Time Evolving Block Decimation Algorithm
Application to bosons on a lattice

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What will it be about

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  Motivation
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Time-Evolving Block Decimation
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  Time evolution algorithm
  Finding the ground state
  Costs and Improvements

Bose-Hubbard example

Extension to an infinite chain

Bose-Hubbard example

Further reading
Motivation

- Many interacting particles systems (bosons, fermions, spins - typical problems of statistical physics, condensed matter, e.g. Ising model)
- Static properties, ground state, low excitations, quantum phase transitions
- Dynamics, time evolution,...

\[ i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle \]

Typowe metody Typical approaches:
- Finite difference method
- Basis sets expansions (or in overcomplete coherent states..)
- Large scale diagonalizations

but ...
Example: Bose-Hubbard Hamiltonian

\[ \hat{H} = -J \sum_{i=0}^{d} \left( \hat{a}_{i+1}^{\dagger} \hat{a}_i + \text{h.a.} \right) + \sum_{i=0}^{d} \epsilon_i \hat{n}_i + \frac{U}{2} \sum_{i=1}^{d} \hat{n}_i (\hat{n}_i - 1), \]

\( \hat{a}_i^{\dagger} (\hat{a}_i) \) are creation (annihilation) operators for a boson at site \( i \)

\( \hat{n}_i = \hat{a}_i^{\dagger} \hat{a}_i \) — occupation number operator

\( J \) - hopping rate, \( U \) - interaction energy,

\( d \) maximal occupation ( \( \text{dim}(\mathcal{H}) = d + 1 \) on each site)

Very sparse matrix of dimension:

\[ D = \frac{(N + M - 1)!}{N!(M - 1)!}, \]

the number of particles is \( N \) and number of lattice sites \( M \).

\( D = 6435 \) for \( N = M = 8 \)

\( D = 92378 \) for \( N = M = 10 \)

\( D = 1352078 \) for \( N = M = 12 \)
Bose-Hubbard Hamiltonian

possibilities:

- Basis truncation
- Lanczos scheme’s
- ...

... as well as novel ideas coming from Quantum Entanglement machinery.
Bose-Hubbard Hamiltonian

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▶ ...

yield a partial gain only..

Alternatives for a static (ground state) problem

▶ Quantum Monte Carlo (QMC)
▶ Density Matrix Renormalization Group (DMRG)
▶ approximations (mean field etc.)

... as well as novel ideas coming from Quantum Entanglement machinery
Quantum Entanglement Primer

Consider a system composed of two parts

- iff \( |\psi\rangle = |\Phi[A]\rangle \otimes |\Phi[B]\rangle \) the state is separable
- otherwise Schmidt’s decomposition possible

\[
|\psi\rangle = \sum_{\alpha=1}^{\chi_A} \lambda_\alpha |\Phi_\alpha^{[A]}\rangle \otimes |\Phi_\alpha^{[B]}\rangle,
\]

\( |\Phi_\alpha^{[A]}\rangle (|\Phi_\alpha^{[B]}\rangle) \) is an eigenvector with eigenvalue \(|\lambda_\alpha|^2 > 0\) of \( \rho^{[A]} = Tr_B(|\psi\rangle\langle\psi|) \) also \( \langle\Phi_\alpha^{[A]}|\psi\rangle = \lambda_\alpha |\Phi_\alpha^{[B]}\rangle \).

The entanglement of \( |\psi\rangle \) is e.g. \( \chi \equiv \max_A \chi_A \).
We assume \( \chi \) is “small”.
Entanglement Primer 2

\[ |\psi\rangle = \sum_{i,j}^{d} C_{ij} |i_{A}\rangle \otimes |j_{B}\rangle \]

Then Singular Value Decomposition does the job

\[ C = \hat{U}\hat{D} V^\dagger; \quad \hat{D} = \text{diag} \lambda_i \]

Now we shall concentrate on states with \textit{hopefully} small entanglement. Also the type of time-evolution that will slowly increase \( \chi \) only.
Vidal’s construction

Consider now a general state for M-site chain:

\[ |\psi\rangle = \sum_{i_1=0}^{d} \cdots \sum_{i_n=0}^{d} c_{i_1 \cdots i_n} |i_1\rangle \otimes \cdots \otimes |i_n\rangle, \]
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The key ingredient of Vidal’s simulation protocol:

$$|\psi\rangle \leftrightarrow \Gamma^{[1]} \lambda^{[1]} \Gamma^{[2]} \lambda^{[2]} \cdots \Gamma^{[l]} \cdots \lambda^{[n-1]} \Gamma^{[n]}.$$

