Finite – temperature Lanczos method



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Outline

Introduction to ED – based method:

- models, lattices

Lanczos based methods:

- T = 0 ground state and correlation functions
- T > 0 Lanczos method: static and dynamical properties
- T >> 0 microcanonical Lanczos method
- advantages and limitations

Examples of application:

- t J model: low T thermodynamics, spectral functions
- frustrated Heisenbeeg model: triangular lattice \rightarrow spin liquid
- many-body localization: high-T dynamics

Numerical calculations - simulations

The only computer experiments worth doing are those that yield a surprise ! (V. Arnold ~ 1970)

Why to investigate model (strongly correlated) systems numerically:

- to discover new phenomena
- to get new ideas for construction of the theory
- to confirm existing theories, concepts, experiments
- to establish the right model for experiments
- to produce reliable model results
- to disprove wrong theories, speculations
- to do something
- to spend computer time

Many – body quantum lattice models of strongly correlated electrons

Limitation of methods based on ED (exact diagonalization):

The size of the Hilbert space: *K* quantum degrees/ site

$$\implies N_{st} = K^N$$

N lattice sites

Heisenberg model: spin systems

$$H = \sum_{\langle ij
angle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$= 1/2 \qquad K = 2 \qquad N_{st} = 2^N$$

taking into account conserved quantities and symmetries:

S

total spin: $S_{tot}^{z} = 0 \Longrightarrow N_{st} = {N \choose N/2} < 2^{N}$ translation + rotation symmetry of the lattice : $\tilde{N}_{st} = N_{st}/N \cdots$ **practical limit** today: $N_{st} < 10^{9} = 1GB \Longrightarrow N = 36$ **t - J model:** doped insulator, HTC cuprates.. $H = -\sum_{\langle ij \rangle s} (t_{ij} \tilde{c}_{js}^{\dagger} \tilde{c}_{is} + \text{H.c.}) + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$ $\tilde{c}_{is}^{\dagger} = (1 - n_{i,-s}) c_{is}^{\dagger}$ $K = 3 \Longrightarrow N_{st} \propto 3^N$

projected fermion operators

symmetries: $S_{tot}^z + \mathbf{q} + N_h$ at present: N = 32 $N_e = 4$

Hubbard model: Mott insulators, correlated metals..

$$\begin{split} H &= -t \sum_{\langle ij \rangle s} (c_{js}^{\dagger} c_{is} + c_{is}^{\dagger} c_{js}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} & \text{electrons with spin} \\ K &= 4 \Longrightarrow N_{st} \propto 4^{N} & \text{at present:} \quad N = 20 \end{split}$$

Lattices

1D systems:



there are more powerful methods than for statics (DMRG ..), but not necessarily for T > 0 dynamical quantities

2D systems: periodic boundary conditions square lattice, tilted (+ distorted) square lattice, frustrated lattices (triangular, Kagome..)



Exact diagonalization

A) Full ED: T > 0 statics and dynamics

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$
 Memory $\propto N_{st}^2$ Operations $\propto N_{st}^3$
 $\langle A\rangle = Z^{-1}\sum_{n=1}^{N_{st}} e^{-E_n/T} \langle \Psi_n | A | \Psi_n \rangle \implies N_{st} < 20000$

Example - Heisenberg S=1/2 model: $N \le 20$

B) Lanczos – based ED: T = 0 ground state, g.s. dynamics

sparse Hamiltonian matrix ! Basis states only locally connected Memory \propto Operations $\propto N_{st}$

Lanczos ED technique

Diagonalization of sparse matrices: - power method

C. Lanczos (1950), R. Haydock, V.Heine (1970)

- 1) start with (random) normalized vector in Hilbert space $|\phi_0\rangle$
- 2) generate orthogonal Lanczos vectors $L_M = \{ |\phi_m, m = 1, M \}$ Krylov space $\{ |\phi_0\rangle, H |\phi_0\rangle, \cdots, H^M |\phi_0\rangle \}$

