Exact Diagonalization Technique

Hai-Qing Lin

Beijing Computational Science Research Center

Refs. PRB 42, 6561 (1990);
Computer in Physics 7, 400 (1993);
Can. J. Phys. 77, 353 (1999).

Outline

- Introduction
- Searching Algorithm
- Iteration Scheme
- Applications
- Current Status and Improvements
- Finite size scaling

Exact Diagonalization

- **Exact solution on finite lattice**
- **Gain insights on correlations**
- **Flexibility (BC, interactions, etc)**
- **Check on approximations and simulations**
- **Finite size scaling scheme is desired**
- **Usually prefer short-range interactions**

Exact Diagonalization Procedure

Eigenvalue problems

- $H_{ij} = \langle i|H|j\rangle$,
  $i, j = 1, 2, \ldots, M$
- $H|\Phi\rangle = \lambda|\Phi\rangle$,
  $|\Phi\rangle = \Sigma_i \alpha_i |i\rangle$
- $\langle O\rangle = \langle\Phi|O|\Phi\rangle$

Orthonomal Basis

- **Hubbard model: 0, ↑, ↓, ↑↓**
  $M = 4^N$, N = number of Lattice
- **Spin model:** $S_i^z = -S, -S+1, \ldots, S$.
  $M = (2S+1)^N$. e.g., Spin-½ , $M = 2^N$
- **Binary representation and bit operation:**
  $I_\sigma = \Sigma_i n_\sigma 2^{i-1}$.
  $I = \Sigma_i s(i)\,(2S+1)^{i-1}$,
  $s(i) \equiv S_i^z + \mathrm{S} = 0, 1, \ldots, 2S$.
  $c_i^\dagger c_j$ + h.c. or $S_i^+ S_j^-$ + h.c.: (1,0) ↔ (0,1)

Search Algorithm

- $H\,|i\rangle = \sum H_{ij}\,|j\rangle$
- *For a give binary representation of spin (electron) configuration, how to find an efficient storage/lookup table?*

  ‘ ‘Direct’ ’ Method

- $J(I) = 1, 2, \ldots, M$, I up to $(2S+1)^N$ (4^N)
- **Length of vector J(I) could be too long**
- **Too many null entries**

Hashing Technique

- **Commonly used in computer science (read)**
- **Hashing function, $h(I) = [I \pmod K] + 1$.**
- **Length of vector $h(I) \geq M$.**
- **Collision, $h(I_1) = h(I_2)$, $I_1 \neq I_2$**
- **Non-vectorizable, hard to parallel, slow.**

TABLE I. Spin configurations, their representations I, their positions in the storage table $J(I)$ by using a naive way of searching (see the text) for a spin-$\frac{1}{2}$ system of size 6. A hashing function $h(I)=[I(\mathrm{mod}K)]+1$ with $K=23$ is also shown.

Configuration	I	$J(I)$	$h(I)$	Configuration	I	$J(I)$	$h(I)$
0 0 0 1 1 1	7	1	8	1 0 0 0 1 1	35	11	13
0 0 1 0 1 1	11	2	12	1 0 0 1 0 1	37	12	15
0 0 1 1 0 1	13	3	14	1 0 0 1 1 0	38	13	16
0 0 1 1 1 0	14	4	15	1 0 1 0 0 1	41	14	19
0 1 0 0 1 1	19	5	20	1 0 1 0 1 0	42	15	20
0 1 0 1 0 1	21	6	22	1 0 1 1 0 0	44	16	22
0 1 0 1 1 0	24	7	2	1 1 0 0 0 1	49	17	4
0 1 1 0 0 1	25	8	3	1 1 0 0 1 0	50	18	5
0 1 1 0 1 0	26	9	4	1 1 0 1 0 0	52	19	7
0 1 1 1 0 0	28	10	6	1 1 1 0 0 0	56	20	11

