
Localchi[i_, u_] := Module[{vec, eig, gs, E0, chi = 0}, vec = Eigenvectors[H[u]];
   eig = Eigenvalues[H[u]];
   gs = vec[[size]];
   E0 = eig[[size]];
   For[k = 1, k < size - 1, k++;
    chi = chi + (gs.OpSz[i].vec[[k]]) ^2 / (eig[[k]] - E0)];
   2 * chi];
Plot[Localchi[1, u], {u, 0, 10}, PlotPoints → 20, MaxRecursion → 1]
```



Staggered susceptibility

```
OpStaggered = Sum[(-1) ^i * OpSz[i], {i, 1, 6}];
Staggeredchi[u_] := Module[{vec, eig, gs, E0, chi = 0}, vec = Eigenvectors[H[u]];
   eig = Eigenvalues[H[u]]; gs = vec[[size]]; E0 = eig[[size]];
   For[k = 1, k < size - 1, k++;
    chi = chi + (gs.OpStaggered.vec[[k]]) ^2 / (eig[[k]] - E0)]; 2 * chi];
Plot[Staggeredchi[u], {u, 0, 10}, PlotPoints → 10, MaxRecursion → 1]
```



Translation symmetry

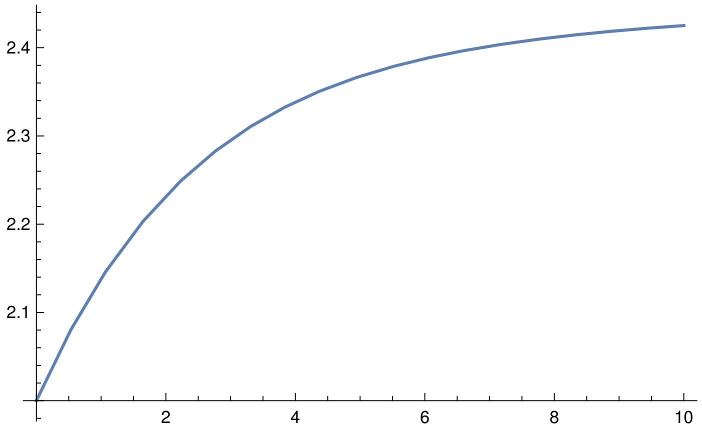
```
klist =.;
klist = Table[Exp[I * 2 π / 6 * n], {n, 0, 5}]
```

$\left\{1, e^{\frac{i\pi}{3}}, e^{\frac{2i\pi}{3}}, -1, e^{-\frac{2i\pi}{3}}, e^{-\frac{i\pi}{3}}\right\}$

Bloch sum

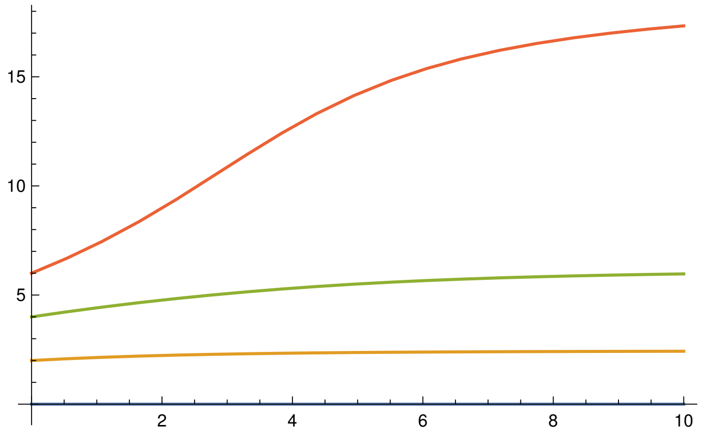
```
SzList = Table[OpSz[i], {i, 1, 6}];
Szk[k_] := N[Sum[klist[[i]]^k * OpSz[i], {i, 1, 6}]];
SzkList = N[Table[Szk[k], {k, 0, 6}]];
SzSzk[k_, u_] := Re[Expect0[SzkList[[k + 1]].SzkList[[6 - k + 1]], u]];
```

```
Plot[Re[Expect0[SzkList[[2]].SzkList[[6]], u]],
 {u, 0, 10}, PlotPoints → 10, MaxRecursion → 1]
```



Correlation function in reciprocal space< Sz (k) Sz (-k) >