 $H|\phi_0\rangle = a_0|\phi_0\rangle + b_1|\phi_1\rangle$

$$H|\phi_i\rangle = b_i|\phi_{i-1}\rangle + a_i|\phi_i\rangle + b_{i+1}|\phi_{i+1}\rangle \quad 1 \le i \le M$$

3) diagonalization of (real) tridiagonal matrix M x M: real a_i, b_i

$$|\psi_j\rangle = \sum_{i=0}^M v_{ji} |\phi_i\rangle$$
 $\langle \psi_i | H | \psi_j \rangle = \epsilon_j \delta_{ij}$ exact ! $i, j \leq M$

approx. eigenfunctions convergence for ground state: $M < 60 \ll N_{st}$

T = 0 dynamics via Lanczos

dynamical (auto)correlation function for operator A

$$C(\omega) = \int_{0}^{\infty} e^{i\omega^{+}t} \langle \Psi_{0} | A^{\dagger}(t) A | \Psi_{0} \rangle = \langle \Psi_{0} | A^{\dagger} \frac{1}{\omega^{+} + E_{0} - H} A | \Psi_{0} \rangle$$
1) start the Lanczos procedure with normalized $|\tilde{\phi}_{0}\rangle = \frac{1}{\alpha} A | \Psi_{0} \rangle$
2) generate Lanczos functions $|\tilde{\phi}_{j}\rangle \Longrightarrow |\tilde{\psi}_{j}\rangle, \quad j = 1, M \text{ and } |\tilde{a}_{j}, \tilde{b}_{j}\rangle$
3) $C(\omega) = \frac{\alpha^{2}}{\omega^{+} + E_{0} - \tilde{a}_{0} - \frac{\tilde{b}_{1}^{2}}{\omega^{+} + E_{0} - \tilde{a}_{1} - \frac{\tilde{b}_{2}^{2}}{\omega^{+} + E_{0} - \tilde{a}_{2} - \dots}}$

frequency moments:
$$\mu_l = -\frac{1}{\pi} \int_{-\infty}^{\infty} \omega^l \text{Im}C(\omega) d\omega = \alpha^2 \langle \tilde{\phi}_0 | (H - E_0)^l | \tilde{\phi}_0 \rangle$$

exact ! for given $|\Psi_0\rangle$ provided $l \leq \tilde{M}$

Matrix elements via Lanczos

How to evaluate matrix element for any operators A, B? $W_{kl} = \langle n | H^k B H^l A | n \rangle$

Perform 2 x Lanczos M > (l, k)!

$$L_{M} : |\phi_{0}\rangle \cdots |\psi_{j}\rangle, \epsilon_{j} \qquad \tilde{L}_{M} : |\tilde{\phi}_{0}\rangle \propto A |\phi_{0}\rangle \cdots |\tilde{\psi}_{j}\rangle, \tilde{\epsilon}_{j}$$

$$W_{kl} = \sum_{i=0}^{M} \sum_{j=0}^{M} \langle \phi_{0} |\psi_{i}\rangle \langle \psi_{i} | B |\tilde{\psi}_{j}\rangle \langle \tilde{\psi}_{j} | A |\phi_{0}\rangle \langle \epsilon_{i}\rangle^{k} (\tilde{\epsilon}_{j})^{l} \qquad \text{exact !} M > (l,k)$$
Proof: projectors $P_{M} = \sum_{i=0}^{M} |\psi_{i}\rangle \langle \psi_{i}| \qquad \tilde{P}_{M} = \sum_{i=0}^{M} |\tilde{\psi}_{i}\rangle \langle \tilde{\psi}_{i}|$

 $W_{kl} = \langle \phi_0 | P_M H P_M H \dots H P_M B \tilde{P}_M H \dots \tilde{P}_M H \tilde{P}_M A | \phi_0 \rangle$

FTLM - T > 0 static quantities

Operator A :

J. Jaklič, PP (1994)

$$\langle A \rangle = \sum_{n=1}^{N_{st}} \langle n | e^{-\beta H} A | n \rangle / \sum_{n=1}^{N_{st}} \langle n | e^{-\beta H} | n \rangle$$