‘ ‘Two-Table’ ’ Technique

- **N = Na + Nb**
- $I_a = \Sigma_i^{N_a}\ s(i)\ (2S+1)^{i-1}$.
  $I_b = \Sigma_i^{N_b} s(i)\ (2S+1)^{i-1}$, $s(i) \equiv S_i^z + S = 0, 1, \ldots, 2S$
- $J(I) = J(I_a) + J(I_b)$.
- **Length of vector** $h(I) \leq \sqrt{M}$ **(reduces memory).**
- **No collision.**
- **Vectorizable (parallelizable), very fast.**
- **Similar for fermions. (how?)**

TABLE II. Spin configurations, their representations I_a and I_b, their base vectors $J_a(I_a)$ and position vectors $J_b(I_b)$ and their positions in the storage table $J(I)$ by using the new coding technique for unsymmetrized basis (see the text) for a spin-$\frac{1}{2}$ system of size six.

Configuration A	I_a	$J_a(I_a)$	Configuration B	I_b	$J_b(I_b)$	$J=J_a+J_b$
1 1 1	7	1	0 0 0	0	0	1
0 1 1	3	1	0 0 1	1	1	2
1 0 1	5	2	0 0 1	1	1	3
1 1 0	6	3	0 0 1	1	1	4
0 1 1	3	1	0 1 0	2	4	5
1 0 1	5	2	0 1 0	2	4	6
1 1 0	6	3	0 1 0	2	4	7
0 1 1	3	1	1 0 0	4	7	8
1 0 1	5	2	1 0 0	4	7	9
1 1 0	6	3	1 0 0	4	7	10
0 0 1	1	1	0 1 1	3	10	11
0 1 0	2	2	0 1 1	3	10	12
1 0 0	4	3	0 1 1	3	10	13
0 0 1	1	1	1 0 1	5	13	14
0 1 0	2	2	1 0 1	5	13	15
1 0 0	4	3	1 0 1	5	13	16
0 0 1	1	1	1 1 0	6	16	17
0 1 0	2	2	1 1 0	6	16	18
1 0 0	4	3	1 1 0	6	16	19
0 0 0	0	1	1 1 1	7	19	20

Symmetries

- $[H, O_s] = 0$
  $H = H_1 \oplus H_2 \oplus \cdots$
- **Translation (Periodic Boundary Condition)**
- **Rotation ($D \geq 2$)**
- **Reflection (may not commute with rotation)**
- $N_\uparrow$, $N_\downarrow$ (S_T^z), S^2

Sparse Matrix

- **There exists many zero matrix elements**
- **Number of operations ~ N log(N), not N^3**

  Ground state properties (low dimensions)
- **No finite temperature phase transitions (Mermin-Wagner)**
- **$E_f \approx 10^5 T$:**
  Low lying excitations determine basic physics

Iteration Scheme

- **Standard approach, basic linear algebra**
- **Power method**
- **Lanczos method**
- **Similar approach: e.g, projection (QMC)**

Power Method

- **Select a state $|\Psi>$**
- **Apply H (or shift by a constant) to $|\Psi>$ and calculate**

$$E^n = <\Psi | H^n | \Psi> / <\Psi | \Psi>$$

- **In the limit $n \rightarrow \infty$, E^n converges to the ground state if $|\Psi>$ is not orthogonal to the ground state**

Lanczös Algorithm

- **Recursion Relation**

$$H|\Phi_j\rangle = \beta_{j-1}|\Phi_{j-1}\rangle + \alpha_j|\Phi_j\rangle + \beta_j|\Phi_{j+1}\rangle$$

- **Tridiagonal matrix**
- **It is a canonical transform**

$$T_{m\times m} = \begin{bmatrix} \alpha_1 & \beta_1 & \cdots & 0 \\ \beta_1 & \alpha_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \beta_{m-1} \\ 0 & \cdots & \beta_{m-1} & \alpha_m \end{bmatrix}$$

