```
In[*]:= SetDirectory@NotebookDirectory[];

[设置目录 __当前笔记本的目录
Import["Qubits_package.m"];

[导入
Import["ExactKrylov_package.m"];
```

Parameters

Model

```
If[StringMatchQ[HamType, "Heisenberg"], (
[··· [字符串匹配判定

EL = funGraph[Nq, GraphType];

Model = funHeisenberg[Nq, EL]

)];

If[StringMatchQ[HamType, "FermiHubbard"], (
[··· [字符串匹配判定

EL = funGraph[Nq / 2, GraphType];

u = 1.;

Model = funFermiHubbard[Nq, EL, u]

)];

Graph[EL]

Out[=]=
```

In[@]:= Ham = funHamiltonianQubit[Model];

Spectrum

```
In[@]:= {EE, ES} = funSpectrum[Ham];
     HamNorm = Max[Abs[EE]];
               _… _ 绝对值
     EE = EE / HamNorm;
     Eg = EE[[1]]
Out[\ \ \ \ ]=\ \ -0.721501
In[@]:= If[StringMatchQ[HamType, "Heisenberg"], (
     L… 上字符串匹配判定
        htot = 3. * Length[EL] / HamNorm
                   长度
      )]
     If[StringMatchQ[HamType, "FermiHubbard"], (
     L··· L字符串匹配判定
        htot = (2. * Length[EL] + u / 4. * Nq / 2.) / HamNorm
                    长度
      )]
Out[\ \ \ \ \ ]= 1.17428
```

Reference state

```
In[*]:= If[StringMatchQ[HamType, "Heisenberg"], (
     ... 字符串匹配判定
          \psi = \text{funPairwiseSinglet[Nq]}
        )];
     If[StringMatchQ[HamType, "FermiHubbard"], (
     L… L字符串匹配判定
          \psi = \text{funHartreeFock}[Nq, EL]
        )];
      \psi = Conjugate[ES].\psi;
          共轭
      \psi = Flatten[\psi];
         压平
      Pro\psi = Abs[\psi]^2;
             绝对值
ln[ \circ ]:= pg = Pro\psi[1]
      ER = Total[Pro\psi * EE];
           总计
      \epsilon R = ER - Eg
Out[*]= 0.60369
Out[\bullet]= 0.0223459
```

