Real Space RG Methods for Quantum Mechanics in >1D

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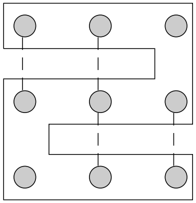
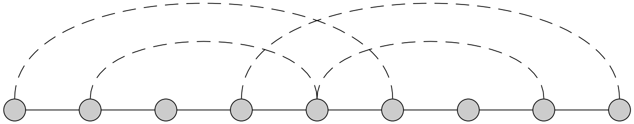
Recent Progress and Prospects in Density–Matrix Renormalization. August 2–13, 2004. Leiden (The Netherlands)

Punctures Renormalization Group (PRG)

• 2D Extension of the DMRG.

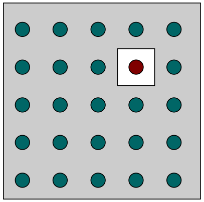




◇ The LEFT–RIGHT distinction creates long-range links.

◇ Is there a *topologically natural* way to break the blocks in $> 1\mathsf{D}$?

THE INSIDE–OUTSIDE DISTINCTION. We split the system into "Block" + "Puncture".



BLOCK (low res.) + PUNCTURE (high res.) Scheme

M.A. Martín-Delgado, J. Rodríguez-Laguna and G. Sierra, Nucl. Phys. B (2001).

Punctures Renormalization Group (PRG)

- SINGLE BLOCK + SINGLE PUNCTURE + SINGLE STATE

Ansatz: $|\psi\rangle = a^B|\phi_B\rangle + a^P|\delta_P\rangle \quad \rightarrow \quad H_{Sb} = \begin{pmatrix} \langle\phi_B|\,H\,|\phi_B\rangle & \langle\phi_B|\,H\,|\delta_P\rangle \\ \langle\delta_P|\,H\,|\phi_B\rangle & \langle\delta_P|\,H\,|\delta_P\rangle \end{pmatrix}$

- SINGLE BLOCK + MANY PUNCTURES + MANY STATES

N_p punctures and m states. Ansatz: $|\phi\rangle = \sum_{i=1}^{m} a_i\,|\psi_i^*\rangle + \sum_{j=1}^{N_p} a_{m+j}\,\big|\delta_{P(j)}\big\rangle$

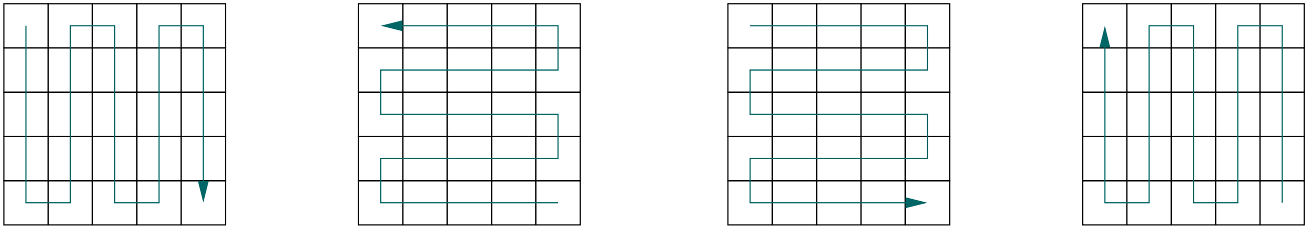
$$H_{Sb} = \left(\begin{array}{ccc|ccc}
\langle\psi_1^*|\,H\,|\psi_1^*\rangle & \cdots & \langle\psi_m^*|\,H\,|\psi_1^*\rangle & \langle\delta_{P(1)}|\,H\,|\psi_1^*\rangle & \cdots & \langle\delta_{P(N_p)}|\,H\,|\psi_1^*\rangle \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\langle\psi_1^*|\,H\,|\psi_m^*\rangle & \cdots & \langle\psi_m^*|\,H\,|\psi_m^*\rangle & \langle\delta_{P(1)}|\,H\,|\psi_m^*\rangle & \cdots & \langle\delta_{P(N_p)}|\,H\,|\psi_m^*\rangle \\
\hline
\langle\psi_1^*|\,H\,|\delta_{P(1)}\rangle & \cdots & \langle\psi_m^*|\,H\,|\delta_{P(1)}\rangle & \langle\delta_{P(1)}|\,H\,|\delta_{P(1)}\rangle & \cdots & \langle\delta_{P(N_p)}|\,H\,|\delta_{P(1)}\rangle \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\langle\psi_1^*|\,H\,|\delta_{P(N_p)}\rangle & \cdots & \langle\psi_m^*|\,H\,|\delta_{P(N_p)}\rangle & \langle\delta_{P(1)}|\,H\,|\delta_{P(N_p)}\rangle & \cdots & \langle\delta_{P(N_p)}|\,H\,|\delta_{P(N_p)}\rangle
\end{array}\right)$$