1) Calculate *M* Lanczos steps for each $|n\rangle$, and corresponding $|\psi_i^n\rangle$

$$\langle A \rangle = Z^{-1} \sum_{n=1}^{N_{st}} \sum_{k=0}^{\infty} \frac{(-\beta)^k}{k!} \langle n | H^k A | n \rangle \qquad Z = \sum_{n=1}^{N_{st}} \sum_{k=0}^{\infty} \frac{(-\beta)^k}{k!} \langle n | H^k | n \rangle$$

$$\langle n | H^k A | n \rangle = \sum_{i=0}^{M} \langle n | \psi_i^n \rangle \langle \psi_i^n | A | n \rangle (\epsilon_i^n)^k \quad \text{correct } k < M, \text{ extended to } k > M !$$

$$\langle A \rangle = Z^{-1} \sum_{n=1}^{N_{st}} \sum_{i=0}^{M} e^{-\beta \epsilon_i^n} \langle n | \psi_i^n \rangle \langle \psi_i^n | A | n \rangle \qquad Z = \sum_{n=1}^{N_{st}} \sum_{i=0}^{M} e^{-\beta \epsilon_i^n} \langle n | \psi_i^n \rangle \langle \psi_i^n | n \rangle$$

reproduces high-T expansion up to the order M !

reproduces correctly also T = 0 result !

$$\begin{split} M &\sim 50 : |\psi_0^n\rangle \sim |\Psi_0\rangle \\ \langle A \rangle &= \sum_{n=1}^{N_{st}} \langle n|\Psi_0\rangle \langle \Psi_0|A|n\rangle \Big/ \sum_{n=1}^{N_{st}} \langle n|\Psi_0\rangle \langle \Psi_0|n\rangle = \langle \Psi_0|A|\Psi_0\rangle / \langle \Psi_0|\Psi_0\rangle \end{split}$$

2) Replace full sum with random sampling

$$\begin{split} N_{st} \text{ states } |n\rangle &\Longrightarrow R \text{ random states } |r\rangle, \ R \ll N_{st} \\ \tilde{A}_{r} &= \langle r|e^{-\beta H}A|r\rangle / \langle r|e^{-\beta H}|r\rangle \quad \text{single random state} \quad \begin{aligned} |r\rangle &= \sum_{n=1}^{N_{st}} \eta_{rn} \eta_{rm} \langle n|e^{-\beta H}A|m\rangle / \sum_{n,m=1}^{N_{st}} \eta_{rn}^{*}\eta_{rm} \langle n|e^{-\beta H}|m\rangle \quad \text{random value, sign} \\ \bar{A}_{r} &= \sum_{n=1}^{N_{st}} |\eta_{rn}|^{2} \langle n|e^{-\beta H}A|n\rangle / \sum_{n=1}^{N_{st}} |\eta_{rn}|^{2} \langle n|e^{-\beta H}|n\rangle \end{split}$$

$$|\eta_{rn}|^{2} = 1/N_{st} + \delta_{rn}$$

$$\langle n|e^{-\beta H}|n\rangle = Z_{n} \text{ and } \langle n|e^{-\beta H}A|n\rangle = Z_{n}A_{n} \quad \text{uncorrelated}$$

$$\bar{A}_{r} = \langle A\rangle(1 + \mathcal{O}(1/\sqrt{\bar{Z}}))$$

$$\bar{Z} = e^{\beta E_{0}}\sum_{n} Z_{n} = \sum_{n=1}^{N_{st}} \langle n|e^{-\beta(H-E_{0})}|n\rangle$$

statistical error: effective number of states Z(T)

$$T \to \infty : \bar{Z} \longrightarrow N_{st}$$

At high T >> 0 single random state is enough to evaluate $\langle A \rangle$!