Run

```
In[*]:= dList = Table[d, {d, 2, 30}];
     plotsRTE = {};
     plotsF = {};
     plots = {};
     \gamma 2 \in K = \{\};
d = dList[[1]];
        Ide = IdentityMatrix[d];
               单位矩阵
        E0 = Eg + 1.;
        {Hmat, Smat} = funMatPower[EE, Pro\psi, d, E0];
        EB = Hmat[[d, d]] / Smat[[d, d]];
        \epsilon B = EB - Eg;
        \log \eta = -15;
        \eta = 10.^{\log \eta};
        {EK, cn} = funDiagonalisation[Hmat + 2. * \eta * Ide, Smat + 2. * \eta * Ide];
        \epsilon K = EK - Eg;
        If [\epsilon K > 1.*^{-2} | \epsilon K < 1.*^{-9}, (
        如果
           Print[\{d, \epsilon K\}];
          打印
           Goto[end];
          转到
          )];
        {\gammaList, \inList} = funGammaEpsilon[Eg, pg, Hmat, Smat, Ide, 1., 1., \log \etaList];
        γListP = γList;
        \epsilonListP = \epsilonList;
        eMin = Min[eList];
                最小值
        If [\epsilon Min < 2. * \epsilon K, (
        如果
           γ = funInterpolation[εList, γList, 2. * εK];
          ),(
           γ = 0.;
          )];
        \gamma P = \gamma;
        E0 = 0;
        {Hmat, Smat} = funMatChebyshev[EE, Pro\psi, d, htot, E0];
        {\gamma List, \epsilon List} = funGammaEpsilon[Eg, pg, Hmat, Smat, Ide, 1., 1., log<math>\eta List];
        γListCP = γList;
        eListCP = eList;
        eMin = Min[eList];
```

```
「おん」、旧
If [\epsilon Min < 2. * \epsilon K, (
如果
   γ = funInterpolation[εList, γList, 2. * εK];
 ),(
   γ = 0.;
 )];
\gammaCP = \gamma;
E0 = Eg;
\tau MIN = 0;
\tauMAX = 64;
Do[(
Do循环
   \tau = (\tau MIN + \tau MAX) / 2.;
   {Hmat, Smat} = funMatGaussianPower[EE, Pro\psi, 1, htot, \tau, E0];
   EK = Hmat[[1, 1]] / Smat[[1, 1]];
   err = EK - Eg;
   If [err > \epsilonB, \tauMIN = \tau];
  如果
   If [err < \epsilonB, \tauMAX = \tau];
  如果
 ), {j, 1, 30}];
\tau = (\tau MIN + \tau MAX) / 2.;
\delta = RandomReal[\{-0.1, 0.1\}];
    伪随机实数
E0 = Eg + \delta;
{Hmat, Smat} = funMatGaussianPower[EE, Pro\psi, d, htot, \tau, E0];
{\gammaList, \inList} = funGammaEpsilon[Eg, pg, Hmat, Smat, Ide, htot, 1., \log \etaList];
γListGP = γList;
\epsilonListGP = \epsilonList;
eMin = Min[eList];
        最小值
If [\epsilon Min < 2. * \epsilon K, (
如果
   γ = funInterpolation[εList, γList, 2. * εK];
 ),(
   γ = 0.;
 )];
\gamma GP = \gamma;
E0 = Eg - 1.;
{Hmat, Smat} = funMatInversePower[EE, Proψ, d, E0];
{\gammaList, \inList} = funGammaEpsilon[Eg, pg, Hmat, Smat, Ide, 1., 1., \log \etaList];
γListIP = γList;
\epsilonListIP = \epsilonList;
eMin = Min[eList];
        最小值
If [\epsilon Min < 2. * \epsilon K, (
如果
   γ = funInterpolation[εList, γList, 2. * εK];