Punctures Renormalization Group (PRG)

PRG SCHEME (case $N_p = 1$ and $m = 1$):

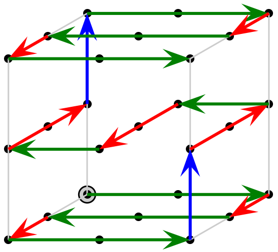
- Choose a (just any!) global wavefunction $|\psi\rangle$ and a site p.
- Make the component on site p vanish and normalize, obtaining $|\phi_B\rangle$.
- Make up the former superblock hamiltonian and diagonalize it.
- Introduce the weights of the ground state into the *Ansatz* and obtain a new $|\psi\rangle$.
- Return to the initial step choosing a new p.

How should we choose the trajectory of the puncture? SEWING.

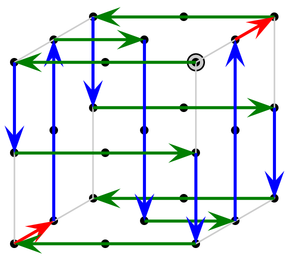


Punctures Renormalization Group (PRG)

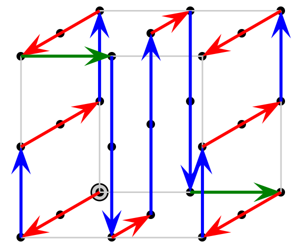
P_z



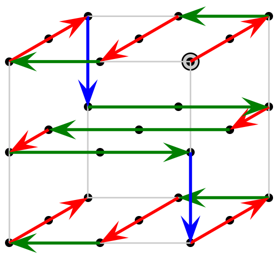
P_x



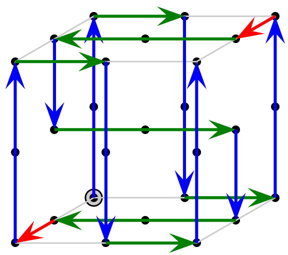
P_y



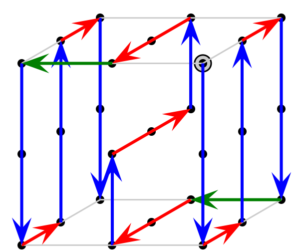
$Q_z(P_z^{-1})$



$Q_x(P_x^{-1})$



$Q_y(P_y^{-1})$

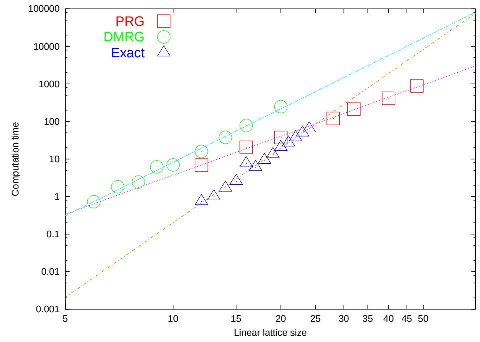


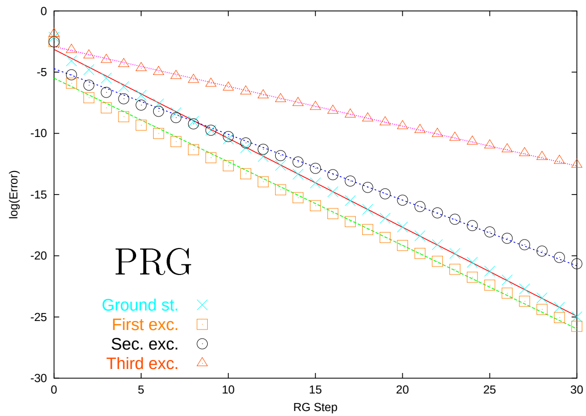
3D Path $\leftarrow$ $Q_y(P_y^{-1})\ Q_x(P_x^{-1})\ Q_z(P_z^{-1})\ P_y\ P_x\ P_z$