Random sampling: $1 \le R \ll N_{st}$

$$\langle A \rangle = \frac{N_{st}}{ZR} \sum_{r=1}^{R} \sum_{j=0}^{M} e^{-\beta \epsilon_j^r} \langle r | \psi_j^r \rangle \langle \psi_j^r | A | r \rangle \quad Z = \frac{N_{st}}{R} \sum_{r=1}^{R} \sum_{j=0}^{M} e^{-\beta \epsilon_j^r} |\langle r | \psi_j^r \rangle|^2$$

$$\delta \langle A \rangle / \langle A \rangle = \mathcal{O}(1/\sqrt{R\bar{Z}})$$

3) Conserved quantities (energy, specific heat..): [H, A] = 0

$$\langle A \rangle = \frac{N_{st}}{ZR} \sum_{r=1}^{R} \sum_{j=0}^{M} e^{-\beta \epsilon_{j}^{r}} |\langle r | \psi_{j}^{r} \rangle|^{2} A_{j}^{r}$$

just few additional lines in the Lanczos code !

 $\langle r|\psi_j^r\rangle = v_{j0}^r$ no need to calculate (and store) Lanczos wf., overlap given by diagonalization of 3-diagonal matrix !

FTLM - T > 0 dynamical (auto)correlations

$$\chi''(\omega) = \pi (1 - e^{-\beta\omega})C(\omega) \qquad C(\omega) = \frac{1}{\pi} \operatorname{Re} \int_0^{+\infty} dt e^{i\omega t} C(t)$$
$$C(t) = \langle A^{\dagger}(t)A(0) \rangle = \frac{1}{Z} \sum_{n} \langle n|e^{(-\beta+it)H} A^{\dagger} e^{-iHt} A|n \rangle$$
$$C(t) = Z^{-1} \sum_{n=1}^{N_{st}} \sum_{k,l=0}^{\infty} \frac{(-\beta+it)^k}{k!} \frac{(-it)^l}{l!} |\langle n|H^k A^{\dagger} H^l A|n \rangle$$

perform 2 x Lanczos with $|\phi_0\rangle = |n\rangle, |\phi_0\rangle \propto A|n\rangle$, exact $l, k \leq M$ extrapolation: j, k > M

$$C(t) = Z^{-1} \sum_{n=1}^{N_{st}} \sum_{i,j=0}^{M} e^{-\beta\epsilon_i^n} e^{it(\epsilon_i^n - \tilde{\epsilon}_j^n)} \langle n | \psi_i^n \rangle \langle \psi_i^n | A^{\dagger} | \tilde{\psi}_j^n \rangle \langle \tilde{\psi}_j^n | A | n \rangle$$

$$C(\omega) = \frac{N_{st}}{ZR} \sum_{r=1}^{R} \sum_{i,j=1}^{M} e^{-\beta\epsilon_i} \langle r | \psi_i^r \rangle \langle \psi_i^r | A^{\dagger} | \tilde{\psi}_j^r \rangle \langle \tilde{\psi}_j^r | r \rangle \delta(\omega - \tilde{\epsilon}_j^r + \epsilon_i^r)$$

Finite – size effects: T_{fs}

Which size or T is large enough to represent the macroscopic result ?

Effective number of MB states: $\bar{Z} = \text{Tr e}^{-\beta(H-E_0)} = Z^*(T_{fs}) > 1$





more frustration, better for FTLM and ED-based methods:

- shorter correlation length
- large density of low lying MB states, therefore lower T_{fs}
- frustrated systems: macroscopic-like results for $T > T_{fs}$

How many Lanczos steps?

1D Heisenberg model $S(q = \pi, \omega) : T >> 0$



T >> 0 oscillations in spectra:

- Lanczos generates equidistant

'levels' in the middle MB spectrum

- no information content ?