- (i) $\lambda^{[0]}$ 
- (ii) $\Gamma^{[1]} \lambda^{[1]}$ 
- (iii) $\lambda^{[0]} \Gamma^{[1]} \lambda^{[1]} \Gamma^{[2]} \lambda^{[2]}$
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\begin{itemize}
  \item $\Gamma^{[l]}_{\alpha \alpha'}$ - tensor associated with site $l$
  \item $\lambda^{[l]}_{\alpha'}$ - the Schmidt splitting $[1 \cdots l]:[(l+1) \cdots n]$.
\end{itemize}

explicitly :-)

$$c_{i_1 i_2 \cdots i_n} = \sum_{\alpha_1, \cdots, \alpha_{n-1}} \Gamma^{[1]}_{\alpha_1 i_1} \lambda^{[l]}_{\alpha_1} \Gamma^{[2]}_{\alpha_1 \alpha_2} \lambda^{[2]}_{\alpha_2} \cdots \Gamma^{[n]}_{\alpha_{n-1} i_n}.$$
Vidal’s construction 2 – How to get $\Gamma$’s

$$|\psi\rangle = \sum_{\alpha_1} \lambda^{[1]}_{\alpha_1} |\Phi^{[1]}_{\alpha_1}\rangle |\Phi^{[2\ldots n]}_{\alpha_1}\rangle$$

$$= \sum_{i_1, \alpha_1} \Gamma^{[1]}_{\alpha_1} |i_1\rangle \lambda^{[1]}_{\alpha_1} |\Phi^{[2\ldots n]}_{\alpha_1}\rangle,$$

(i) expand $|\Phi^{[2\ldots n]}_{\alpha_1}\rangle$

$$|\Phi^{[2\ldots n]}_{\alpha_1}\rangle = \sum_{i_2} |i_2\rangle |\tau^{[3\ldots n]}_{\alpha_1 i_2}\rangle;$$

(ii) express via Schmidt decomposition of $2 : [3\ldots n]$

$$|\tau^{[3\ldots n]}_{\alpha_1 i_2}\rangle = \sum_{\alpha_2} \Gamma^{[2]}_{\alpha_1 \alpha_2} |\Phi^{[3\ldots n]}_{\alpha_2}\rangle;$$

(iii) make all substitutions

$$|\psi\rangle = \sum_{i_1, \alpha_1, i_2, \alpha_2} \Gamma^{[1]}_{\alpha_1} |i_1\rangle \lambda^{[1]}_{\alpha_1} \Gamma^{[2]}_{\alpha_1 \alpha_2} |i_2\rangle \lambda^{[2]}_{\alpha_2} |\Phi^{[3\ldots n]}_{\alpha_1}\rangle.$$
(iv) move to site 4,5,...
Remarks:

- close links to “finitely correlated states” (Fannes et al.)
- close links to “matrix product states” (Öslund and Rommer)
- thus very similar to DMRG scheme
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- simple study of time dependence
- similar approach for ground state solution
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So what is new?

- simple study of time dependence
- similar approach for ground state solution
- natural extension to truly infinite systems
Time evolution

Consider a Hamiltonian

\[ H = \sum_{i=1}^{M} H_1^{[i]} + \sum_{i=1}^{M} H_2^{[i,i+1]}; \]

\[ |\Psi(T)\rangle = \exp(-iHT) |\Psi(0)\rangle \]

done, as usual, in small steps

\[ |\Psi(t+\tau)\rangle = \exp(-iH\tau) |\Psi(t)\rangle \]

Decompose \( H \) as

\[ H = F + G, \]

\[ F \equiv \sum_{\text{even}} l F^{[l]} \equiv \sum_{\text{even}} l (H^{[l]}_1 + H^{[l],l+1}_2), \]

\[ G \equiv \sum_{\text{odd}} l G^{[l]} \equiv \sum_{\text{odd}} l (H^{[l]}_1 + H^{[l],l+1}_2), \]

Observe:

\[ [F^{[l]}, F^{[l']}] = 0 \quad [G^{[l]}, G^{[l']}] = 0 \] but

\[ [F, G] \neq 0. \]
Time evolution

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\[
F \equiv \sum_{\text{even } l} F^{[l]} \equiv \sum_{\text{even } l} \left( H_1^{[l]} + H_2^{[l,l+1]} \right),
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\]

