Numerical Methods in Many-body Physics

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Electron-Electron Interactions in Solids

Literature:

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Outline

I. Exact Diagonalization
- *(i)* Introduction to interacting quantum systems
- *(ii)* Representation of many-body states
- *(iii)* Complete Diagonalization
- *(iv)* Iterative Diagonalization (Lanczos and Davidson)
- *(v)* Dynamics
- *(vi)* Finite temperature

II. Numerical Renormalization Group
- *(i)* Anderson and Kondo problems
- *(ii)* Numerical RG for the Kondo problem
- *(iii)* Numerical RG for quantum lattice problems
- *(iv)* Numerical RG for a noninteracting particle

III. From the NRG to the Density Matrix Renormalization Group
- *(i)* Better methods for the noninteracting particle
- *(ii)* Density Matrix Projection for interacting systems
- *(iii)* DMRG Algorithms
- *(iv)* DMRG-like algorithm for the noninteracting particle

IV. The DMRG in Detail
- *(i)* Programming details
- *(ii)* Measurements
- *(iii)* Wavefunction transformations
- *(iv)* Extensions to higher dimension

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- *(i)* Classical transfer matrices
- *(ii)* Finite temperature
- *(iii)* Dynamics
- *(iv)* Quantum chemistry
- *(v)* Time evolution
- *(vi)* Matrix product states
- *(vii)* Quantum information

VI. Quantum Monte Carlo Methods
- *(i)* Review of classical Monte Carlo
- *(ii)* Variational and Green's function QMC
- *(iii)* World-line QMC
- *(iv)* Determinantal QMC
- *(v)* Loop Algorithm
- *(vi)* Stochastic Series Expansion (SSE)
- *(vii)* Diagrammatic QMC

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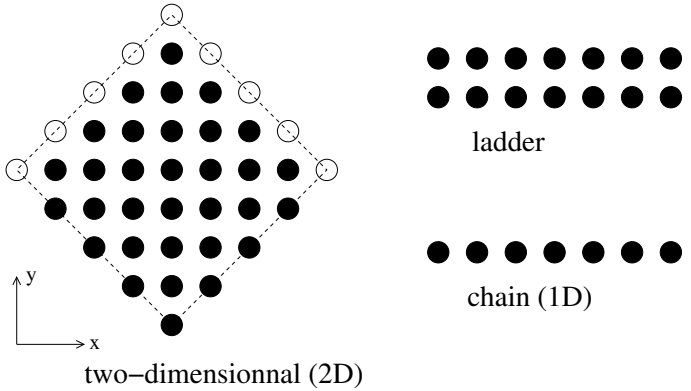
I. Exact Diagonalization

Direct diagonalization of Hamiltonian matrix on finite clusters



Goals

- ground state properties
- low-lying excitations
- dynamics, finite T, ...

Advantages

- almost any system can be treated
- almost any observable can be calculated
- quantum-number resolved quantities
- numerically exact (for finite cluster)

Limitation: exponential in lattice size

Largest sizes reached

- $S = 1/2$ spin models
  square lattice: $N = 40$ triangular lattice: $N = 39$, star lattice: $N = 42$
  maximum dimension of basis: 1.5 billion
- t-J models
  checkerboard lattice with 2 holes: $N = 32$
  square lattice with 2 holes: $N = 32$
  maximum dimension of basis: 2.8 billion
- Hubbard models
  square lattice at half filling: $N = 20$
  quantum dot structure: $N = 20$
  maximum dimension of basis: 3 billion
- Holstein models
  chain with $N = 14$ + phonon pseudo-sites
  maximum dimension of basis: 30 billion

I (i) Interacting Quantum Systems

Here: discrete, finite case

- system of N quantum mechanical subsystems, $\ell = 1, \ldots, N$
- finite number of basis states per subsystem

$$|\alpha_\ell\rangle \,, \qquad \alpha_\ell = 1, \ldots, s_\ell$$

- more general case: $s_\ell \to \infty$ (continuum or thermodynamic limit)

$N \to \infty$ (thermodynamic limit)

$\ell \to x$ (continuous quantum field)

Properties:

- Basis *direct product* of component basis

$$|\alpha_1, \alpha_2, \ldots, \alpha_N\rangle \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ldots \otimes |\alpha_N\rangle$$

$\Rightarrow$ total number of states: $\prod_{\ell=1}^{N} s_\ell$

- arbitrary state in this basis

$$|\psi\rangle = \sum_{\{\alpha_\ell\}} \psi(\alpha_1, \alpha_2, \ldots, \alpha_N)\, |\alpha_1, \alpha_2, \ldots, \alpha_N\rangle$$

- behavior governed by Schrödinger equation

$$H\,|\Psi(t)\rangle = i\hbar\,\frac{\partial}{\partial t}\,|\Psi(t)\rangle \quad \text{or} \quad H\,|\psi\rangle = E\,|\psi\rangle \quad \text{(time-independent)}$$

Hamiltonians

In general, Hamiltonians can connect arbitrary numbers of subsystems

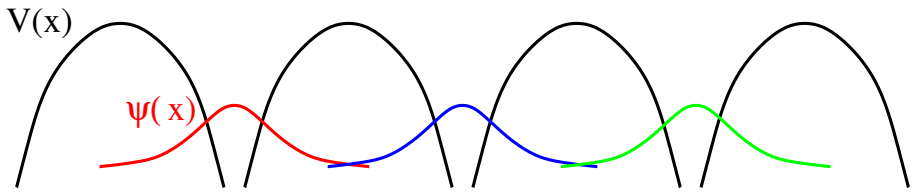
$$H = \sum_{\ell} H^{(1)}_{\ell} + \sum_{\ell,m} H^{(2)}_{\ell m} + \ldots + \sum_{\ell,m,p} H^{(4)}_{\ell mnp} + \ldots$$

