Collective Phenomena in Nanoscience:
The Role of Quantum Monte Carlo and Diagonalization Solvers

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Albuquerque, NM

Outline

Defining the Theory Problem

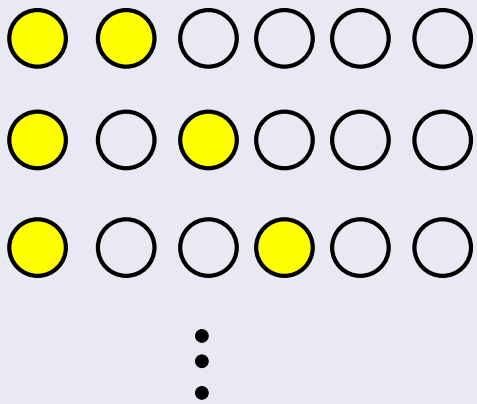
$$H = -\sum_{i=1}^{Nc} \frac{\hbar^2 \nabla^2}{2m_e} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \cdots \quad (1)$$

- Ground state energies, Magnetic and spin orders and correlations. Magnetization measurements: SQUID
- Superconducting orders and gaps. Superconducting gaps: Andreev spectroscopy
- $A(k, \omega)$. ARPES measurements
- $N(r, \omega)$. STM measurements
- $S(k, \omega)$. neutron scattering measurements

The Exponential Problem in Second Quantization

$$H = \sum_{ij} t_{i,\gamma,j,\gamma'} c^{\dagger}_{i\gamma} c_{j\gamma'} + \frac{e^2}{4\pi\epsilon_0} \sum_{i}^{N_c} \sum_{i<j}^{N+c} \frac{n_i n_j}{|\vec{r}_i - \vec{r}_j|} + \cdots \qquad (2)$$

Example: 6 sites, 2 electrons leads to $C_2^6 = 15$ states

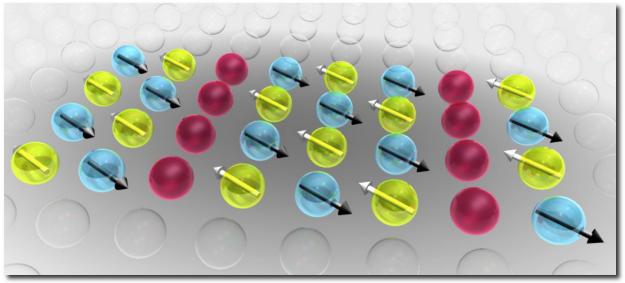


What does exponential mean?

- Assume N_f "flavors" or orbitals (including spin), N sites
- Assume no symmetries (won't change the argument much)
- Then complexity is $2^{N \times N_f}$.
- Assume a more or less realistic problem: $N_f = 10$, $N = 10$
- Exact diagonalization would take $\approx 10^6$ billion years to complete

Quantum Monte Carlo

- Calculates observables exactly (error can be made arbitrary)
- Has a complexity that scales with N^4
- Does previous problem in 6 months to 1 year



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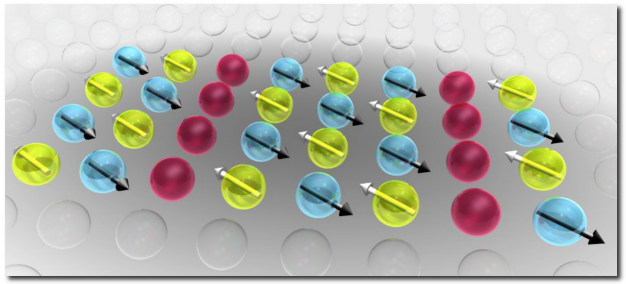

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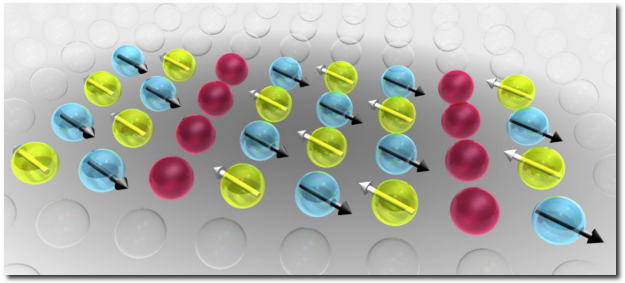
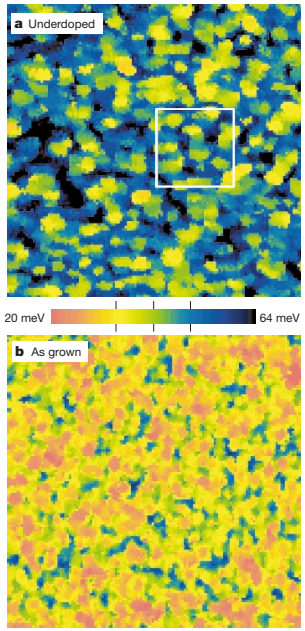
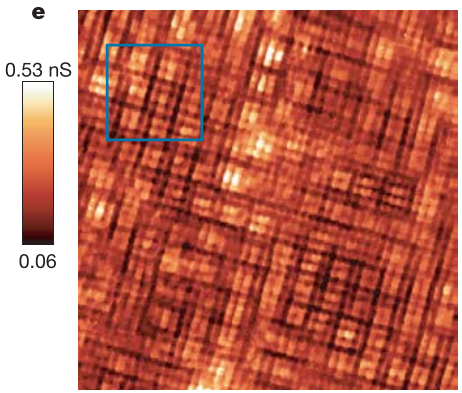
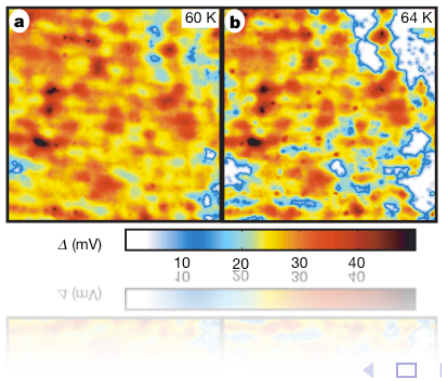