 ),(
```

```
γ = 0.;
 )];
\gammaIP = \gamma;
E0 = Eg;
\tauMIN = 0;
\tauMAX = 64;
Do[(
Do循环
   \tau = (\tau MIN + \tau MAX) / 2.;
   {Hmat, Smat} = funMatITE[EE, Pro\psi, d, \tau, E0];
   EK = Hmat[[d, d]] / Smat[[d, d]];
   err = EK - Eg;
   If [err > \epsilonB, \tauMIN = \tau];
   If [err < \epsilonB, \tauMAX = \tau];
  如果
 ), {j, 1, 30}];
\tau = (\tau MIN + \tau MAX) / 2.;
E0 = Eg;
{Hmat, Smat} = funMatITE[EE, Pro\psi, d, \tau, E0];
{\gammaList, \inList} = funGammaEpsilon[Eg, pg, Hmat, Smat, Ide, 1., 1., \log \etaList];
γListITE = γList;
eListITE = eList;
eMin = Min[eList];
        最小值
If [\epsilon Min < 2. * \epsilon K, (
如果
   γ = funInterpolation[εList, γList, 2. * εK];
 ),(
  γ = 0.;
 )];
\gammaITE = \gamma;
ΔtList = Table \left[\frac{2.*PI}{100} j, {j, 1, 100}\right];
\epsilonKList = \DeltatList;
Do [ (
   \Delta t = \Delta t List[j];
   {Hmat, Smat} = funMatRTE[EE, Pro\psi, d, \Deltat, E0];
   \log \eta = -15;
   \eta = 10.^{\log \eta};
   {EK, cn} = funDiagonalisation[Hmat + 2. * \eta * Ide, Smat + 2. * \eta * Ide];
   err = EK - Eg;
   ∈KList[j] = err
  ), {j, 1, Length[∆tList]}];
```

```
Δt = ΔtList[Position[εKList, Min[εKList]][1, 1]]];
                                     最小值
AppendTo[plotsRTE, ListLogPlot[Transpose[{∆tList, eKList}], PlotRange → Full]];
                        点集的对数图 上转置
                                                                                | 绘制范围
E0 = Eg;
{Hmat, Smat} = funMatRTE[EE, Pro\psi, d, \Deltat, E0];
{\gammaList, \epsilonList} = funGammaEpsilon[Eg, pg, Hmat, Smat, Ide, 1., 1., \log \etaList];
γListRTE = γList;
∈ListRTE = ∈List;
eMin = Min[eList];
        最小值
If [\epsilon Min < 2. * \epsilon K, (
   \gamma = \text{funInterpolation}[\epsilon \text{List}, \gamma \text{List}, 2. * \epsilon \text{K}];
 ),(
  γ = 0.;
 )];
\gammaRTE = \gamma;
\Delta E = 0.;
E0 = Eg;
\tauMIN = 0;
\tau MAX = 64;
Do [ (
Do循环
   T = (\tau MIN + \tau MAX) / 2.;
   {Hmat, Smat} = funMatFilter[EE, Pro\psi, d, T, E0, \DeltaE];
   EK = Hmat[[1, 1]] / Smat[[1, 1]];
   err = EK - Eg;
   If [err > \epsilonB, \tauMIN = T];
   If [err < \epsilonB, \tauMAX = T];
  如果
 ), {j, 1, 30}];
T = (\tau MIN + \tau MAX) / 2.;
ΔEList = Table \left[\frac{2.}{d * 100} * j, {j, 1, 100}\right];
\epsilonKList = \DeltaEList;
Do [ (
LDo循环
   \Delta E = \Delta E List[[j]];
   E0 = Eg;
   {Hmat, Smat} = funMatFilter[EE, Pro\psi, d, T, E0, \DeltaE];
   log\eta = -15;
   \eta = 10.^{\log \eta};
   {EK, cn} = funDiagonalisation[Hmat + 2. * \eta * Ide, Smat + 2. * \eta * Ide];
   err = EK - Eg;

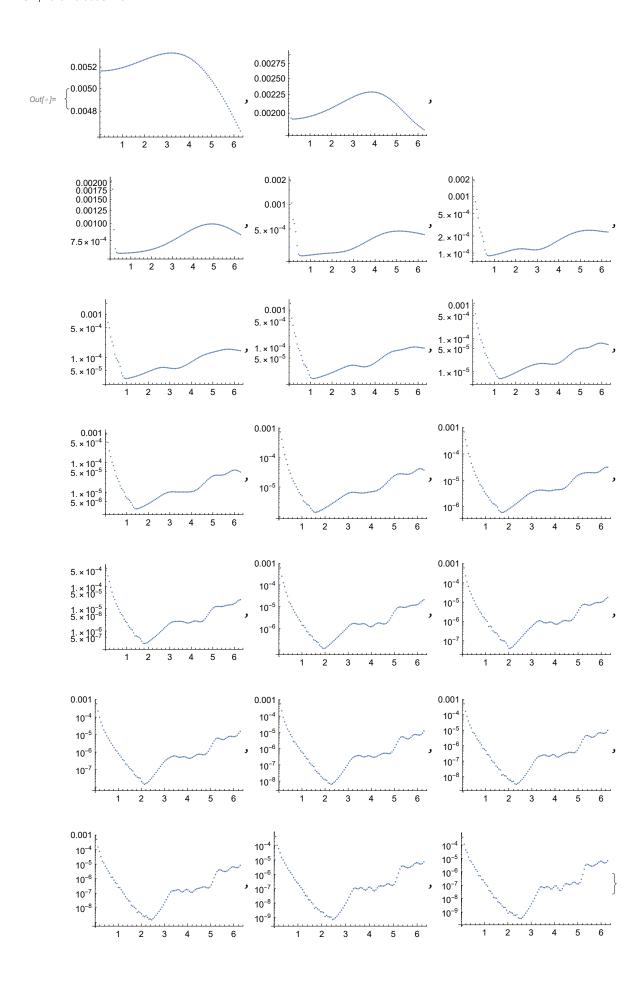
ϵKList[j] = err;
```