- $H^{(1)}_{\ell}$ usually determines $|\alpha_\ell\rangle$
- $H^{(2)}_{\ell m}$, sometimes $H^{(4)}_{\ell mnp}$ will be important here
- $H^{(2)}_{\ell m}$ often short-ranged

Typical terms:

- tight-binding term:

$$H^{\rm tb} = -\sum_{\ell,m,\sigma} t_{\ell m}\, c^{\dagger}_{\ell,\sigma} c_{m,\sigma}$$



- localized Wannier orbitals (unfilled d- or f- orbitals in transition metals)
- states $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$ per orbital $\rightarrow 4^N$ degrees of freedom
- overlap between near orbitals – "hopping" t_{lm} short ranged (n.n., possibly n.n.n.)

- local (Anderson) disorder

$$H_\ell^{\rm A} = \sum_\sigma \lambda_\ell \, n_{\ell,\sigma} \quad , \qquad n_{\ell,\sigma} \equiv c^\dagger_{\ell,\sigma} c_{\ell,\sigma}$$

- Coulomb interaction between electrons $\quad H^{\rm C}_{\ell m} = \dfrac{e^2}{|\mathbf{r}_\ell - \mathbf{r}_m|}$

  screening leads to
  - on-site (Hubbard) interaction

$$H_\ell^{\rm U} = U \; n_{\ell,\uparrow} n_{\ell,\downarrow}$$

  - near-neighbor Coulomb interaction

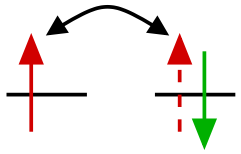
$$H^{\rm V}_{\ell m} = V \; n_\ell \; n_{\ell+\hat{\mathbf{r}}} \quad , \; (n_\ell \equiv \textstyle\sum_\sigma n_{\ell,\sigma}) \qquad \text{etc.}$$

- Spin models
  - $\mathbf{S}_i$ localized quantum mechanical spins ($S = 1/2, 1, 3/2, \ldots$)

    states $|-S\rangle \; |-S+1\rangle \ldots |S\rangle \Rightarrow (2S+1)^N$ degrees of freedom
  - Heisenberg exchange

$$H^{\rm Heis}_{\ell m} = J \; \mathbf{S}_\ell \cdot \mathbf{S}_m = J^z \; S^z_\ell S^z_m + \frac{1}{2} J^{xy} \left(S^+_\ell S^-_m + S^-_\ell \, S^+_m \right)$$

  - strong coupling limit of the Hubbard model at $n = 1$ ($S = 1/2$)



AF exchange $\rightarrow J = \frac{4t^2}{U}$

  - variations: $J^z \neq J^{xy}$ (Ising or XY anisotropy), $H^n_\ell = D(S^z_\ell)^2$ (single-ion),

$$H^{bq}_{\ell m} = J_2 \; \left(\mathbf{S}_\ell \cdot \mathbf{S}_m \right)^2 \text{ (biquadratic)}$$

- t–J model: strong-coupling limit of doped Hubbard

$$H^{tJ}_{\ell m} = \mathcal{P}\, H^{tb}_{\ell m}\, \mathcal{P} + J\, \left(\mathbf{S}_\ell \cdot \mathbf{S}_m \, - \, \frac{1}{4} n_\ell \, n_m \right)$$

  double occupancy projected out ($\mathcal{P}$) - 3 states/site

- Anderson impurity - hybridized d (or f) orbital with on-site interaction

$$H^{AI}_\ell \; = \; \varepsilon_d n^d_\ell \; + \; V \left(d^\dagger_{\ell,\sigma} c_{\ell,\sigma} + \text{H.c.} \right) \; + \; U n^d_{\ell,\uparrow} n^d_{\ell,\downarrow}$$

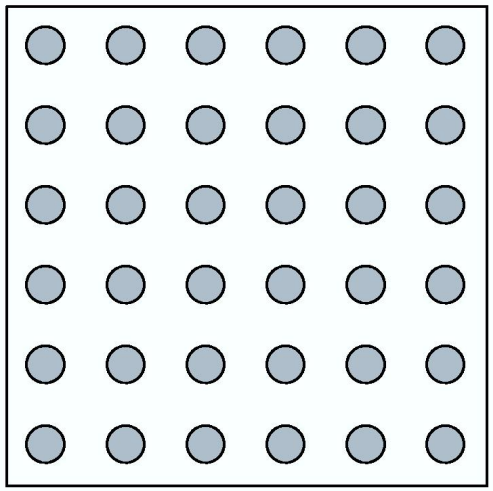
  single impurity or lattice (PAM) possible