Electronic Inhomogeneities in Cuprates

- Spin and charge stripes (Tranquada et al., '95; Mook et al., '00)
- Checkerboard charge modulations (Hanaguri, Davis et al., '04)
- Random superconducting gap modulations (Lang, Davis eta l., '02; Gomes, Yazdani et al., '07)

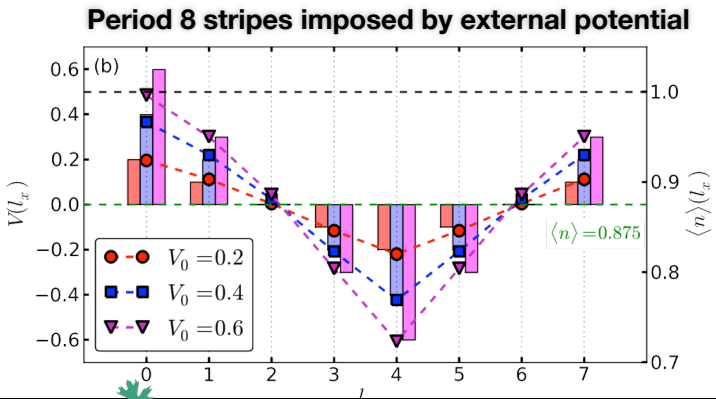






Inhomogeneities in Cuprates

- Question: What is the effect of stripes on the pairing correlations and T_c?
- Answer: It can enhance both of them [Maier et al., PRL 2010]



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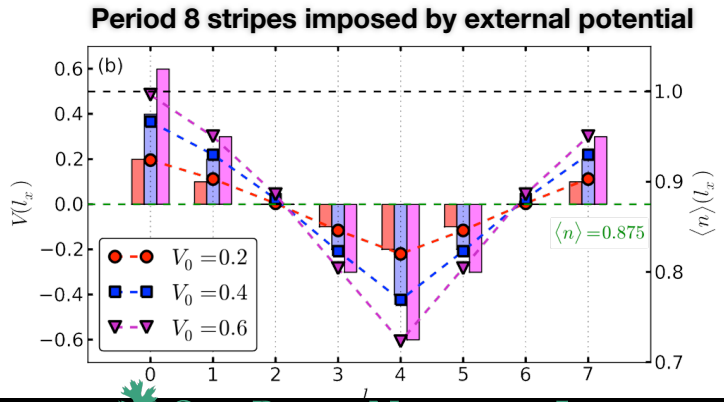
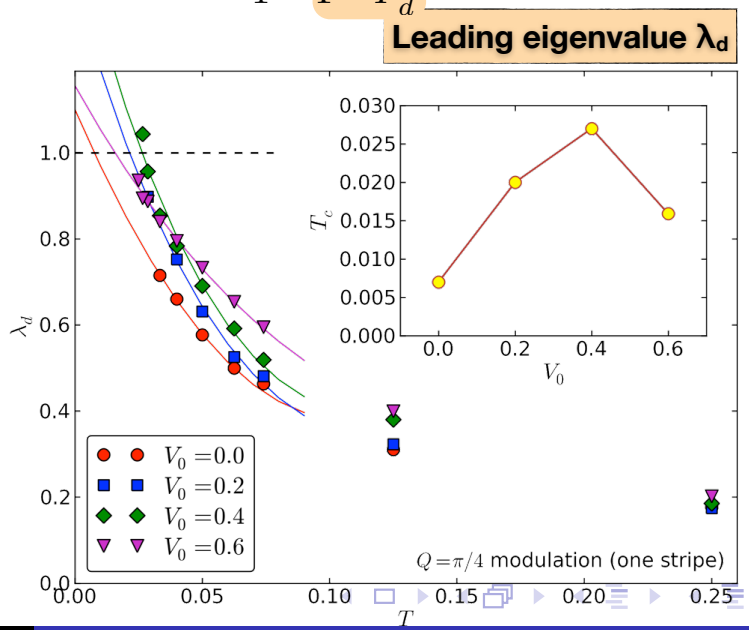
$$P_d = \frac{P_d^0}{1 - \Gamma^{pp} P_d^0}$$

Leading eigenvalue λ_d





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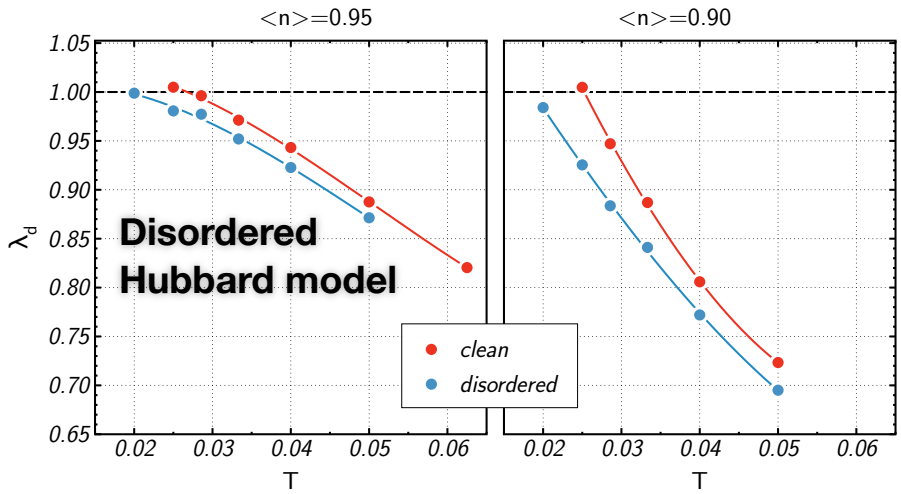