Observe: \([F^{[l]}, F^{[l']]} = 0 ([G^{[l]}, G^{[l']]} = 0) \text{ but } [F, G] \neq 0.\]
Apply Trotter expansion of order $p$ for $\exp(-iH\tau)$

$$\exp(-i(F + G)\tau) \approx f_p[\exp(-iF\tau), \exp(-iG\tau)]$$

$$f_1(x, y) = xy, \quad f_2(x, y) = x^{1/2}yx^{1/2},$$
Apply Trotter expansion of order $p$ for $\exp(-iH\tau)$

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$$f_1(x, y) = xy, \quad f_2(x, y) = x^{1/2}yx^{1/2},$$

And we get a chain of two-site gates:

$$\exp(-iF\tau) = \prod_l \exp(-iF^{[l]}\tau) = \prod_l \exp(-i(H_1^{[l]} + H_2^{[l,l+1]})\tau) = \prod_l U^{[l]}$$

**Vidal's lemma:** Updating $|\Psi\rangle$ expressed as

$$|\Psi\rangle \longleftrightarrow \Gamma^{[1]}\lambda^{[1]}\Gamma^{[2]}\lambda^{[2]} \ldots \Gamma^{[l]} \ldots \lambda^{[n-1]}\Gamma^{[n]}.$$ 

is a LOCAL operation affecting $\Gamma^{[l]}$, $\lambda^{[l]}$ and $\Gamma^{[l+1]}$. 
Recall that there are at most $\chi$ links of our $l$ and $l+1$ sites.

$|\Psi\rangle = \chi \sum_{\alpha,\beta,\gamma = 1}^{d} \sum_{i,j = 0}^{\Gamma[l]} \lambda^{B}[l]_{\alpha \beta} \lambda^{A}[l]_{\beta \gamma} |\alpha_{ij}\gamma\rangle$,

$|\Psi'\rangle = U(l) |\Psi\rangle = \chi \sum_{\alpha,\gamma = 1}^{d} \sum_{i,j = 0}^{\Theta} \Theta_{ij \alpha \gamma} |\alpha_{ij}\gamma\rangle$,

where $\Theta_{ij \alpha \gamma} = \sum_{\beta, kn} V_{ij kn} \lambda^{A}[l]_{\beta \lambda} \lambda^{B}[l+1]_{\beta \gamma}$. 

Time evolution 3
Recall that there are at most $\chi$ links of our $l$ and $l+1$ sites

$$|\psi\rangle = \sum_{\alpha,\beta,\gamma=1}^{\chi} \sum_{i,j=0}^{d} \Gamma^{[l]}_{\alpha\beta} \lambda^{[l]}_{\beta\gamma} \Gamma^{[l+1]}_{\lambda\beta} |\alpha ij\rangle,$$

$$|\psi'\rangle = U^{(l)}|\psi\rangle = \sum_{\alpha,\gamma=1}^{\chi} \sum_{i,j=0}^{d} \Theta^{ij}_{\alpha\gamma} |\alpha ij\rangle,$$

where

$$\Theta^{ij}_{\alpha\gamma} = \sum_{\beta} \sum_{kn} V^{ij}_{kn}\Gamma^{[l]}_{\alpha\beta} \lambda^{[l]}_{\beta\gamma} \Gamma^{[l+1]}_{\lambda\beta} |\beta\gamma|.$$
Time evolution 4

Now singular value decomposition of $\Theta$ grouping indexes as $[\alpha i] : [j \gamma]$:

$$\Theta = \sum_\beta X_{[\alpha i] \beta} \tilde{\lambda}_\beta^{(l)} Y_{\beta [j \gamma]}$$
Time evolution 4

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And

$$\tilde{\Gamma}_{\alpha \beta}^{[\ell] i} = X_{[\alpha i] \beta} / \lambda_{\alpha}^{(l-1)}; \quad \tilde{\Gamma}_{\alpha \beta}^{[\ell+1] i} = Y_{[\alpha i] \beta} / \lambda_{\beta}^{(l+1)}$$
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▶ Note: $\alpha \in [1, \chi]$, i.e. $[\alpha i]$ leads to $\chi(d + 1)$ as dimension of $\Theta$. 
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- SVD yields $\tilde{\lambda}^{[l]}$ of that length, normalized so as
  $$\sum (\tilde{\lambda}^{[l]}_{\alpha})^2 = 1.$$
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► **Note:** $\alpha \in [1, \chi]$, i.e. $[\alpha i]$ leads to $\chi(d + 1)$ as dimension of $\Theta$.