```
Plot[{SzSzk[0, u], SzSzk[1, u], SzSzk[2, u], SzSzk[3, u]},
 {u, 0, 10}, PlotPoints → 10, MaxRecursion → 1]
```



Time dependent correlations

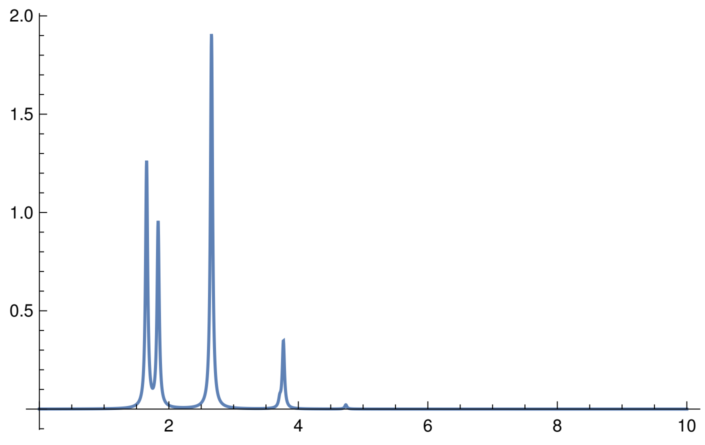
Matrix elements, Lorentzians, Re and Im susceptibility

```
Szzw[u_, i_, j_] := Module[{vec, eig, gs, E0, chi}, vec = Eigenvectors[H[u]];
   eig = Eigenvalues[H[u]];
   gs = vec[[size]];
   E0 = eig[[size]];
   chi = 0 * eig;
   For[k = 1, k < size, k++;
    chi[[k]] = (gs.OpSz[i].vec[[k]]) * (vec[[k]].OpSz[j].gs)]; chi];
Szzkw[u_, i_, j_] := Module[{vec, eig, gs, E0, chi}, vec = Eigenvectors[H[u]];
   eig = Eigenvalues[H[u]]; gs = vec[[size]]; E0 = eig[[size]];
   chi = 0 * eig;
   For[k = 1, k < size, k++;
    chi[[k]] = (gs.SzkList[[i]].vec[[k]]) * (vec[[k]].SzkList[[j]].gs)];
   chi];
L[w_, x_, G_] := G / (2 Pi) * 1 / ((w - x) ^2 + G^2);
RL[w_, x_, G_] := (w - x) / ((w - x) ^2 + G^2);
Spect[w_, G_, M_, eig_] := Module[{t = 0}, For[i = 1, i <= Length[M],
    i++, If[Abs[M[[i]]] ^2 > 0.000001, t = t + L[w, eig[[i]], G] * M[[i]]]];
   t];
RSpect[w_, G_, M_, eig_] := Module[{t = 0}, For[i = 1, i ≤ Length[M], i++,
    If[Abs[M[[i]]] ^2 > 0.000001, t = t + RL[w, eig[[i]], G] * M[[i]]]];
   -t];

eig = Eigenvalues[H[1]] - Eigenvalues[H[1]][[-1]];
```

Local spin-spin correlation function (spectrum = Im part)