- Kondo impurity - localized d spin $\mathbf{S}$

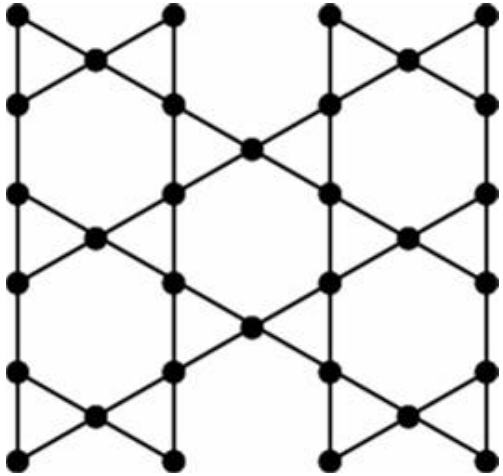
$$H^K_\ell = \frac{J_K}{2}\, \mathbf{S}_\ell \cdot \left(c^\dagger_{\ell,\alpha} \boldsymbol{\sigma}_{\alpha,\beta} c_{\ell,\beta} \right)$$

  limit of symmetric Anderson impurity at strong U

Lattices

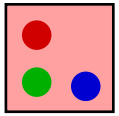


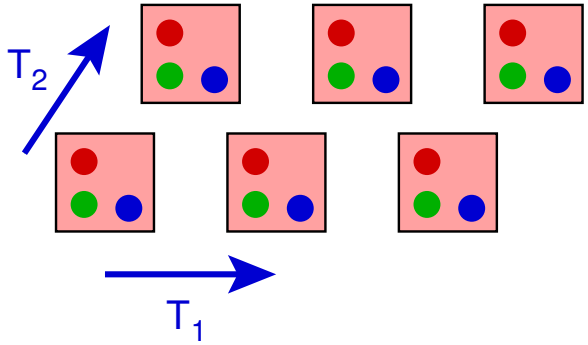
square lattice



Kagomé lattice

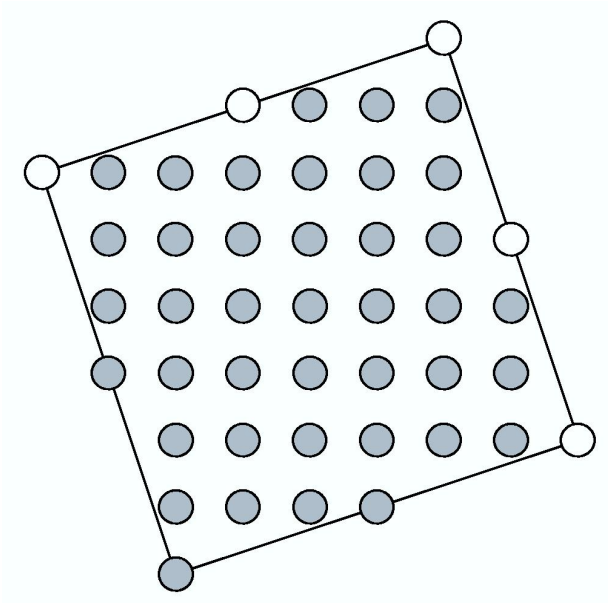
Described by

- unit cell 
- Bravais lattice: translation vectors $\mathbf{T}_1$, $\mathbf{T}_2$ (2D)



- finite lattices: finite multiples of $\mathbf{T}_1$, $\mathbf{T}_2$ and boundary conditions
  - periodic, antiperiodic
  - open
- lattice symmetries:
  - translation – multiples of Bravais lattice vector + periodic (AP) BCs
  - rotations – e.g., $\pi/2$ for a square lattice (group C_{4v})
  - reflection – about symmetry axis

Tilted clusters



40-site cluster, square lattice ($a = 1$)

$$\mathbf{T}_1 = (1, 0)\ ,\ \mathbf{T}_2 = (0, 1)$$

Spanning vectors:

$$\mathbf{F}_1 = (6, 2)\ ,\ \mathbf{F}_2 = (-2, 6)$$

In general,

$$\mathbf{F}_1 = (n, m)\ ,\ \mathbf{F}_2 = (-m, n)$$
$$N = n^2 + m^2$$

translational symmetry satisfied

$\Rightarrow$ reflection/rotation symmetries become more complicated

I (ii) Representation of Many-Body States

mapping to (binary) integers:

- spin-1/2 Heisenberg:

$$|\uparrow_1\downarrow_2\ldots\uparrow_{N-1}\uparrow_N\rangle \rightarrow 1_1 0_2 \ldots 1_{N-1} 1_N$$

  spin flip = bit flip

- Hubbard

$$|N_\ell^\uparrow N_\ell^\downarrow\rangle \rightarrow N_\ell^\uparrow N_\ell^\downarrow \qquad \text{or} \qquad |N_\ell^e S_\ell^z\rangle$$

  with $N_\sigma = \{0, 1\}$

- other models (t–J, $S = 1$ Heisenberg, ...) more complicated

Symmetries: given group $\mathcal{G}$ with generators $\{g_p\}$

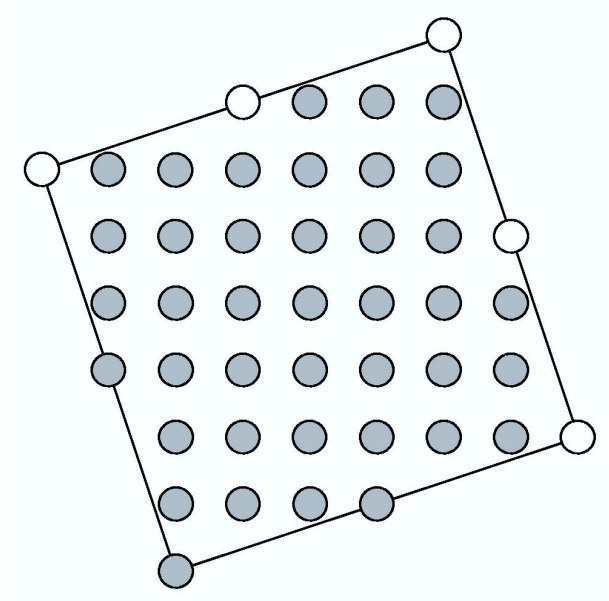
$[H, g_p] = 0 \rightarrow H$ block diagonal (Hilbert space can be divided)