► SVD yields $\tilde{\lambda}^{[\eta]}$ of that length, normalized so as 

$$\sum (\tilde{\lambda}^{[\eta]}_\alpha)^2 = 1.$$ 

► Numerically we want to limit the length of $\lambda$ to some $\chi_e$ so we drop smallest and renormalize:

$$\lambda^{[\eta]}_\alpha = \left[ \sum_{\alpha=1}^{\chi_e} |\tilde{\lambda}^{[\eta]}_\alpha|^2 \right]^{-\frac{1}{2}} \tilde{\lambda}^{[\eta]}_\alpha$$

And that’s the end of the story!!
Finding the ground state

(one of the methods)

Start with

\[ |\Phi\otimes\rangle \equiv |\phi^1\rangle \otimes \cdots \otimes |\phi^n\rangle, \quad \langle \Phi\otimes |\psi_{gr}\rangle \neq 0, \]

(expansion into \(\lambda\)'s and \(\Gamma\)'s) trivial.
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(expansion into \(\lambda\)'s and \(\Gamma\)'s) trivial.

► Use the scheme to simulate an evolution in imaginary time \(t\) according to \(H\),

\[ |\psi_{gr}\rangle = \lim_{t\to\infty} \frac{\exp(-Ht)|\Phi\otimes\rangle}{\| \exp(-Ht)|\Phi\otimes\rangle \|}; \]
Finding the ground state

(one of the methods)

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- Use the scheme to simulate an evolution in imaginary time $t$ according to $H$,

\[ |\psi_{gr}\rangle = \lim_{t \to \infty} \frac{\exp(-Ht)|\Phi\otimes\rangle}{\| \exp(-Ht)|\Phi\otimes\rangle \|}; \]

- The procedure converges almost always :-)
Costs and Improvements

Generally execution time scales as $((d + 1)\chi_e)^3$
Further simple improvements:

- Global selection rules
- The procedure is easy to parallelize :-)
- But yet to be done :-(
- Further difficult (under construction) improvements
  - Long range interactions
  - Renormalizable entanglement
  - Tree structures
  - Multidimensions - - projected entangled pair states, MERA
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![Diagram](image-url)
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![Diagram](image)

But yet to be done :-(

Further difficult (under construction) improvements

- Long range interactions
- Renormalizable entanglement
- Tree structures
- Multidimensions - - Projected entangled pair states, MERA
Bose-Hubbard example

Comparison with high order perturbation theory\(^{(1)}\)

\[
\hat{H} = -J \sum_{i=0}^{d} \left( \hat{a}_{i+1}^{\dagger} \hat{a}_i + \text{h.a.} \right) + \sum_{i=0}^{d} \epsilon_i \hat{n}_i + \frac{U}{2} \sum_{i=1}^{d} \hat{n}_i (\hat{n}_i - 1),
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Bose-Hubbard example

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\]

\[
\frac{\varepsilon}{4} = -J^2 + J^4 + \frac{68}{9} J^6 - \frac{1267}{81} J^8 + \frac{44171}{1458} J^{10} - \frac{4902596}{6561} J^{12} - \frac{802092135607}{2645395200} J^{14} + O(J^{16}).
\]

\[
\frac{\text{Var}(\hat{n})}{\sqrt{2}} = 2J - 3J^3 - \frac{1441}{36} J^5 + \frac{32045}{648} J^7 - \frac{3105413}{5184} J^9 - \frac{6979423019}{839808} J^{11} - \frac{207832615291307}{5290790400} J^{13}, \quad (4)
\]

Treatment of infinite systems

Let $H = \sum_r H^{[r,r+1]}$ be invariant under $r \to r + 1$ transformation. If $|\psi_0\rangle$ is also translationally invariant, evolution preserves that. Now we can treat truly infinite systems

$$|\psi\rangle = \sum_{\alpha=1}^\chi \lambda^{(r)}_\alpha |\Phi^{(<r)}_\alpha\rangle \otimes |\Phi^{(r+1)}_\alpha\rangle;$$

where

$$|\Phi^{(<r+1)}_\alpha\rangle = \sum_{\beta=1}^\chi \sum_{i=1}^D \lambda_\beta^{(r)} \Gamma^{(r+1)}_{i\beta\alpha} |\Phi^{(<r)}_\beta\rangle |i^{(r+1)}\rangle,$$