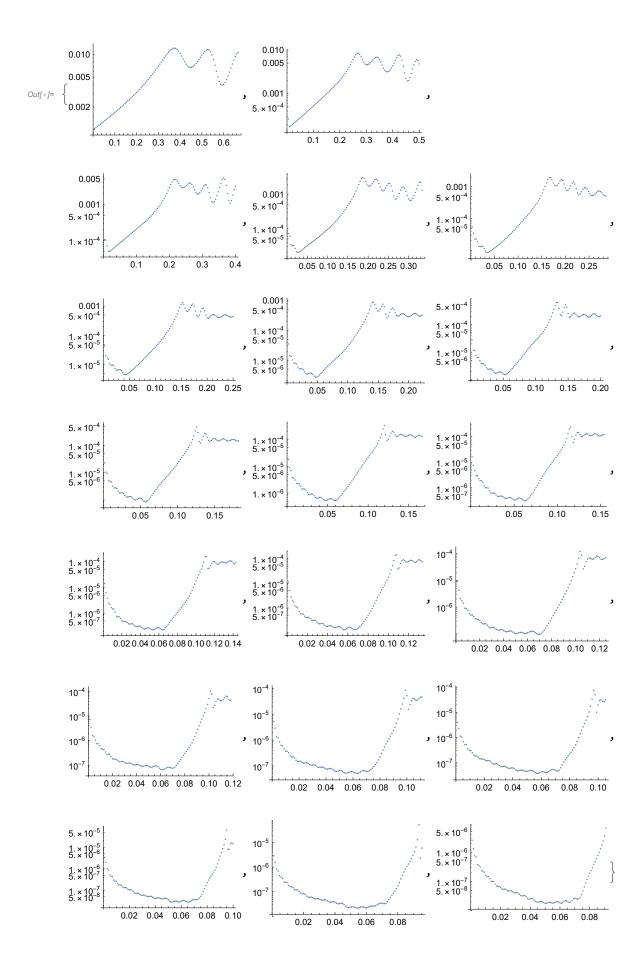
```
), {j, 1, Length[∆EList]}];
             长度
  \Delta E = \Delta EList[Position[\epsilon KList, Min[\epsilon KList]][1, 1]]];
                                  最小值
               付置
  AppendTo[plotsF, ListLogPlot[Transpose[{∆EList, eKList}], PlotRange → Full]];
                     点集的对数图 转置
                                                                    绘制范围
  上附加
  E0 = Eg;
  {Hmat, Smat} = funMatFilter[EE, Pro\psi, d, T, E0, \DeltaE];
  {\gammaList, \inList} = funGammaEpsilon[Eg, pg, Hmat, Smat, Ide, 1., 1., \log \etaList];
  γListF = γList;
  eListF = eList;
  eMin = Min[eList];
         最小值
  If [\epsilon Min < 2. * \epsilon K, (
  如果
    γ = funInterpolation[εList, γList, 2. * εK];
   ),(
    γ = 0.;
   )];
  \gamma F = \gamma;
  AppendTo[plots, ListLogLogPlot[
                    点集的双对数图
     {Transpose[{\gamma ListP, 0. * eListP + eK}], Transpose[{\gamma ListP, 0. * eListP + 2. * eK}],}
     上转置
      Transpose[{γListP, εListP}], Transpose[{γListCP, εListCP}],
      转置
                                       转置
      Transpose[{γListGP, εListGP}], Transpose[{γListIP, εListIP}],
      Transpose[{γListITE, εListITE}], Transpose[{γListRTE, εListRTE}],
      Transpose[\{\gamma ListF, \epsilon ListF\}]}, PlotRange \rightarrow PR, Joined \rightarrow True,
                                        绘制范围
                                                         连接点
                                                                  真
      | 转置
     PlotStyle → {Cyan, Brown, Red, Yellow, Blue, Green, Orange, Purple, Magenta}]];
    绘图样式
                  L蓝绿色 L棕色 L红色 L黄色 L蓝色 L绿色 L橙色
                                                                   紫色
  AppendTo[\gamma2\epsilonK, {\gammaP, \gammaCP, \gammaGP, \gammaIP, \gammaITE, \gammaRTE, \gammaF}];
  上附加
  Label[end];
  Print[{"d", d, ∈K, ToString[Now]}];
                      转换为…
  , {1, 1, Length[dList]}
\gamma 2 \in K = Transpose[\gamma 2 \in K];
       转置
{2, 0.0110074}
{d, 2, 0.0110074, DateObject[{2022, 12, 10, 11, 49, 51.0045883}, Instant, Gregorian, 8.]}
{d, 3, 0.00516331, DateObject[{2022, 12, 10, 11, 49, 51.6409754}, Instant, Gregorian, 8.]}
{d, 4, 0.00192308, DateObject[{2022, 12, 10, 11, 49, 52.4794042}, Instant, Gregorian, 8.]}
```