Lanczös Algorithm

Orthogonality

- $\langle \Phi_i | \Phi_j \rangle = \delta_{ij}$
- $\alpha_i = \langle \Phi_j | H | \Phi_j \rangle$
- $\beta_i = \langle \Phi_{j+1} | H | \Phi_j \rangle$

Pseudocode

$q(1{:}n) = 0;\ \beta_0 = 0;\ j = 0$
while $\beta_j \neq 0$
  if $j \neq 0$
    for $i = 1{:}n$
      $t = b_i;\ b_i = q_i/\beta_j;\ q_i = -\beta_j/t$
    end
  end
  $q = q + \mathtt{mult}(A,b)$
  $j = j + 1;\ \alpha_j = b^T q;\ q = q - \alpha_j b;\ \beta_j = \|q\|$
end

Iteration

- **Eigenvalues of the matrix $T_{m\times m}$**

  $$\lambda_i(m+1) \le \lambda_i(m)$$

- **The ground state energy of H**

  $$E_0 = \lim_{m\to M} \lambda_1$$

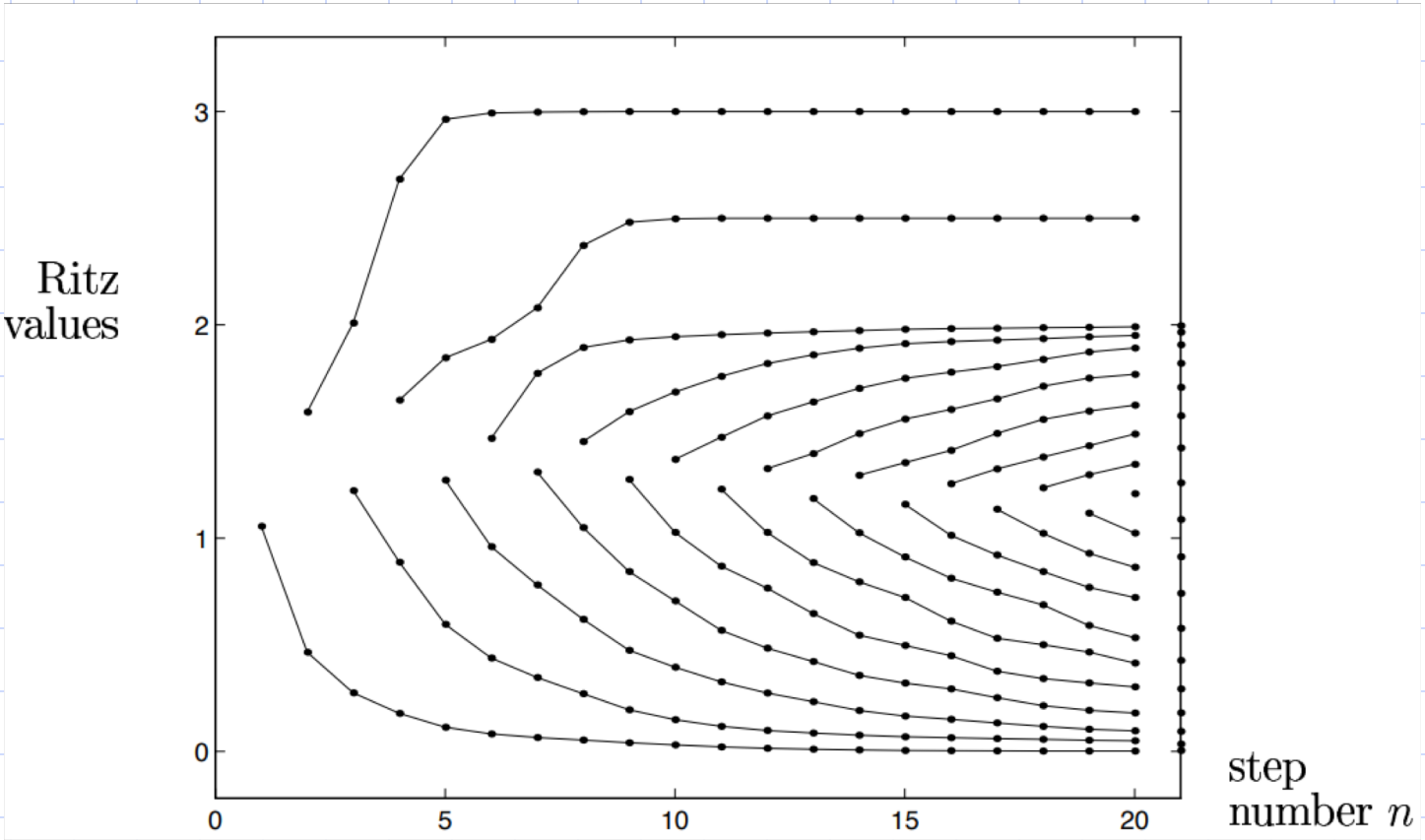
- **The ground state wave function**

  $$|\Psi_0\rangle = \sum_{j=1}^{m} z(j,1)\,|\Phi_j\rangle$$

  where $z(j,1)$ is eigenvector of $\lambda_1(m)$

- **In practice, m = 30 – 100 (10 digits in E_0).**

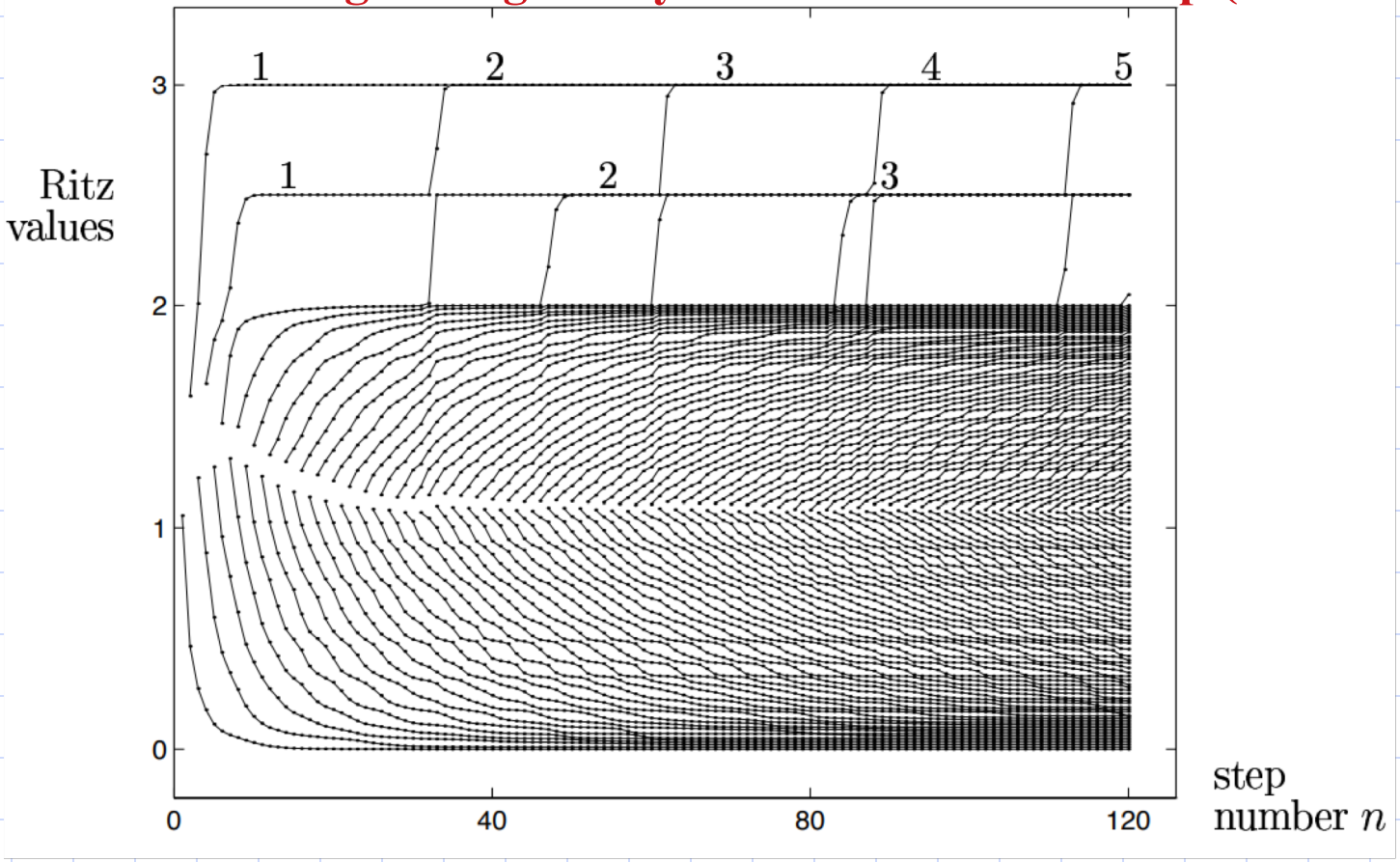
Convergence



- **Convergence to endpoint eigenvalues in a few steps**

Convergence

Solution: enforcing orthogonality of the basis at each step (more expensive)



- **Rounding errors are the source of ghost eigenvalues → loss of orthogonality between the basis vectors.**

Symmetry and Conservation Quantities