```
weigh = Szzw[1, 1, 1];
Plot[Spect[x, 0.02, weigh, eig], {x, 0, 10}, PlotRange → Full]
```



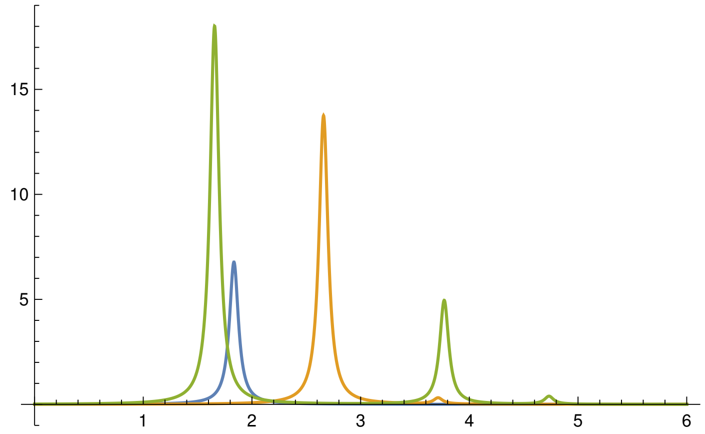
```
Round[weigh, 0.0001]
```

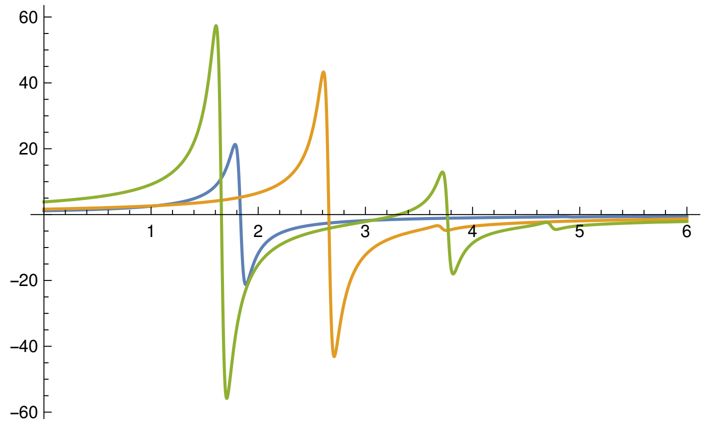
```
{0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.0001, 0.0001,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.0003, 0., 0.,
 0., 0., 0., 0., 0., 0., 0.0027, 0.0006, 0., 0., 0., 0., 0.0001, 0., 0., 0., 0., 0.,
 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0.0432, 0.0024, 0.0026, 0., 0., 0.,
 0., 0., 0., 0., 0., 0.0534, 0.1866, 0., 0., 0., 0., 0., 0.1133, 0.005, 0.1572, 0.}
```

k-dependent correlation function < S (k, w) S (-k, w) >

```
weigh1 = Szzkw[1, 2, 6];
weigh2 = Szzkw[1, 3, 5];
weigh3 = Szzkw[1, 4, 4];
```

```
Plot[{Spect[x, 0.05, weigh1, eig], Spect[x, 0.05, weigh2, eig],
  Spect[x, 0.05, weigh3, eig]}, {x, 0, 6}, PlotRange → Full]
Plot[{RSpect[x, 0.05, weigh1, eig], RSpect[x, 0.05, weigh2, eig],
  RSpect[x, 0.05, weigh3, eig]}, {x, 0, 6}, PlotRange → Full]
```





Electronic propagators

construct subspaces with n+1 and n-1 particles

```
s1p = s1 + 1;
s1m = s1 - 1;
basep =.;
basem =.;
jp = 0;
jm = 0;
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 == s1p, jp++;
  basep[jp] = vec];
 If[n2 == s2 && n1 == s1m, jm++;
  basem[jm] = vec]]
sizep = jp
sizem = jm
```

```
300
```

```
300
```

construct the Hamiltonians in these subspaces

```
H2p = DiagonalMatrix[Table[nn[basep[i]], {i, 1, sizep}]];
H2m = DiagonalMatrix[Table[nn[basem[i]], {i, 1, sizem}]];
H1p = Table[0, {i, 1, sizep}, {j, 1, sizep}];
For[i = 1, i ≤ Length[hop], i++, cre = hop[[i]][[1]];
  anh = hop[[i]][[2]];
  For[bra = 1, bra ≤ sizep, bra++,
   For[ket = 1, ket ≤ sizep, ket++, If[HopTest[basep[bra], basep[ket], cre, anh],
     H1p[[bra]][[ket]] = HopSign[basep[bra], cre] * HopSign[basep[ket], anh]]]]];
H1m = Table[0, {i, 1, sizem}, {j, 1, sizem}];
For[i = 1, i ≤ Length[hop], i++, cre = hop[[i]][[1]];
  anh = hop[[i]][[2]];
  For[bra = 1, bra ≤ sizem, bra++, For[ket = 1, ket ≤ sizem, ket++,
    If[HopTest[basem[bra], basem[ket], cre, anh], H1m[[bra]][[ket]] =
      H1m[[bra]][[ket]] + HopSign[basem[bra], cre] * HopSign[basem[ket], anh]]]]];
```

calculated eigenenergies and eigenvectors

```
Hp[u_] := N[H1p + u * H2p + DiagonalMatrix[Table[E0 (s1 + s2 + 1), {i, 1, sizep}]]];
Ep[u_] := Eigenvalues[Hp[u]];
Hm[u_] := N[H1m + u * H2m + DiagonalMatrix[Table[E0 (s1 + s2 - 1), {i, 1, sizem}]]];
Em[u_] := Eigenvalues[Hm[u]];
```

construct the creation n->n+1 and anihilation n->n-1 operators (on site and in k-space)