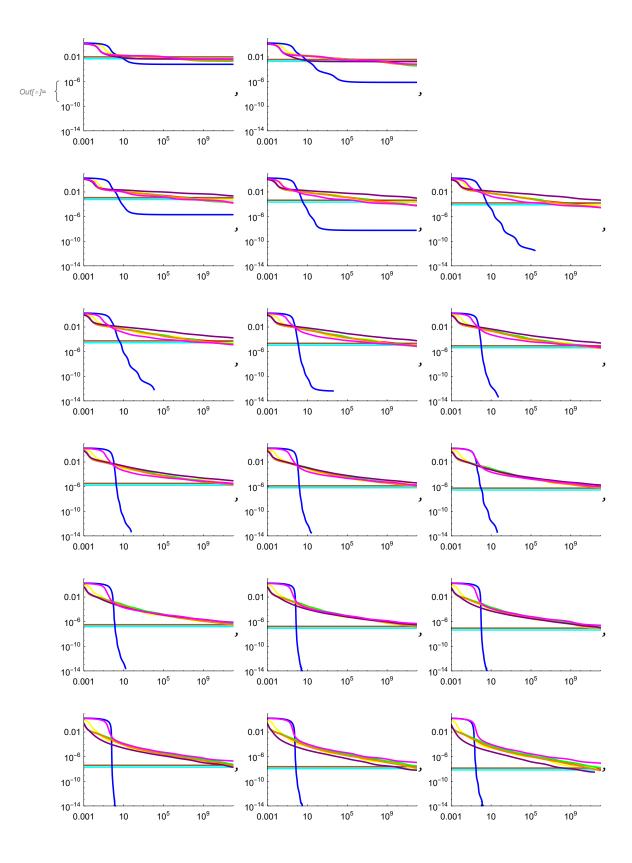
```
{d, 5, 0.000602236, DateObject[{2022, 12, 10, 11, 49, 53.4082409}, Instant, Gregorian, 8.]}
{d, 6, 0.000229127, DateObject[{2022, 12, 10, 11, 49, 54.5744971}, Instant, Gregorian, 8.]}
{d, 7, 0.0000830542, DateObject[{2022, 12, 10, 11, 49, 56.0325346}, Instant, Gregorian, 8.]}
{d, 8, 0.0000279942, DateObject[{2022, 12, 10, 11, 49, 57.7839061}, Instant, Gregorian, 8.]}
{d, 9, 0.0000111243, DateObject[{2022, 12, 10, 11, 49, 59.8469732}, Instant, Gregorian, 8.]}
\{d, 10, 4.36578 \times 10^{-6}, DateObject[\{2022, 12, 10, 11, 50, 2.2534840\}, Instant, Gregorian, 8.]\}
\{d, 11, 1.69961 \times 10^{-6}, DateObject[\{2022, 12, 10, 11, 50, 5.0665694\}, Instant, Gregorian, 8.]\}
\{d, 12, 6.82016 \times 10^{-7}, DateObject[\{2022, 12, 10, 11, 50, 8.4258071\}, Instant, Gregorian, 8.]\}
\{d, 13, 2.8792 \times 10^{-7}, DateObject[\{2022, 12, 10, 11, 50, 12.6528769\}, Instant, Gregorian, 8.]\}
\{d, 14, 1.61108 \times 10^{-7}, DateObject[\{2022, 12, 10, 11, 50, 20.5740825\}, Instant, Gregorian, 8.]\}
{d, 15, 8.56406 \times 10^{-8}, DateObject[{2022, 12, 10, 11, 50, 30.2744736}, Instant, Gregorian, 8.]}
\{d, 16, 4.4359 \times 10^{-8}, DateObject[\{2022, 12, 10, 11, 50, 40.6851590\}, Instant, Gregorian, 8.]\}
{d, 17, 2.01177\times10<sup>-8</sup>, DateObject[{2022, 12, 10, 11, 50, 52.9903669}, Instant, Gregorian, 8.]}
\{d, 18, 1.18725 \times 10^{-8}, DateObject[\{2022, 12, 10, 11, 51, 9.0967416\}, Instant, Gregorian, 8.]\}
{d, 19, 7.04174\times10<sup>-9</sup>, DateObject[{2022, 12, 10, 11, 51, 37.5559958}, Instant, Gregorian, 8.]}
\{d, 20, 3.74192 \times 10^{-9}, DateObject[\{2022, 12, 10, 11, 52, 8.5206633\}, Instant, Gregorian, 8.]\}
\{d, 21, 2.0856 \times 10^{-9}, DateObject[\{2022, 12, 10, 11, 52, 41.5691291\}, Instant, Gregorian, 8.]\}
\{d, 22, 1.37236 \times 10^{-9}, DateObject[\{2022, 12, 10, 11, 53, 24.0047987\}, Instant, Gregorian, 8.]\}