MCLM: Microcanonical Lanczos method

Dynamical correlations at high T >> 0: might be nontrivial ? if **dynamics singular:** high – ω required, i.e., large M > 100instead FTLM use MCLM: no wf. needed !

$$C(\omega,\lambda) = \langle \Psi_{\lambda} | A^{\dagger} \frac{1}{\omega^{+} + \lambda - H} A | \Psi_{\lambda} \rangle \qquad \lambda = \langle H \rangle(T)$$

wf. with ~ good energy: $\sigma_E / \Delta E < 10^{-3}$ $\sigma_E^2 = \langle \Psi_\lambda | V | \Psi_\lambda \rangle$ perform Lanczos with $V = (H - \lambda)^2$ $M_1 \sim 1000$



Heisenberg: frustrated J_1 - J_2 chain dynamical (spin) conductivity

Numerical methods for T > 0 dynamics



Lanczos – based T > 0 methods

FTLM: T > 0

- represent (optimal ?) interpolation between T=0 Lanczos and HTE
- most valuable for **dynamical correlations**, where not many alternatives
- easy to implement: analogous to T = 0 method + matrix elements
- easy to control: very pedagogical ! code without evident errors usually OK !!
- best for frustrated systems with high entropy !
- similar methods: low-T LM, FTD-DMRG
- limitations: storage of Lanczos wf., full Hilbert space N_{st}

MCLM: T >> 0

- requirements the same as T = 0 (g.s.) code, possibly M >> 100
- interesting for dynamics of nontrivial systems (integrable, disordered MB..)
- similar methods: typicality approach..

t – J model

interplay : electron hopping + spin exchange

single band model for strongly correlated electrons

$$H = -\sum_{i,j,s} t_{ij} \tilde{c}_{js}^{\dagger} \tilde{c}_{is} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)$$

$$t_{ij} = t$$
 n.n. hopping

$$\tilde{c}_{is}^{\dagger} = (1 - n_{i,-s})c_{is}^{\dagger}$$

$$t_{ij} = t'$$
 n.n.n. hopping
etc.

projected fermionic operators: no double occupation of sites





Cuprates: phase diagram



Hole-doped cuprates: ARPES

Fermi surface reconstruction:



 $La_{2-x}Sr_xCuO_4$: Yoshida et al 06



Na-CCOC : K.Shen et al 05



Spectral functions

$$G(\mathbf{k},\omega) = -i \int_0^\infty dt e^{i(\omega+\mu)t} \langle \{\tilde{c}_{\mathbf{k}s}(t), \tilde{c}_{\mathbf{k}s}^{\dagger}\}_+ \rangle \qquad \text{projected operators}$$

$$G(\mathbf{k},\omega) = \frac{\alpha}{\omega - \zeta_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)} \qquad |\Sigma(\mathbf{k},\omega) \to \pm \infty)| \propto 1/\omega$$

 $\alpha = (1 + c_h)/2$ normalization

$$\zeta_{\mathbf{k}} = \int d\omega \omega A(\mathbf{k},\omega)/lpha$$

'free' term

Finite size lattice:

Continuous **k**: $t_{ij} \rightarrow \tilde{t}_{ij} = t_{ij} \exp(i\vec{\theta} \cdot \vec{r}_{ij})$ **k** = **k**_l + $\vec{\theta}$ Regularization: with FTLM calculate $G(\mathbf{k}, \omega) \longrightarrow \Sigma(\mathbf{k}, \omega)$ \longrightarrow average $\Sigma(\mathbf{k}, \omega)$ over $\delta k \sim 0.3 \longrightarrow G(\mathbf{k}, \omega)$ **Pseudogap:** spectral function and self energy along the 'Fermi line'



calculated for lowest $T = T_{fs}$! macroscopic result ?



 $-\Sigma_{MFL}^{\prime\prime}(\mathbf{k},\omega\sim0)\sim a_{\mathbf{k}}+b_{\mathbf{k}}|\omega|$

marginal FL damping

intermediate (optimum) doping:

 $c_{h} = 0.17$





 $c_{h} = 0.05$

 $c_{h} = 0.17$



Fermi surface evolution: A(k,ω=0)

Pseudogap evolution:



pseudogap large:

- a) antinodal region
- b) low doping



density of states: integrated pseudogap

t – J model: transport properties

dynamical (optical) conductivity:



2D Heisenberg model: unfrustrated vs. frustrated (2017)



Many-body localization: goal

Create a macroscopic quantum MB system which does not thermalize at any temperature and retains the information locally ?