$$|\Phi^{(r)}_\alpha\rangle = \sum_{\beta=1}^\chi \sum_{i=1}^D \Gamma^{(r+1)}_{i\alpha\beta} \lambda^{(r+1)}_\beta |i^{(r)}\rangle |\Phi^{(r+1)}_\beta\rangle.$$

$$|\psi\rangle = \sum_{\alpha,\beta,\gamma=1}^\chi \sum_{i,j=1}^D \lambda^{(r-1)}_{i\alpha\beta} \Gamma^{(r)}_{i\beta\gamma} \lambda^{(r)}_{j\beta\gamma} \Gamma^{(r+1)}_{j\gamma\alpha} \lambda^{(r+1)}_{\gamma} |i^{(r)}\rangle |j^{(r+1)}\rangle |\Phi^{(<r)}_\alpha\rangle |\Phi^{(r+2)}_\gamma\rangle.$$
Infinite systems 2

$|\psi\rangle$ – shift invariant – $(r)$ is not needed, but.. We need to act with the two-side gate:

$$U^{[r,r+1]} \equiv \exp(-iH^{[r,r+1]}\delta t), \quad \delta t \ll 1$$

that breaks for a moment the symmetry. Thus

$$\Gamma^{[2r]} = \Gamma^A, \quad \lambda^{[2r]} = \lambda^A, \quad \Gamma^{[2r+1]} = \Gamma^B, \quad \lambda^{[2r+1]} = \lambda^B, \quad r \in \mathbb{Z}.$$
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Bose-Hubbard example

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Note the presence of the chemical potential \( \mu \).

Challenging problem: The tip of the quantum phase transitions
Bose-Hubbard example 2

Various methods used (mean-field, Bethe-ansatz, diagonalization $N = M = 12$, QMC, DMRG...)
The most stable approach - the slope of the correlation function $C(s) = \langle \Psi_{gr} | \hat{a}^\dagger_{r+s} \hat{a}_r | \Psi_{gr} \rangle$.

- exponential decay for large $s$ in Mott Insulator Phase.
- power law decay for large $s$ in Superfluid Phase $C(s) \propto s^{-K/2}$ with $K = 1/2$ at transition.
Bose-Hubbard example 3

T. Kühner, S.R. White, H. Monien, Phys. Rev. B61, 12474 (2000) give $J_c = 0.297 \pm 0.01$ (DMRG).
Our simulation\(^{(2)}\) yields $J_c = 0.2958 \pm 0.0003$.

Table: The location of the critical point $J_c$ for different ranges of $s$ value in the correlation function $C(s)$

<table>
<thead>
<tr>
<th>$s$</th>
<th>KWM 2000</th>
<th>This work</th>
</tr>
</thead>
<tbody>
<tr>
<td>$4 \leq s \leq 8$</td>
<td>$0.2874 \pm 0.0001$</td>
<td>$0.2868 \pm 0.0006$</td>
</tr>
<tr>
<td>$8 \leq s \leq 16$</td>
<td>$0.2938 \pm 0.0001$</td>
<td>$0.2915 \pm 0.0002$</td>
</tr>
<tr>
<td>$16 \leq s \leq 32$</td>
<td>$0.2968 \pm 0.0003$</td>
<td>$0.29383 \pm 0.00006$</td>
</tr>
<tr>
<td>$32 \leq s \leq 48$</td>
<td>$0.3062 \pm 0.0003$</td>
<td>$0.29525 \pm 0.00005$</td>
</tr>
<tr>
<td>$48 \leq s \leq 64$</td>
<td>$0.3107 \pm 0.01$</td>
<td>$0.29610 \pm 0.00001$</td>
</tr>
<tr>
<td>$10 \leq s \leq 150$</td>
<td></td>
<td>$0.29529 \pm 0.00005$</td>
</tr>
<tr>
<td>$50 \leq s \leq 150$</td>
<td></td>
<td>$0.29580 \pm 0.00002$</td>
</tr>
</tbody>
</table>

\(^{(2)}\)J. Zakrzewski and D. Delande, in preparation (2006)
Bose-Hubbard example 4

And that is converged (thanks to ICM...)
Further reading

- the infinite case: G. Vidal cond-mat/0605597.
- relation to DMRG A.J. Daley et al. cond-mat/0403313; DMRG review U. Schollwoeck, Rev. Mod. Phys. 77, 259 (2005) and cond-mat/0409292.
- attempts for multidimensions F. Verstraete and J.I. Cirac cond-mat/0407066 (PEPS); G. Vidal cond-mat/0610099.
- Entanglement renormalization: G. Vidal, cond-mat/0512165.
- ....