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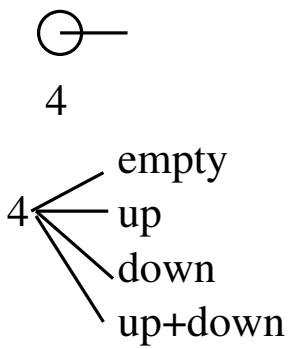
Current trends in QMC for Strongly Correlated Electrons

- Continuous time auxiliary field algorithm (expand in U) [Rubtsov et al., 2005; Werner et al., 2006, Gull et al. 2007]
- Hybridization expansion algorithm (expand in t)

DMRG Basics: Wilson's RG



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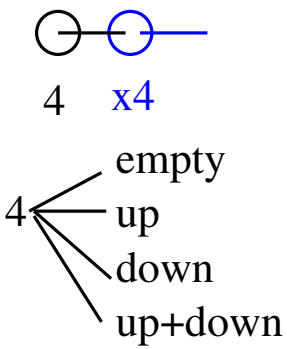

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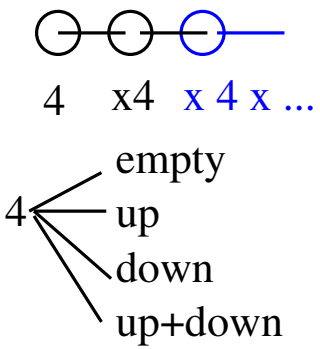

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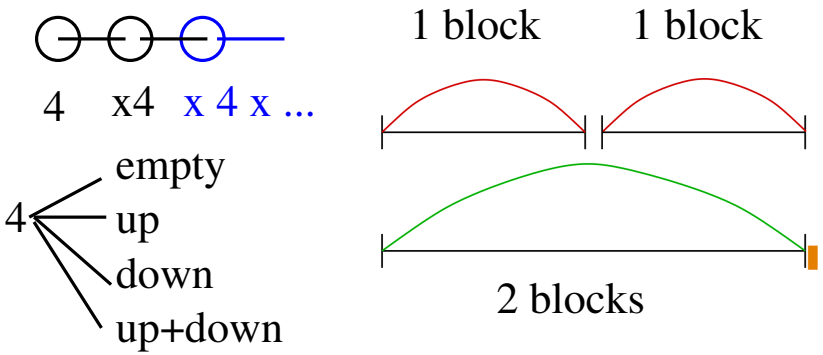

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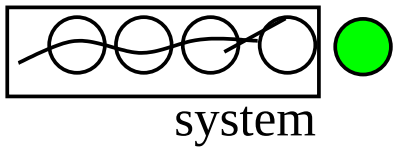

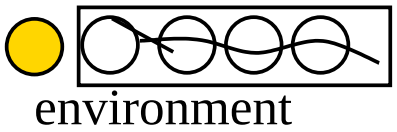

- Algorithm: “Density Matrix Renormalization Group” [White, PRL ’92 and PRB ’92]
- Discard (an exponential number of) states. Keep m states in Hibert space at all times.
- Controlled error, exponentially decaying with m for most 1D systems.

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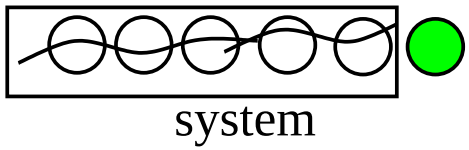

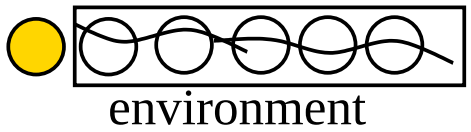

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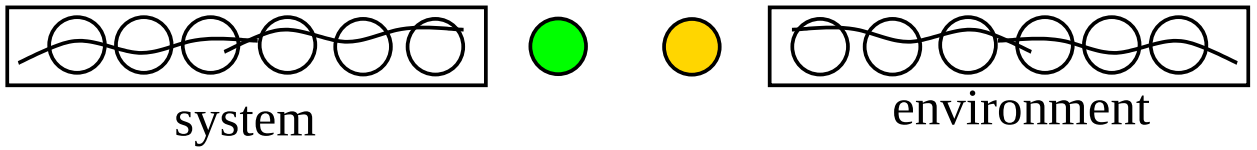

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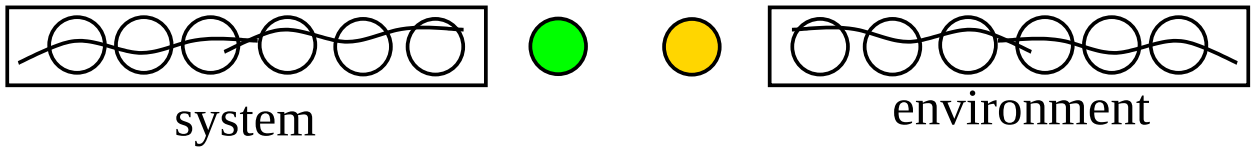