\{23, 8.43686 \times 10^{-10}\}
\{d, 23, 8.43686 \times 10^{-10}, DateObject[\{2022, 12, 10, 11, 53, 24.0792446\}, Instant, Gregorian, 8.]\}
\{24, 5.08429 \times 10^{-10}\}
\{d, 24, 5.08429 \times 10^{-10}, DateObject[\{2022, 12, 10, 11, 53, 24.2023464\}, Instant, Gregorian, 8.]\}
\{25, 3.31254 \times 10^{-10}\}
\{d, 25, 3.31254 \times 10^{-10}, DateObject[\{2022, 12, 10, 11, 53, 24.3205044\}, Instant, Gregorian, 8.]\}
\{26, 2.25562 \times 10^{-10}\}
\{d, 26, 2.25562 \times 10^{-10}, DateObject[\{2022, 12, 10, 11, 53, 24.4426243\}, Instant, Gregorian, 8.]\}
\{27, 1.31702 \times 10^{-10}\}
\{d, 27, 1.31702 \times 10^{-10}, DateObject[\{2022, 12, 10, 11, 53, 24.5630324\}, Instant, Gregorian, 8.]\}
\{28, 8.07604 \times 10^{-11}\}
\{d, 28, 8.07604 \times 10^{-11}, DateObject[\{2022, 12, 10, 11, 53, 24.6967698\}, Instant, Gregorian, 8.]\}
\{29, 5.79942 \times 10^{-11}\}
\{d, 29, 5.79942 \times 10^{-11}, DateObject[\{2022, 12, 10, 11, 53, 24.8707436\}, Instant, Gregorian, 8.]\}
\{30, 4.40111 \times 10^{-11}\}
\{d, 30, 4.40111 \times 10^{-11}, DateObject[\{2022, 12, 10, 11, 53, 25.0564772\}, Instant, Gregorian, 8.]\}
```

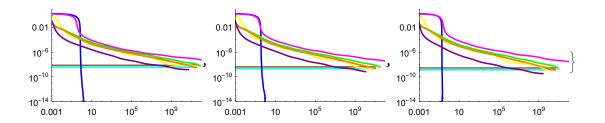
Plots

In[@]:= plotsRTE plotsF plots









Data

```
ln[*]:= If[! StringMatchQ[GraphType, "Chain"] && ! StringMatchQ[GraphType, "Ladder"],
    如果 字符串匹配判定
                                             字符串匹配判定
      GraphType = "Random"];
In[*]:= path =
      ToString[HamType] <> "-" <> ToString[GraphType] <> "-Nq=" <> ToString[Nq] <> ".dat";
                                L转换为字符串
                                                                转换为字符串
      转换为字符串
    CreateFile[path];
    创建文件
    file = File[path];
          文件位置的符号表示
In[@]:= Data = {};
    AppendTo[Data, "γ2εΚ:"];
    Data = Join[Data, \gamma 2 \in K];
          连接
    AppendTo[Data, ""];
    Export[file, Data];
    导出
```