Ideal noneqilibrium system = absence of thermalizationno d.c. transportat any T !nonergodicity of (all) correlationslocal quantitites : qubitsno leakage of quantum information

Numerical challenge: $T >> 0 + low-\omega$ (long t) dynamics !

What is MBL and why is it so interesting ?

Nonergodic behaviour in a macroscopic MB quantum system: T > 0

- non-interacting (NI) fermions on disordered lattice: Anderson localization
- integrable MB models: Heisenberg chain etc...
- systems undergoing phase transition (macroscopic ordering at $T < T_c$)



systems = correlations + large disorder ?

Basko, Aleiner, Altshuler (2006):

-MI transition at $T=T^*$ at fixed disorder W

-MI transition at W=W_c even at $T = \infty$!

> 700 theoretical papers after 2006 > 100 papers / year

Does MBL exist (phase transition or crossover ..) ? Which are properties of the ergodic and non-ergodic phase ?

'Standard' model of many-body localization

1D isotropic (or anisotropic) Heisenberg model + random fields:

$$H = J \sum_{i} \left[\frac{1}{2} (S_{i+1}^{+} S_{i}^{-} + S_{i+1}^{-} S_{i}^{+}) + \Delta S_{i+1}^{z} S_{i}^{z} \right] + \sum_{i} h_{i} S_{i}^{z} \qquad h_{i} \in [-W, W]$$

Jordan – Wigner transformation (1D)

equivalent to disordered chain of interacting spinless fermions

= Anderson model + interaction
$$t = J/2$$

 $H = -t \sum_{i} (c_{i+1}^{\dagger}c_{i} + h.c.) + \sum_{i} h_{i}n_{i} + V \sum_{i} n_{i+1}n_{i}$ $V = J\Delta$

T ~ ∞ : **phase diagram** (approximate ?)



 $H = -t \sum_{i} (c_{i+1}^{\dagger} c_{i} + h.c.) + \sum_{i} h_{i} n_{i} + V \sum_{i} n_{i+1} n_{i}$ Bar Lev et al, PRL (2015) ergodic phase: W < W_c (V) nonergodic (MBL) phase: W > W_c (V)

$W > W_c$:

- Poisson MB level statistics
- vanishing d.c. transport spin (particle), energy
- area (log) law for entanglement entropy increase
- non-ergodic behaviour of (all) correlation functions, no thermalization
- local integrals of motion

Numerical methods for MBL (dynamics)



MBL numerical problem: T >> 0 + very long times - low ω !
+ large sizes ?

Characteristic feature: dynamical conductivity and d.c. transport

Barišić et al, PRB (2010, 2016)

vanishing d.c. transport σ_0 for W > W_c ~ 5 $\sigma(\omega) \sim \sigma_0 + \zeta |\omega|^{\alpha} \qquad \alpha \sim 1$



Characteristic feature: nonergodicity and universal dynamics

Mierzejewski et al., PRB (2016)



density-wave (imbalance) correlation function: $T = \infty$, V = t (Δ =0.5), ED, L = 16

$$C(\omega) = \frac{1}{\pi} \operatorname{Re} \int_0^\infty \mathrm{d}t \, \mathrm{e}^{\imath \omega^+ t} \langle n_{q=\pi}(t) n_{q=\pi}^\dagger \rangle$$

a) real-time dynamics: $C(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} C(\omega)$ oscillations emerging from NI physics

b) 'quasi'-time dynamics: $\tilde{C}(\tau) = \int_{-1/\tau}^{1/\tau} d\omega C(\omega)$ the same long-time variation

$$\tilde{C}(\tau) \sim C_0 + a t^{-\gamma}$$

nonergodic (MBL) phase: $W > W^* \sim 4$ $C_0 = C(t=\infty) > 0$ + anomalous time dependence $C(\omega) = C_0 \delta(\omega) + C_{reg}(\omega)$ Many open question and numerical challenges !