```
ctest[x_, y_, i_] := norm[x - y] == 1 && x[[i]] == 0 && y[[i]] == 1;
OpC[site_] := Module[{t = Table[0, {i, 1, sizem}, {j, 1, size}]},
  For[bra = 1, bra ≤ sizem, bra++, For[ket = 1, ket ≤ size, ket++, If[
     ctest[basem[bra], base[ket], site], t[[bra]][[ket]] = HopSign[base[ket], site]]]];
  t]
OpCd[site_] := Module[{t = Table[0, {i, 1, sizep}, {j, 1, size}]},
  For[bra = 1, bra ≤ sizep, bra++, For[ket = 1, ket ≤ size, ket++, If[ctest[base[ket],
      basep[bra], site], t[[bra]][[ket]] = HopSign[basep[bra], site]]]];
  t]
Ck[k_] := N[Sum[klist[[i]]^k * OpC[i], {i, 1, n}]] / Sqrt[n];
Cdk[k_] := N[Sum[klist[[i]]^(-k) * OpCd[i], {i, 1, n}] / Sqrt[n]];
```

define the matrix elements |<n+1|a^+|g>|^2 and |<n-1|a|g>|^2

```
Gpw[u_, i_, j_] := Module[{vec, chi = ConstantArray[0, sizep],
     X = gs[u].Transpose[OpCd[i]], Y = OpCd[j].gs[u]}, vec = Eigenvectors[Hp[u]];
   For[k = 1, k < sizep, k++;
    chi[[k]] = (X.vec[[k]]) * (vec[[k]].Y)]; chi];
Gmw[u_, i_, j_] := Module[{vec, chi = ConstantArray[0, sizem],
     X = gs[u].Transpose[OpC[i]], Y = OpC[j].gs[u]}, vec = Eigenvectors[Hm[u]];
   For[k = 1, k < sizem, k++;
    chi[[k]] = (X.vec[[k]]) * (vec[[k]].Y)]; chi];
Gkpw[u_, j_] := Module[
   {vec, chi = ConstantArray[0, sizep], Y = Cdk[j].gs[u]}, vec = Eigenvectors[Hp[u]];
   For[k = 1, k < sizep, k++;
    chi[[k]] = (Abs[vec[[k]].Y])^2]; chi];
Gkmw[u_, j_] := Module[
   {vec, chi = ConstantArray[0, sizem], Y = Ck[j].gs[u]}, vec = Eigenvectors[Hm[u]];
   For[k = 1, k < sizep, k++;
    chi[[k]] = (Abs[vec[[k]].Y])^2];
   chi];
```

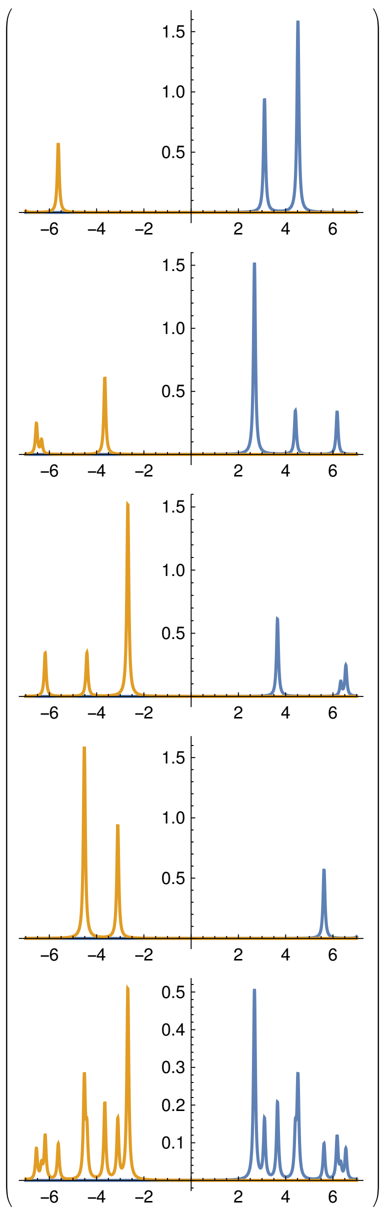
precompute the matrix elements