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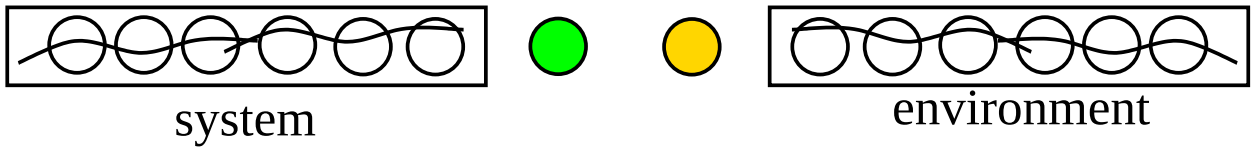

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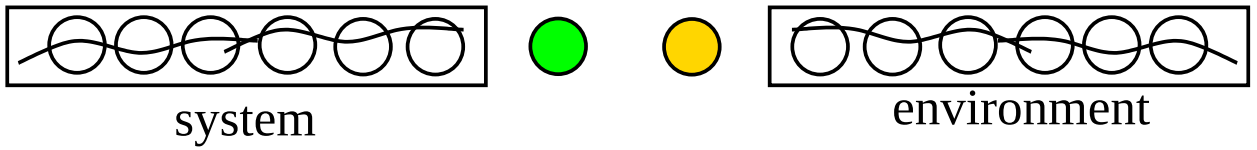

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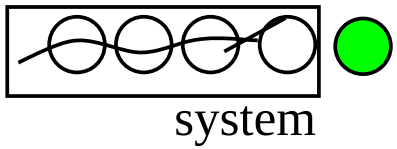

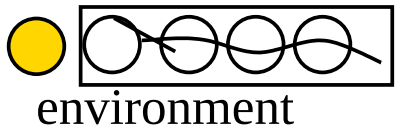

- After adding a site the Hilbert space of system and environment (separately) is transformed by a linear transformation $|k'\rangle = \sum_k W_{k',k}|k\rangle$
- Operators are transformed by $A' = W^\dagger A W$
- Transformations "stack":
  $\tilde{A} = \cdots W_3^\dagger W_2^\dagger W_1^\dagger W_0^\dagger A W_0 W_1 W_2 W_3 \cdots$

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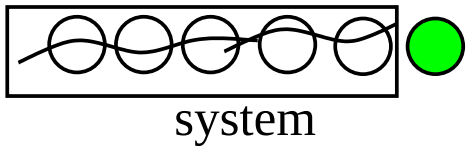

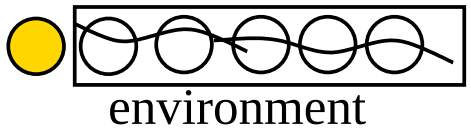

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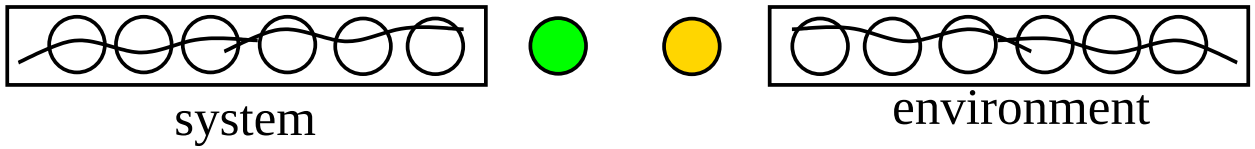

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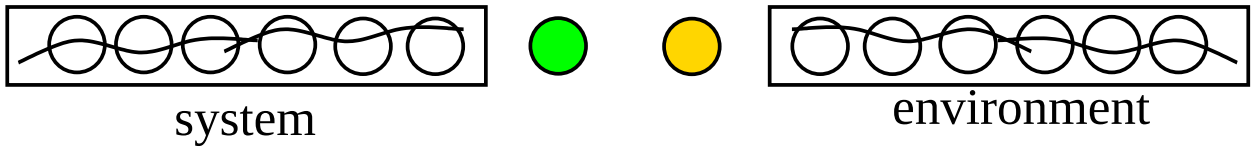

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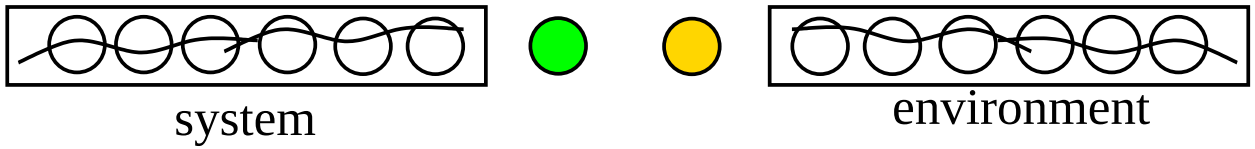

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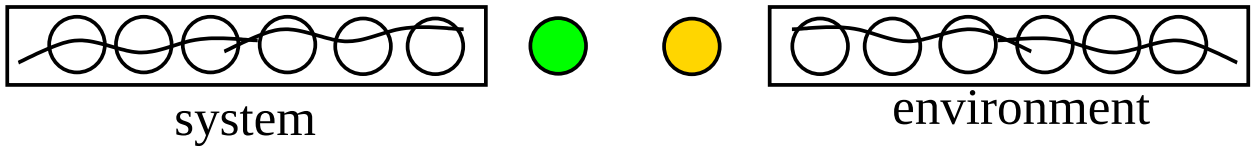

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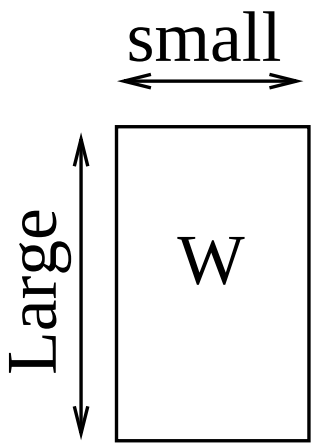