- Continuous
  - conservation of particle number, S^z – U(1) $\Rightarrow$ permutations of bits
  - total spin SU(2) difficult to combine with space group
    $\Rightarrow$ spin inversion (Z_2) can be used
- Space group
  - translation: abelian local states
  - point group (reflections and rotations): non-abelian in general

$\Rightarrow$ form symmetrized linear combination of local states

Example

Reduction of Hilbert space for $S = 1/2$ Heisenberg on $\sqrt{40} \times \sqrt{40}$ cluster



- full Hilbert space: dim$= 2^{40} = 10^{12}$
- constrain to $S_z = 0$: dim$= 138 \times 10^9$
- using spin inversion: dim$= 69 \times 10^9$
- utilizing all 40 translations: dim$= 1.7 \times 10^9$
- using all 4 rotations: dim$= 430,909,650$

I (iii) Complete Diagonalization

To solve $H\,|\psi\rangle = E\,|\psi\rangle$ (H real, symmetric)

Method (*Numerical Recipes*, Ch. 11)

1. Householder transformation - reduction to tridiagonal form T
   - $\approx 2n^3/3$ operations ($4n^3/3$ with eigenvectors)
2. Diagonalization of a tridiagonal matrix
   - roots of secular equation: inefficient
   - QL (QR) algorithm - factorization $T = Q\,L$,
     Q orthogonal, L lower triangular
     $\approx 30n^2$ operations ($\approx 3n^3$ with eigenvectors)

Useful for:

- Simple problems, testing
- Matrix H dense
- Many eigenstates required

But

- H must be stored
- entire matrix must be diagonalized

I (iv) Iterative Diagonalization

Idea: project H onto a cleverly chosen subspace of dimension $M \ll N$

$\Rightarrow$ good convergence of extremal eigenstates

Methods

- Power method $|v_n\rangle = H^n|v_0\rangle$
  - conceptually simple, but converges poorly
  - needs only two vectors, $|v_n\rangle$ & $|v_{n-1}\rangle$
- Lanczos: orthogonal vectors in Krylov subspace (spanned by $\{|v_n\rangle\}$)
  - simple to implement
  - memory efficient - only 3 vectors needed at once
  - works well for sparse, short-range H
- Davidson: subspace expanded by diagonal approximation to inverse iteration
  - higher-order convergence than Lanczos (usually)
  - implementation more complicated
  - works best for diagonally-dominated H
- Jacobi-Davidson: generalization of Davidson
  - nontrivial problem-specific preconditioner (approximation to inverse)
  - can be applied to generalized eigenvalue problem

$$A\,|x\rangle = \lambda\, B\,|x\rangle \qquad (A,\ B \text{ general, complex matrices})$$

Lanczos Algorithm

0) choose $|u_0\rangle$ (random vector, $|\tilde{\psi}_0\rangle$ from last iteration, ...)

1) form $|u_{n+1}\rangle = H\ |u_n\rangle - a_n|u_n\rangle - b_n^2\ |u_{n-1}\rangle$

   where $a_n = \frac{\langle u_n|H|u_n\rangle}{\langle u_n|u_n\rangle}$ and $b_n^2 = \frac{\langle u_n|u_n\rangle}{\langle u_{n-1}|u_{n-1}\rangle}$

2) Is $\langle u_{n+1}|u_{n+1}\rangle < \varepsilon$?

   yes: do 4) then stop

   no: continue

3) repeat starting with 1) until $n = M$ (maximum dimension)

4) diagonalize $\langle u_i|H|u_j\rangle$ (tridiagonal) using QL algorithm

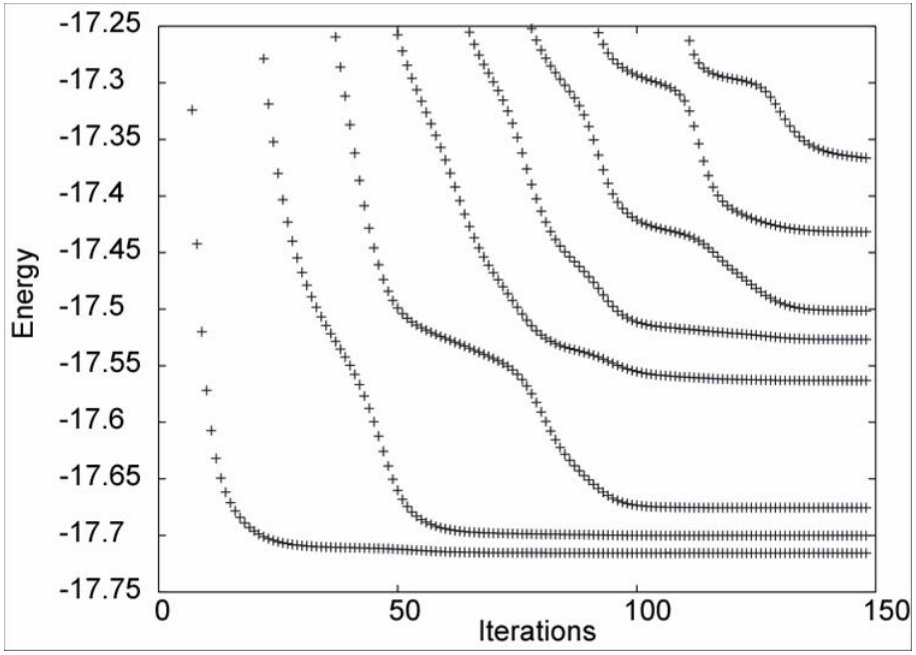
   diagonal elements $\mathbf{D} = (a_0, a_1, \ldots, a_n)$,