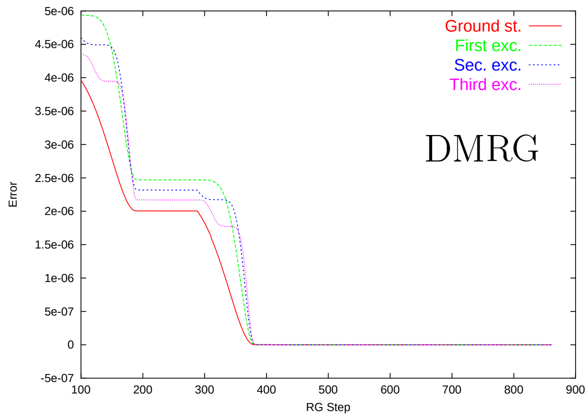
PRG Performance

DIAGONALIZATION TIME: $t \propto L^{\alpha}$. Low energy spectrum of the Hydrogen Atom (3D):

- Exact Diagonalization: $\alpha \approx 9.5 \pm 0.6$.
- PRG $(3 \times 3 \times 3)$: $\alpha \approx 5.6 \pm 0.3$.



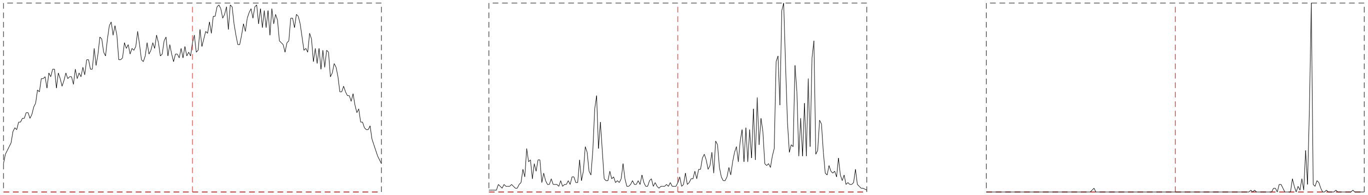




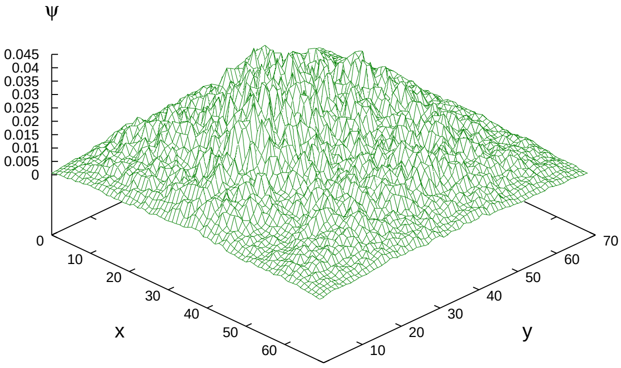
Testing Anderson Localization with Long-Range Couplings

Rodríguez, Malyshev, Sierra, Martín-Delgado, Rodríguez-Laguna and Domínguez-Adame, PRL 2003.

$$\mathcal{H} = \sum_i \epsilon_i \left|\delta_i\right\rangle \left\langle\delta_i\right| + \sum_{i,j} J_{ij} \left|\delta_i\right\rangle \left\langle\delta_j\right| \qquad \begin{cases} \epsilon \text{ is a } \textit{uniform deviate} \text{ in } [-\Delta/2, \Delta/2] \\ J_{ij} = J\,|i-j|^{-\alpha} \end{cases}$$



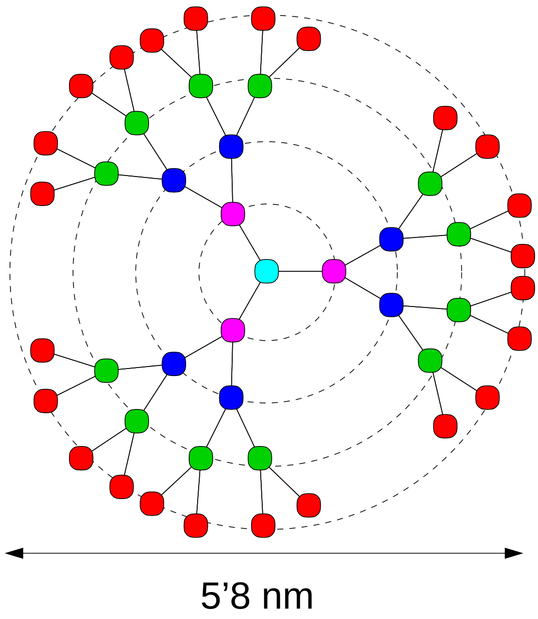
$\alpha = 3/2$, $N = 1000$, $\Delta = 1$, 8 and 30.