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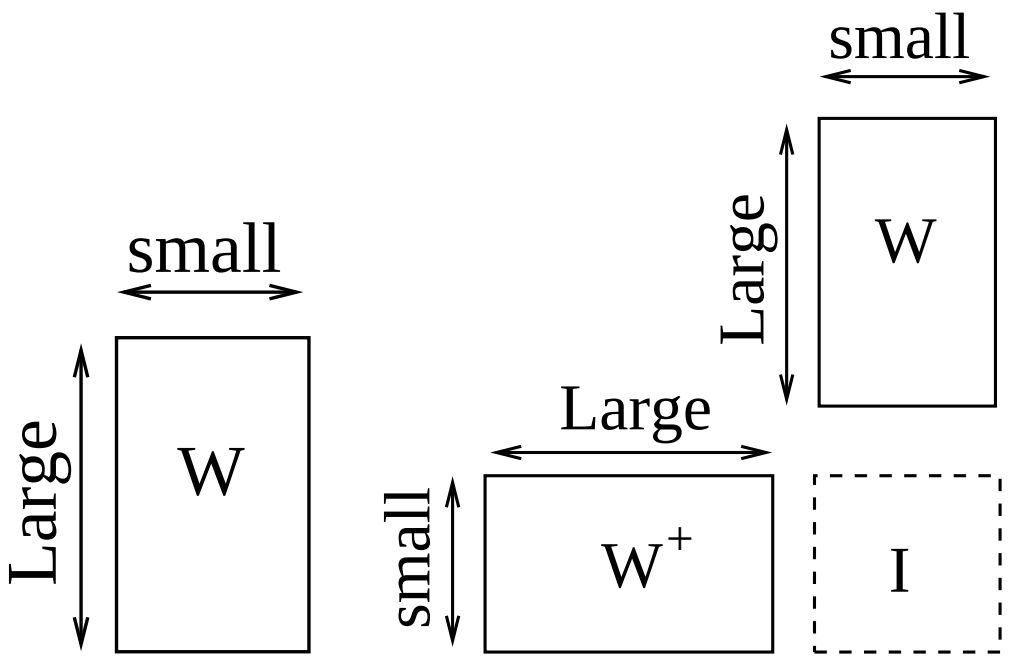

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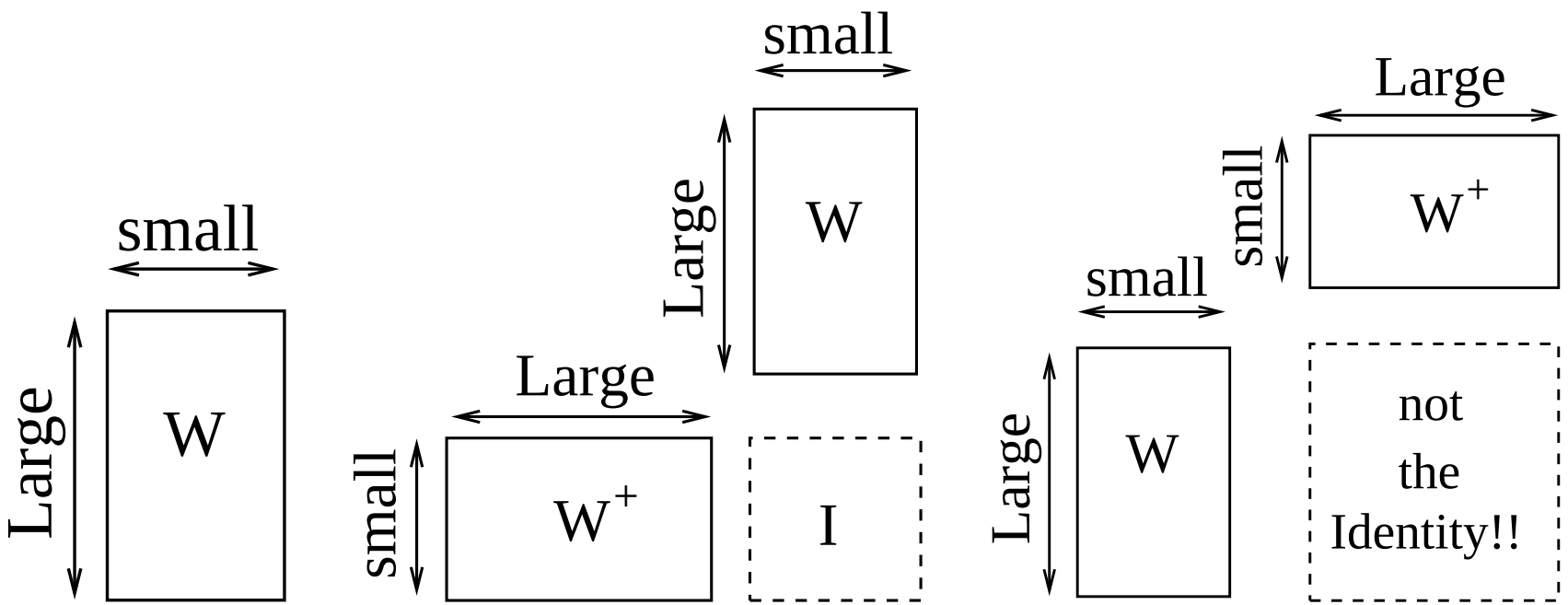

The DMRG Transformation

- $W^\dagger W = I$ *but* $WW^\dagger \neq I$ (i.e., there is no right inverse)
- Let A_i be an operator that lives on the Hilbert space for a single site i in the real space basis

Definition of $\tilde{A}$

Define $\tilde{A}_i = \cdots W_3^\dagger W_2^\dagger W_1^\dagger W_0^\dagger A_i W_0 W_1 W_2 W_3 \cdots$. Note that:

1. $\tilde{A}_i$ acts on a larger Hilbert space than A_i
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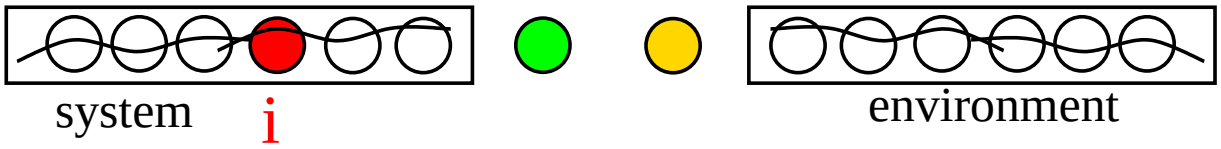

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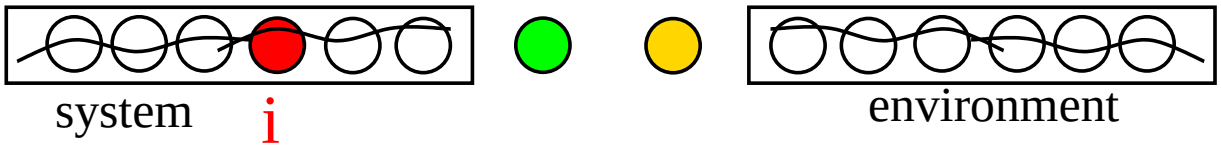

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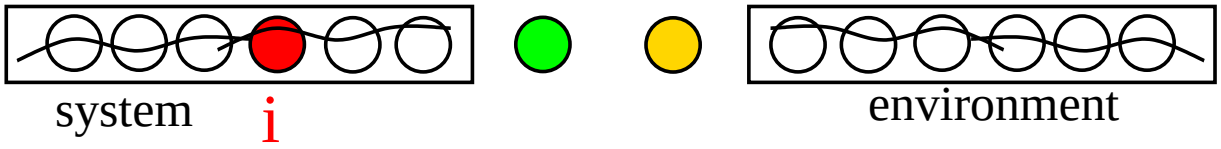
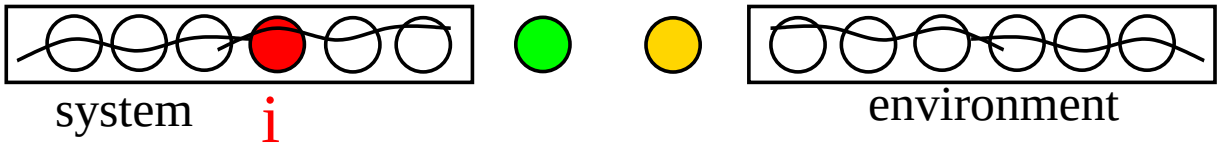
Assembling The Hamiltonian



- Current DMRG basis for system and environ.
- "Assembler operators" $X^0, X^1, \cdots X^l$.
- Let $A_i = \prod_{t \in \mathcal{T}} X^t$, where $\mathcal{T}$ is a subset of $\{0, 1, \cdots 2l-1\}$, $X^{l+r} = (X^r)^\dagger$. Let A_i, B_i, C_i, etc. act on i
- $H_{onsite} = C_i$ and $H_{connections} = A_i B_j$
- Keep H_{system} and $H_{environment}$ on current DMRG basis but build superblock Hamiltonian on the fly

Assembling The Hamiltonian



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- "Assembler operators" $X^0, X^1, \cdots X^l$.
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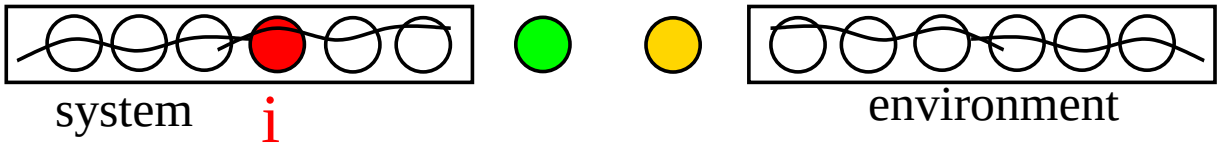

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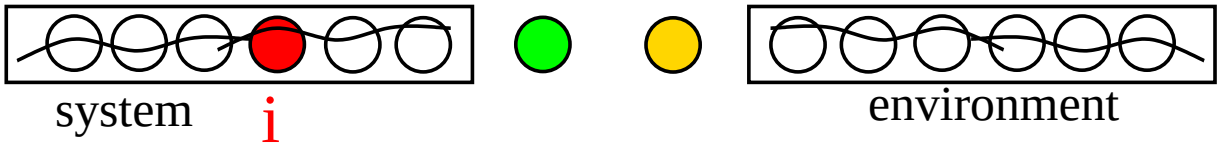

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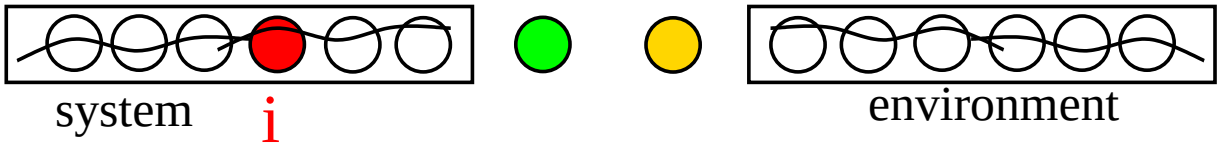

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Types of Hamiltonian Connections