```
U = 8.;
weighp11 = Gpw[U, 1, 1];
eigp = Eigenvalues[Hp[U]] - Egs[U];
weighm11 = Gmw[U, 1, 1];
eigm = Eigenvalues[Hm[U]] - Egs[U];
mu = 10 + U / 2;
weightkp0 = Gkpw[U, 0];
weightkm0 = Gkmw[U, 0];
weightkp1 = Gkpw[U, 1];
weightkm1 = Gkmw[U, 1];
weightkp2 = Gkpw[U, 2];
weightkm2 = Gkmw[U, 2];
weightkp3 = Gkpw[U, 3];
weightkm3 = Gkmw[U, 3];
plot4 =
  {Plot[{Spect[x, 0.05, weightkp0, eigp - mu], Spect[-x, 0.05, weightkm0, eigm + mu]},
     {x, -7, 7}, PlotRange → Full], Plot[{Spect[x, 0.05, weightkp1, eigp - mu],
      Spect[-x, 0.05, weightkm1, eigm + mu]}, {x, -7, 7}, PlotRange → Full],
   Plot[{Spect[x, 0.05, weightkp2, eigp - mu], Spect[-x, 0.05, weightkm2, eigm + mu]},
     {x, -7, 7}, PlotRange → Full], Plot[{Spect[x, 0.05, weightkp3, eigp - mu],
      Spect[-x, 0.05, weightkm3, eigm + mu]}, {x, -7, 7}, PlotRange → Full],
   Plot[{Spect[x, 0.05, weighp11, eigp - mu], Spect[-x, 0.05, weighm11, eigm + mu]},
     {x, -7, 7}, PlotRange → Full]};
```

Plot Im G(w) for positive (electron addition) and negative (electron removal) frequencies for U=1, 2,4,8

```
{MatrixForm[plot1], MatrixForm[plot2], MatrixForm[plot3], MatrixForm[plot4]}
{plot1, plot2, plot3, plot4}
```

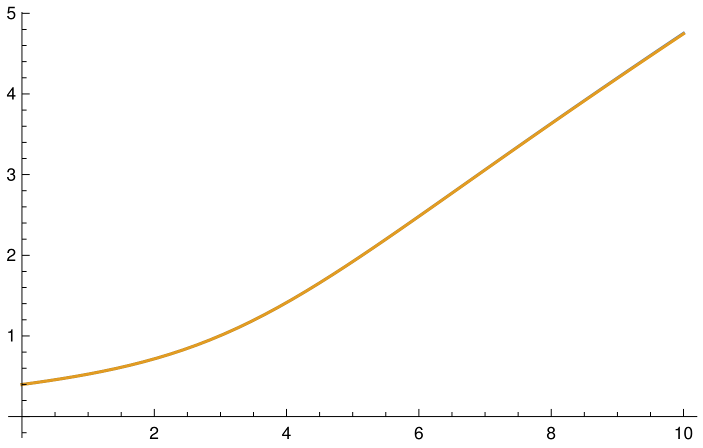
```
MatrixForm[plot4]
```



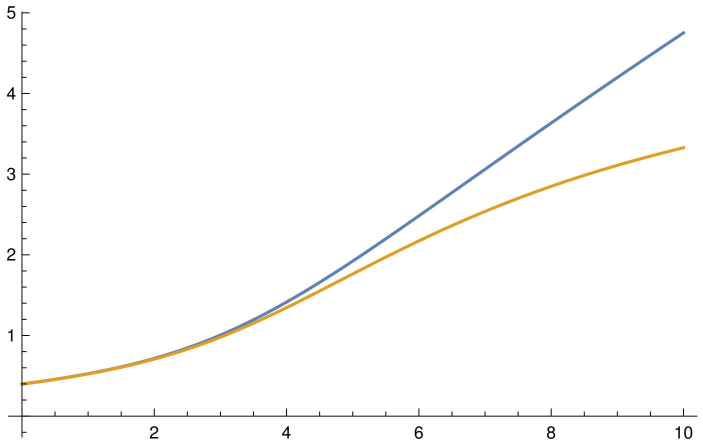
Finite field calculation of local susceptibility

```
field = 0.01;
Htest =.;
gtest =.;
chitest =.;
Htest[u_, x_] := H[u] - x * OpSz[1];
gtest[u_, x_] := Eigenvectors[Htest[u, x]][[-1]];
chitest[u_, x_] := gtest[u, x].OpSz[1].gtest[u, x] / x;
```

```
Plot[{Localchi[1, u], chitest[u, 0.01]}, {u, 0, 10}]
```



```
Plot[{Localchi[1, u], chitest[u, 0.2]}, {u, 0, 10}]
```



5
4
3
2
1
2
4
6
8
10