- If $[H, O_s] = 0$, and $|\Phi_1\rangle$ is in a subspace of O_s, then all $|\Phi_j\rangle$ are in the subspace of O_s and so is $|\Psi_0\rangle$.
- $|\Phi_{j=1,2,\ldots,m}\rangle$ belongs to an invariant subspace of H.
- Choosing different initial state.
- 4×4 Hubbard, $Ne = 8 + 8$,
  $M = 4^{16} = 4\ 294\ 967\ 296$
  $\rightarrow (16)!/(8!)^2 = 601\ 080\ 390 \rightarrow 1\ 310\ 242$ (90 sec.)

Programming and Improvements

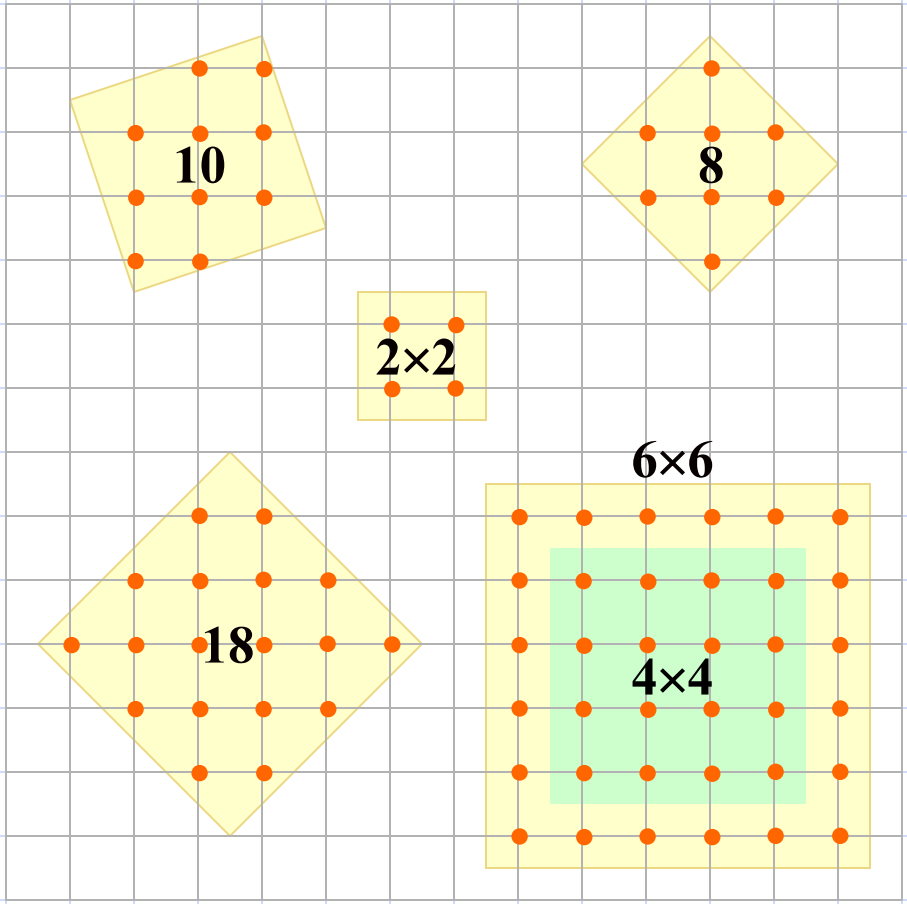
- **Notes on Programming**
- **Good initial trial state (physics)**
- **Reorthogonalization**
- **Fast I/O**
- **Lift degeneracy**
- **Picking up important configurations?**