Onsite Terms: trivial, add when fresh site added

Connections

- Connection I: With a new site: Fluff up:
  $(\cdots W_2^\dagger W_1^\dagger W_0^\dagger A_i W_0 W_1 W_2 \cdots) B_j \equiv \tilde{A}_i B_j$
- Connection II: Between old sites: Caveat, no right inverse!
  $W^\dagger A_i B_j W \neq (W^\dagger A_i W)(W^\dagger B_j W)$, i.e. $\widetilde{A_i B_j} \neq \tilde{A}_i \tilde{B}_j$
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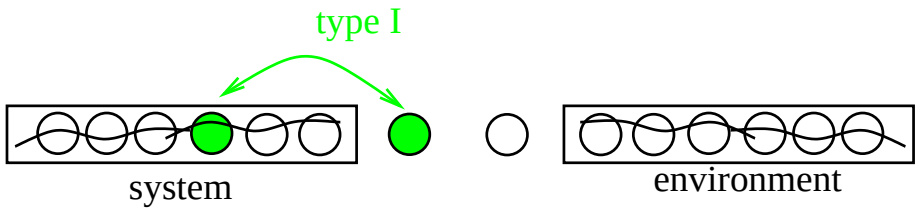

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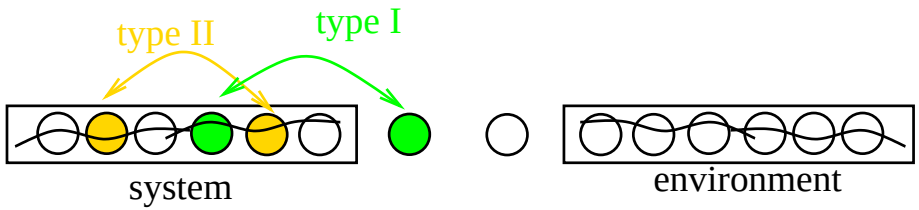

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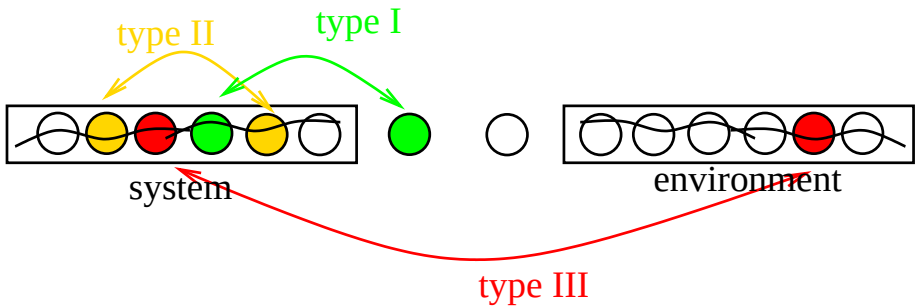

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- CPU intensive part: sum over connections of form $c_i^\dagger c_j$ (Hubbard), $S_i^+ S_j^-$, $S_i^z S_j^z$ (Heisenberg), and generally:

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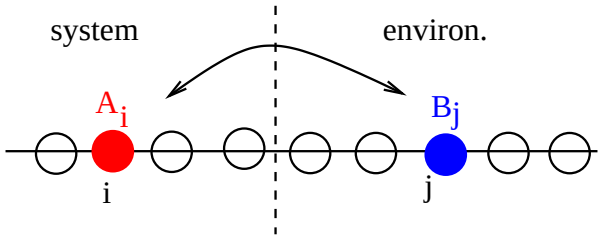

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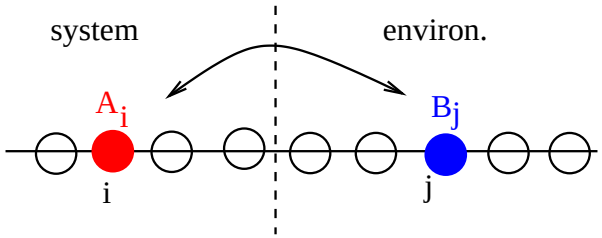

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$$\sum_{\text{connections}\, i,j} A_i B_j \qquad (3)$$

can be parallelized efficiently using *pthreads*.

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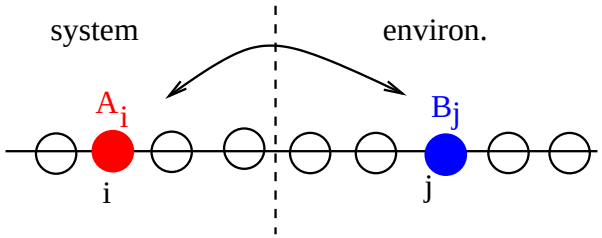
$$(A^S B^E)_{c,c'} = \sum_{a,b,a',b'} G^{SE}_{P^{SE}(c),a+bN_s} \left(\tilde{s}_a A^S_{a,a'} B^E_{b,b'} \right) \times G^{SE}_{P^{SE}(c'),a'+b'N_s}$$



