Week 8 assignment

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Quantum Information and Computation

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N spins; dimension $2^N \times 2^N$, opposite sign than usual

$$\mathcal{H}_{\mathcal{N}} = \lambda \sum_i^N \sigma_z^i - \sum_i^{N-1} \sigma_x^{i+1} \sigma_x^i$$

2N spins, subsystems A and B

$$\mathcal{H}_{2N} = \mathcal{H}_N^A \otimes \mathbb{I}_N + \mathbb{I}_N \otimes \mathcal{H}_N^B - A \otimes B$$
$$A = \mathbb{I}^1 \otimes \mathbb{I}^2 \cdots \otimes \sigma_x^N \; ; \quad B = \sigma_x^1 \otimes \mathbb{I}^2 \cdots \otimes \mathbb{I}^N$$

RSRG Algorithm

- $\tilde{\mathcal{H}} = \mathcal{H} \otimes \mathbb{I}_N + \mathbb{I}_N \otimes \mathcal{H} - A \otimes B$
- Diagonalize $\tilde{\mathcal{H}}$, first 2^N eigenvalues are columns of P.
- Restrict to the lowest important eigenvalues via

$$\mathcal{H} = P^T \tilde{\mathcal{H}} P \tag{1}$$

  and compute physical quantities with Eq. (1).
- $\tilde{A} = A \otimes \mathbb{I}_N$, $\tilde{B} = \mathbb{I}_N \otimes B$; redefine A, B with $P^T(\tilde{A}, \tilde{B})P$ and restart

```
function Ham_Double(H, A, B) result(H_2N)
            complex*16, dimension(:,:), allocatable :: H_2N
        t = size(H,1)
    H_2N = TPROD(H, cEYE(t)) + TPROD(cEYE(t), H) + TPROD(A,B)
```

```
subroutine INIT_INTERACTION(N, d, A, B)
    complex*16, dimension(:,:), allocatable :: A, B
    sigma_x = reshape([0, 1, 1, 0], shape(sigma_x), order = [2,1] )
    A = TPROD( cEYE(d**(N-1)), sigma_x)
    B = TPROD( sigma_x, cEYE(d**(N-1)))
```

```
!RSRG algorithm
        do while( ABS(1 - old_egs/e_gs) > threshold  )
                old_egs = e_gs
                H_double = HAM_DOUBLE(H_single, A, B)
                A_double = TPROD( A, cEYE(2**N))
                B_double = TPROD(cEYE(2**N), B)

                call C_EIGENVECTORS(H_double, eig_vec, eigs )
                P = dcmplx(eig_vec(:, :2**N))

                !the 2N system becomes the one to double in the next iteration
                H_single = PROJECT(H_double, P)
                A = PROJECT(A_double, P)
                B = PROJECT(B_double, P)
                system_size = 2 * system_size

                e_gs = eigs(1)/ system_size
                deallocate(eigs, eig_vec)
        end do
```

Test (first iteration)

RSRG $N = 1, \lambda = 1 \rightarrow \mathcal{H}_1 = \sigma_z \, ; \; A = \sigma_x$

$$\mathcal{H}_2 = \sigma_z \otimes \mathbb{I} + \mathbb{I} \otimes \sigma_z - \sigma_x \otimes \sigma_x$$

Eigenvalues: -2.23, -1, 1, 2.23

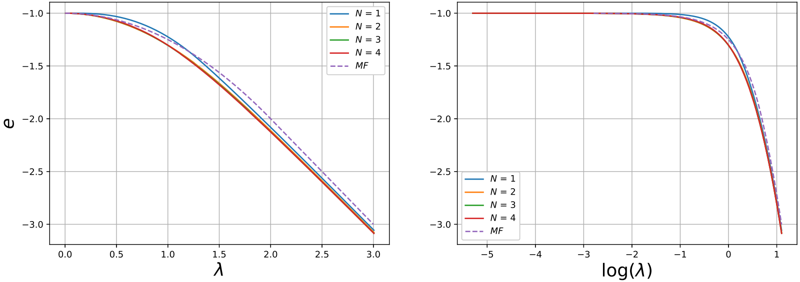
```
beefyboy@beefyboy:~/rgweek8$ gfortran n2.f90 -o example -llapack
beefyboy@beefyboy:~/rgweek8$ ./example
 This is H_2
{         2.00000,          0.00000} {         0.00000,          0.00000} {         0.00000,          0.00000} {        -1.00000,          0.00000}
{         0.00000,          0.00000} {         0.00000,          0.00000} {        -1.00000,          0.00000} {         0.00000,          0.00000}
{         0.00000,          0.00000} {        -1.00000,          0.00000} {         0.00000,          0.00000} {         0.00000,          0.00000}
{        -1.00000,          0.00000} {         0.00000,          0.00000} {         0.00000,          0.00000} {        -2.00000,          0.00000}
 This is P^T H_2 P
{        -2.23607,          0.00000} {         0.00000,          0.00000}
{         0.00000,          0.00000} {        -1.00000,          0.00000}
 This is GS energy density
  -1.1180339887498949
```

The projection correctly leaves only $-2.23, -1$

Threshold $\epsilon = 10^{-13}$, convergence condition $\left(1 - \frac{e_{old}}{e_{new}}\right) < \epsilon$.

Mean field prediction

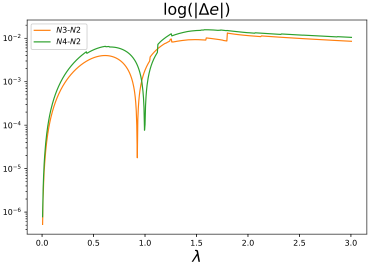
$$e = \begin{cases} -1 - \frac{\lambda^2}{4} & \lambda \in [-2, 2] \\ -|\lambda| & \lambda \notin [-2, 2] \end{cases}$$

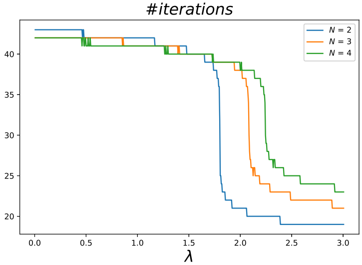


- MF and $N = 1$ are not precise approximations
- $(\log \lambda, e(\lambda))$ plot makes clear $\lambda \approx 1$ transition

Graph on the left:

- $e(N=3) - e(N=2), e(N=4) - e(N=2)$ difference suddenly drops down around $\lambda \approx 1$
- $N = 4$ differs more from $N = 2$ and the drop associated to $\lambda_{critical}$ is moving to the right with N





Graph on the right:

- *iterations* required for convergence drop down around $\lambda \approx 2$
- tradeoff: smaller N-s require more iterations at the beginning but less in the end.
- similar *iterations* $\rightarrow$ different end system sizes $N \cdot 2^{\#iterations}$