Summary

- **Achievements**
  - **Hubbard model, $N = 18$, $M = 16{,}445{,}304$**
  - **Heisenberg model, $N = 36$, $M \approx 16$ M**
- **Applications**
  - **Widely used currently**
  - **LRO in AFH, and other models**
  - **ΔE, Pairing correlations, etc**

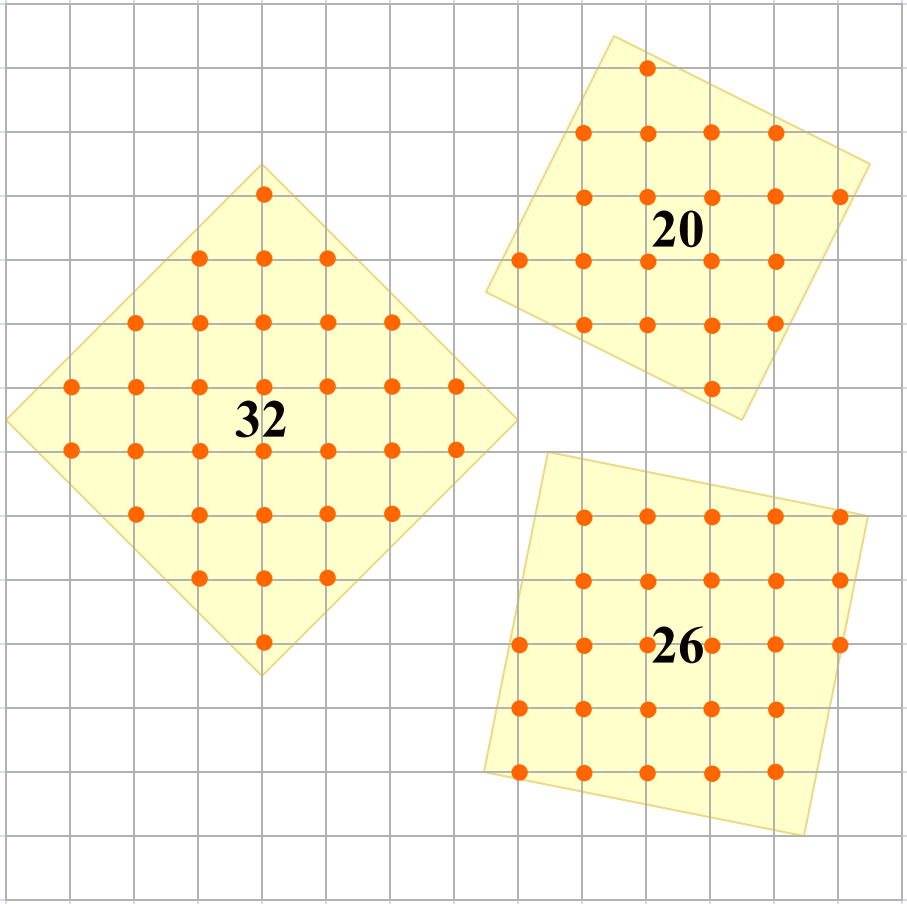
Square Lattice (Oitma and Betts, 1978)