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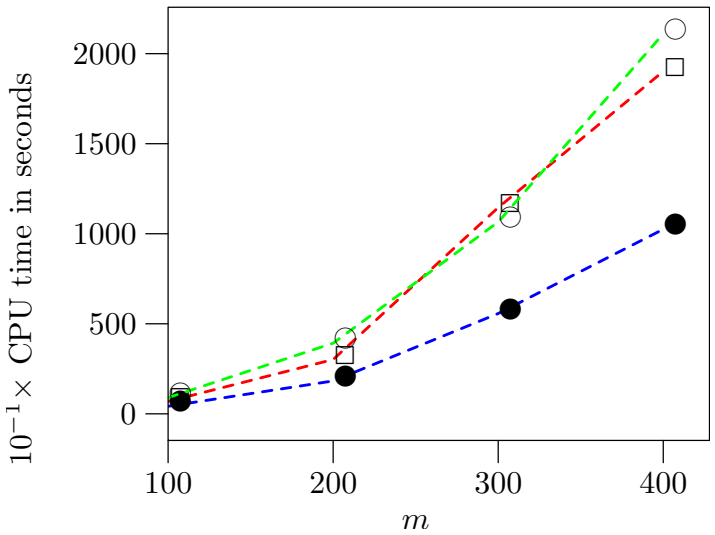
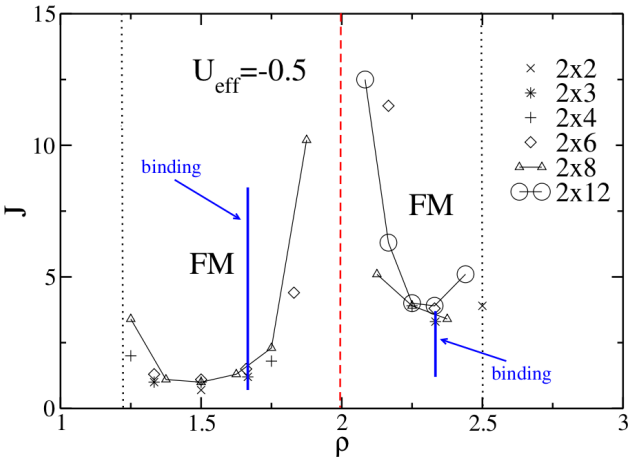
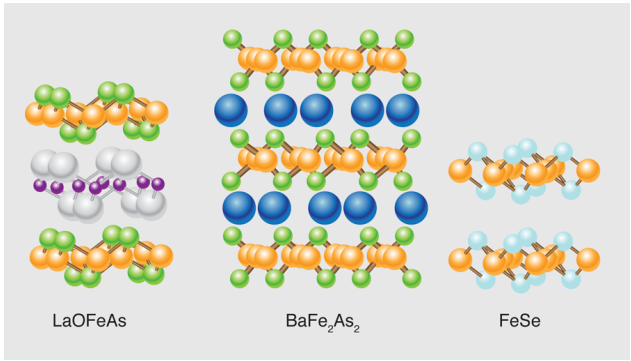
DMRG Parallelization



- Figure: Serial (red/green lines) vs. Parallel (blue lines)
- [G. Alvarez, arXiv:1003.1919]; [K. Hallberg et al. CPC]
- Also: [G. Alvarez, Comp. Phys. Comm. (2009)]
- But: Scalability still an open problem. Big pay-off if solved

Coexistence of Ferromagnetism and Pairing





M. Johannes, Physics 2008

- Computed Phase Diagram of a Model for Iron Pnictides
- User Project: [Xavier et al., PRB 2010]

Current trends in DMRG

- Other models (e.g. t-j model) and other geometries (e.g. "trees")
- Parallelization
- Time dependent DMRG (We are doing this now!)
- Temperature: METTS, [S. White PRL 102, 190601 (2009)]

- Race to solve the 2D problem: MERA, PEPS, too many new algorithms to list all

DFT does not apply to model Hamiltonians

Consider [Schlindmayr and Godby, PRB 1995]:

$$\hat{H} = -t \sum_{i=-\infty}^{\infty} \sum_{\sigma} (c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + \text{H.c.}) + U \sum_{i=-\infty}^{\infty} n_{i\uparrow} n_{i\downarrow} \qquad (4)$$

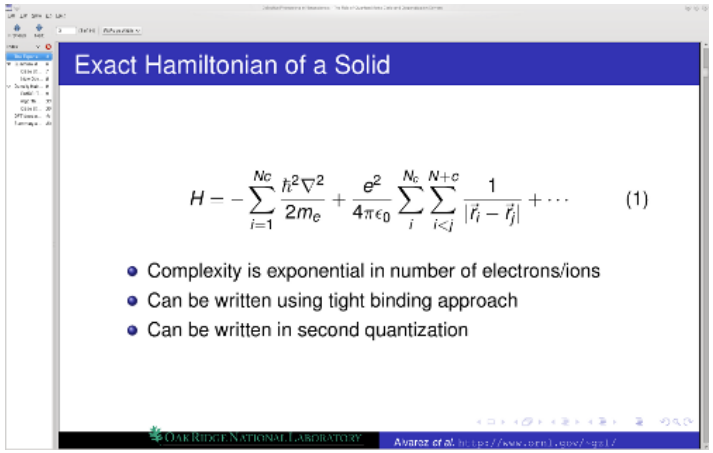
- Translational invariant chain or ring: density is constant
- Properties (*e.g.* kinetic energy) of $U = 0$ and $U \neq 0$ systems different
- But: Kohn-Sham predicts that they are the same

Hohenberg-Kohn Theorem does not apply

- Energy not a functional of (only) the density $E \neq E[\rho]$
- Depends also on U
- Or on $\frac{e^2}{4\pi\epsilon_0}$

Relevant because:

1. Fully reductionist approach not always useful
2. Interest in:
   - Emergent behavior at the nanoscale
   - What interactions are the most relevant for a given solid



Our Interests and Future Research

- If you want to solve the exponential problem exactly...
- ...consider using Quantum Monte Carlo: continuous time, hybridation expansion, ...
- ...and Density Matrix Renormalization Group

Thanks to: E. Dagotto, L. Dias da Silva, M. Eisenbach, S. Manmana, I.P. McCulloch, J. A. Riera, and J. Xavier.


http://www.ornl.gov/~gz1/


http://arxiv.org/abs/1003.1919


http://arxiv.org/abs/0902.3185

Credit Line

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