   off-diagonal elements $\mathbf{O} = (b_1, b_2, \ldots, b_n)$

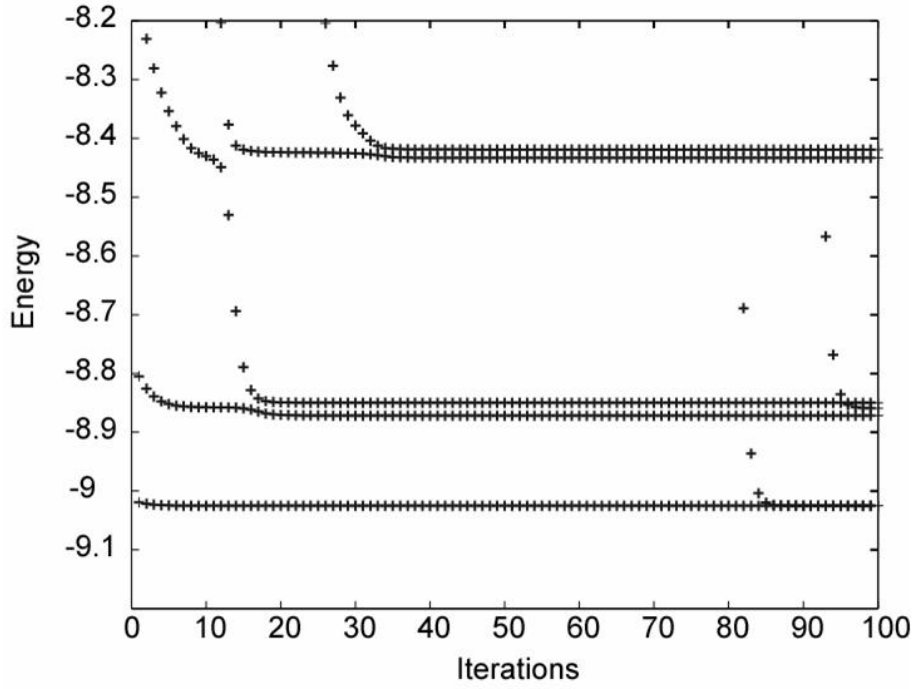
   $\Rightarrow$ eigenvalue $\tilde{E}_0$, eigenvector $|\tilde{\psi}_0\rangle$

5) repeat starting with 0), setting $|u_0\rangle = |\tilde{\psi}_0\rangle$

Convergence of Lanczos Algorithm



- eigenvalues converge starting with extremal ones
- excited states can get "stuck" for a while

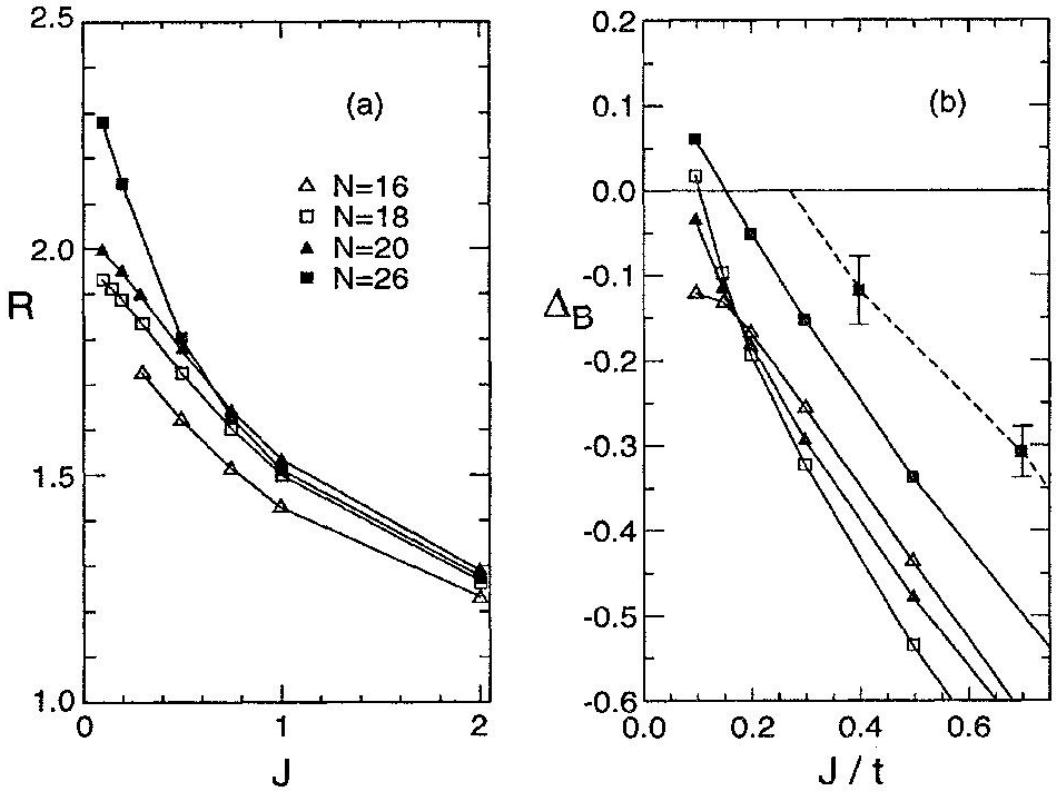


at longer times:

- true eigenvalus converged
- spurious or "ghost" eigenvalues produced
- multiplicity of eigenstates increases

Example: 2D t-J Model

Binding of 2 holes



R: average hole-hole distance
Δ_B: binding energy

(Poiblanc, Riera, & Dagotto, 1993)

- holes closer than two lattice spacings
- pair binding for $J > J_c$, but large finite-size effects

$\Rightarrow$ Does binding persist for larger lattices and constant doping (more holes)?