- $l^2 + m^2 = n$
- l, m, n are integers
- $l + m$ = even



Square Lattice (Oitma and Betts, 1978)

- $l^2 + m^2 = n$
- l, m, n are integers
- $l + m$ = even



More Bipartite Square Lattice (Betts, Lin, Flynn)

- Old:

  $N =$ **8, 10, 4 × 4, 18, 20, 26, 32, 6 × 6 (8 total)**

- New:

  $N =$ **12, 16, 18, 22, 24 (4), 26, 28 (2), 30, 32, 34 (14 additions)**

- **Topological bipartite imperfection, $I_B(N)$**
- **QMC: 16 × 16**

Comparison of estimates of the energy per vertex, ε_0, and the staggered magnetization per vertex, m^+, of the $S = ½$ Heisenberg antiferromagnet on the infinite square lattice at $T = 0$

$-\varepsilon_0(\infty)$	$m^+(\infty)$	**Method**	**Reference**
0.6657(4)	–	Variational	[32] Liang, Doucet, Anderson
0.6638	–	Variational	[33] Hulse, Elser
0.66968	0.31	Coupled cluster	[34] Zeng, Farnell, Bishop
0.66934(3)	0.3075(25)	Quantum Monte Carlo	[35, 36] Runge
0.669437(5)	0.3070(3)	Series expansion QMC	[37] Sandvik
0.669442(26)	0.3077(4)	Green function MC	[38] Buonaura, Sorella
0.66999	0.3069	Third order spin wave	[39] Hamer, Zheng
0.66949	0.30686(10)	Fourth order spin wave	[40] Zheng, Hamer
0.668(1)	0.33(3)	t expansion	[41] Zheng, Oitmaa, Hamer
0.6696(3)	0.303(8)	Series expansion	[42] Singh
0.6693(1)	0.307(1)	Series expansion	[43] Wiese, Ying
0.669(1)	0.325	ED on finite lattices	[19] Schaltz, Ziman, Poilblanc
0.6513(8)	0.20(1)	Ditto	[15] Horsch, von der Linden
0.66960(13)	**0.303(2)**	**Ditto**	**Present estimates**

Related Issues

- **Density Matrix Renormalization (DMRG)**
- **Finite temperature Lanczos method**
- **Monte Carlo Simulation of Eigenvectors**
- Finite size scaling:
  - **scaling function, e.g., spin-wave theory**
  - **establish bounds, e.g., variation principle**
  - **…**

Spectral Function

$$A(\omega) = \sum_m \left|\langle \Phi_m \mid A \mid \Phi_1 \rangle\right|^2 \delta\left(\omega + \lambda_1 - \lambda_m\right)$$

$$= -\frac{1}{\pi} \operatorname{Im} \lim_{\varepsilon \to 0} \langle \Phi_0 \mid A^+ \frac{1}{zI - H} A \mid \Phi_0 \rangle$$

$$= -\frac{1}{\pi} \operatorname{Im} \lim_{\varepsilon \to 0} \cfrac{1}{z - \alpha_1 - \cfrac{\beta_1^2}{z - \alpha_2 - \cfrac{\beta_2^2}{\ddots}}}$$

$$z = \omega + \lambda_1 + i\varepsilon$$

- **A = current operator: $A(\omega)$ is optical conductivity.**
- **$A = S^+$ or S^-: $A(\omega)$ is magnetic susceptibility.**

Perturbation Theory

- For $H = H_0 + V$, $H_0|\Phi_0\rangle = E_0|\Phi_0\rangle$, we compute the Greens function $((E + i\varepsilon)I - H)^{-1}$ and obtain the continued fraction
- Pade approximation
- Brillouin-Wigner perturbation theory