I (v) Dynamics with Exact Diagonalization

Time-dependent correlation functions

$$C(t) = -i\langle\psi_0|A(t)\ A^\dagger(0)|\psi_0\rangle$$

Fourier transform to frequency space (retarded)

$$\tilde{C}(\omega + i\eta) = \langle\psi_0|\, A\ (\omega + i\eta - H + E_0)^{-1}\ A^\dagger\,|\psi_0\rangle \qquad \text{(resolvent)}$$

Spectral function

$$I(\omega) = -\frac{1}{\pi}\lim_{\eta\to 0^+} \mathrm{Im}\,\tilde{C}(\omega + i\eta)$$

Examples from theory and experiment

name	notation	operators	experiment
single-particle spectral weight	$A(\mathbf{k},\omega)$	$A = c_{\mathbf{k},\sigma}$	photoemission
structure factor	$S_{zz}(\mathbf{q},\omega)$	$A = S^z_{\mathbf{q}}$	neutron scattering
optical conductivity	$\sigma_{xx}(\omega)$	$A = j_x$	optics
4-spin correlation	$R(\omega)$	$\sum_{\mathbf{k}} R_{\mathbf{k}}\, \mathbf{S}_{\mathbf{k}} \cdot \mathbf{S}_{-\mathbf{k}}$	Raman scattering

Methods

Krylov space method (continued fraction)

restart Lanzcos procedure with

$$|u_0\rangle = \frac{1}{\sqrt{\langle\psi_0| A\ A^\dagger |\psi_0\rangle}} A^\dagger |\psi_0\rangle$$

In this Lanczos basis,

$$\tilde{C}(z = \omega + i\eta + E_0) = \cfrac{\langle\psi_0| A\ A^\dagger |\psi_0\rangle}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \cfrac{b_3^2}{z - a_3 - \ldots}}}$$

Interpretation:

- calculation of eigenvector not needed
- consider Lehmann representation of spectral function

$$I(\omega) = \sum_n |\langle\psi_n|A^\dagger|\psi_0\rangle|^2\, \delta(\omega - E_n + E_0)$$

  $\Rightarrow$ poles and weights of $\tilde{C}(z)$ determine $I(\omega)$
- weight decreases with $n \rightarrow$ truncate after M steps
- spectrum discrete $\rightarrow$ finite broadening η

Correction vector method (Soos & Ramasesha, 1984)

Calculate vectors

$$|\phi_0\rangle = A^\dagger |\psi_0\rangle \ , \qquad |\phi_1\rangle = (\omega + i\eta - H + E_0)^{-1} \ |\phi_0\rangle$$

directly, then

$$I(\omega) = \frac{1}{\pi} \, \mathrm{Im} \, \langle \phi_0 | \phi_1 \rangle$$

Advantages:

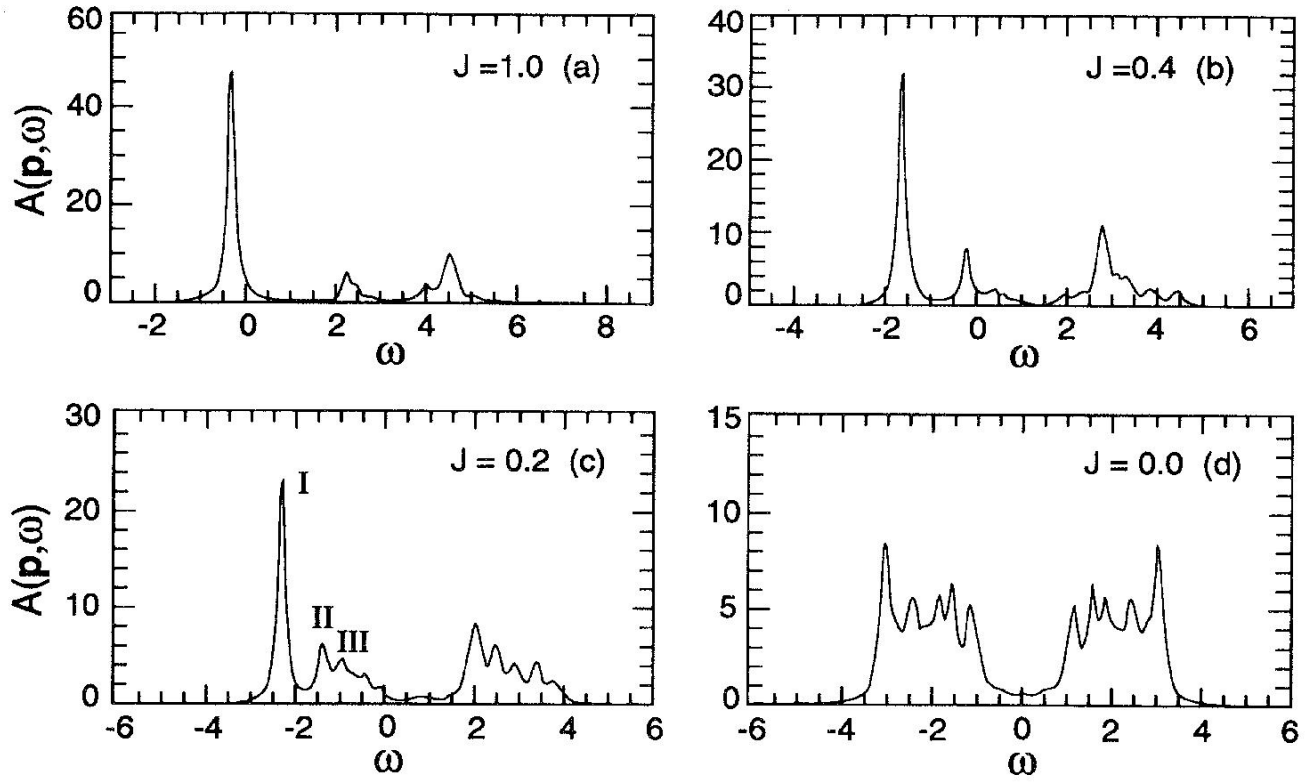
- spectral weight calculated exactly for a given range
- nonlinear spectral functions computed by higher order correction vectors
- can be run in conjunction with Davidson algorithm

Disadvantage: system $(H - z)|\phi_1\rangle = |\phi_0\rangle$ must be solved for each ω desired

Example: Dynamics in 2D t-J Model

Single-particle spectral weight $A(\mathbf{k}, \omega)$ at $\mathbf{k} = \mathbf{k}_F = (\pi/2, \pi/2)$ for one hole

4×4 lattice (Dagotto, Joynt, Moreo, Bacci, & Gagliano, 1993)



Does a single quasiparticle propagate in an antiferromagnet?

- strongly localized hole with string excitations at $J/t = 1.0$
- quasiparticle peak remains until $J/t = 0.4$
- "lump" with pseudogap at $J/t = 0.2$
- pseudogap due to finite-size effects at $J/t = 0$ (symmetric in ω)

I (vi) Finite Temperature with Exact Diagonalization

To calculate finite-T properties in orthonormal basis $|n\rangle$

$$\langle A\rangle = \frac{1}{Z}\sum_{n}^{N}\langle n|Ae^{-\beta H}|n\rangle\ , \qquad Z = \sum_{n}^{N}\langle n|e^{-\beta H}|n\rangle\ ,$$

Problem: expensive to calculate for all $|n\rangle$

Idea: stochastic sampling of Krylov space (Jaklic & Prelovsek, 1994)

$$\langle A\rangle \approx \frac{1}{Z}\sum_{s}\frac{N_s}{R}\sum_{r}^{R}\sum_{m}^{M} e^{-\beta\varepsilon_m^{(r)}}\langle r|\Psi_m^{(r)}\rangle\langle\Psi_m^{(r)}|A|r\rangle$$

where

$$Z \approx \sum_{s}\frac{N_s}{R}\sum_{r}^{R}\sum_{m}^{M} e^{-\beta\varepsilon_m^{(r)}}\left|\langle r|\Psi_m^{(r)}\rangle\right|^2$$

- $\sum_s$ over symmetry sectors of dimension N_s
- $\sum_r$ average over R random starting vectors $|\Psi_0^{(r)}\rangle$
- $\sum_m$ Lanczos propagation of starting vectors: $|\Psi_m^{(r)}\rangle$ at step m

$\Rightarrow$ useful if convergence good when $M \ll N_s$ and $R \ll N_s$

Properties

- related to high-T expansion – $T \to \infty$ limit correct
- high to medium T properties in thermodynamic limit
- low-temperature limit correct (on finite lattice), up to sampling error

  reduction of (large) sampling error: (Aichhorn *et al.*, 2003)

  start with:

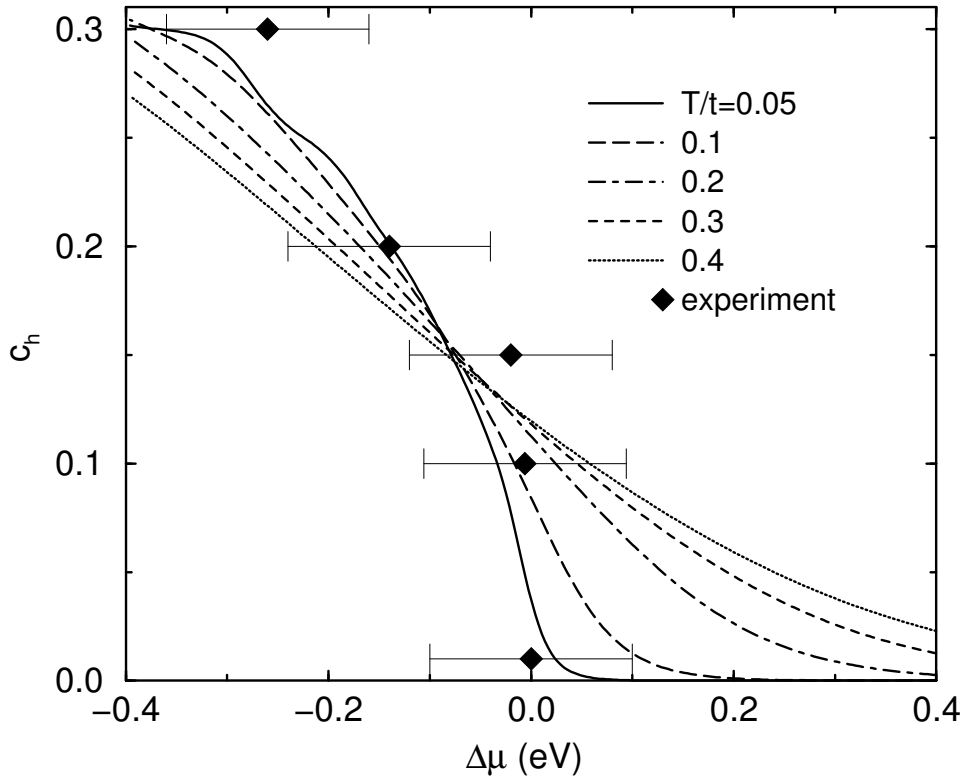
$$\langle A \rangle = \frac{1}{Z} \sum_{n}^{N} \langle n | e^{-\beta H/2} \, A \, e^{-\beta H/2} | n \rangle \ ,$$

  $\Rightarrow$ twofold insertion of Lanczos basis $\rightarrow$ smaller fluctuations at low T
- can calculate
  - thermodynamic properties: specific heat, entropy, static susceptibility, ...
  - static correlation functions
  - dynamics: $A(\mathbf{k}, \omega)$, $S_{zz}(\mathbf{q}, \omega)$, $\sigma_{xx}(\omega)$, ...

Example: t-J Model at finite T

Hole concentration $c_h(=x)$ vs. chemical potential shift $\Delta\mu = \mu_h - \mu_h^0$

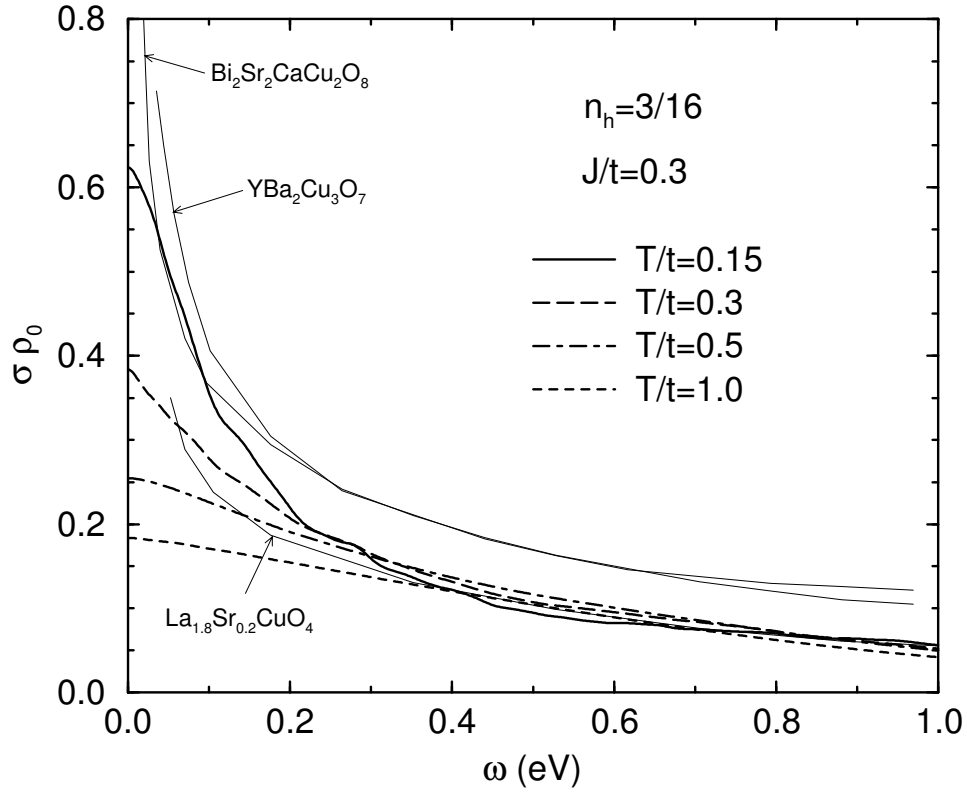
2D t-J model, 16, 18, 20 sites, $t/J = 0.3$, $t = 0.4$eV



(Jaklic & Prelovsek, 1998)

- experimental results for LSCO from photoemission shift (Ino *et al.*, 1997)
- holes only when $\mu < \mu_h^0 \approx -1.99t$ as $T \to 0$
- compressibility finite $\Rightarrow$ no phase separation

Optical conductivity compared with various cuprates at intermediate doping



(Jaklic & Prelovsek, 1998)

- Cuprates measured at $T < 200$K, c_h somewhat uncertain
- high-T falloff slower for materials – transitions to higher excited states?
- experimental curves:
  - LCSO, $c_h \sim x = 0.2$ (Uchida *et al.*, 1991)
  - BISCCO, $c_h \sim 0.23$ (Romero *et al.*, 1992)
  - YBCO, $c_h \sim 0.23$ (Battlogg *et al.*, 1994)

Discussion: Exact Diagonalization

- Method conceptually straightforward, numerically exact
- Iterative diagonalization allows the treatment of surprisingly large matrices
- Efficient implementation using symmetries useful
- System sizes nevertheless strongly restricted
- Extensions to basic method can calculate
  - dynamical correlation functions
  - finite temperature properties
- Not mentioned here, but also possible:
  calculation of full time evolution of quantum state with Lanczos

$\Rightarrow$ Benchmark for other methods, useful when other methods fail