$\alpha = 3$, $\Delta = 5$, $N = 70 \times 70$

Dendrimers

DENDRIMERS are highly branched polymeric self-similar molecules.



- Controlled synthesis → low polydispersity.
- High proportion of active monomers.

[*Molecule recognition, contrast agents for magnetic resonance, building blocks for nanotechnology...*]

- Large internal voids: encapsulation.

[*Drug delivery, gene therapy, antiviral treatments...*]

- Self–similar structure.

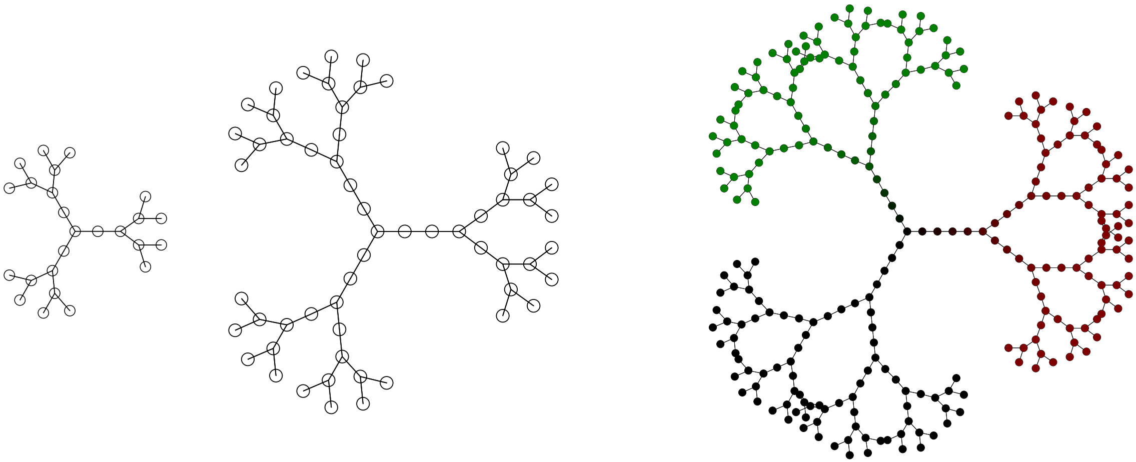
[*Photovoltaic converters, molecular antennae*]

WHICH MONOMERS?

Aminoacids, glucids, polyamidoamines, DNA bases, organo-inorganic compounds... We focus on phenyl rings with acetylene links.

Extended Dendrimers

THE EXTENDED DENDRIMERS FAMILY: *corridors* of decreasing length.



Kopelman et al. (PRL 1997) studied exp. the *Optical Absorption Edge* (OAE).

COMPACT DENDRIMERS. OAE independent of molecule size → *exciton localization*.

EXTENDED DENDRIMERS. OAE decreases with molecular size → *exciton mobility*.

Models for Excitons in Polymers

- Non-interacting excitons: Frenkel model ($\approx$ Tight Binding Model).
- Interacting electrons: e.g. Pariser-Parr-Pople hamiltonian, including Coulomb interaction.

HARIGAYA'S MODEL. (Int. J. Mod. Phys. B, 13, 19, 2531 (1999)). Hypothesis:

◇ Single exciton approach.
◇ Hopping due to dipole interaction between monomers, with random direction.
◇ Localization is related to disorder.
◇ Conclusion: OFF-DIAGONAL DISORDER.

Harigaya Hamiltonian:

$$H = \sum_{i=1}^{N} E|\delta_i\rangle\langle\delta_i| + \sum_{\langle i,j\rangle}(J_{i,j}|\delta_i\rangle\langle\delta_j| + h.c.)$$

E: empirical constant ($37.200\,cm^{-1}$)

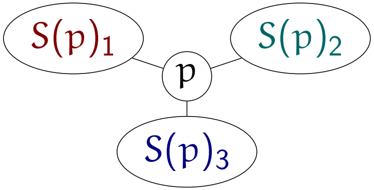
$J_{i,j}$: *gaussian variate* with $\mu = 0$ and $\sigma = 3.552\,cm^{-1}$

- We need good statistics $\rightarrow$ a REALLY FAST SOLVER for Schrödinger Equation.

DMRG climbing the trees

Martín-Delgado, Rodríguez-Laguna and Sierra, PRB 2002.

- DMRG finds its natural place on TREES:

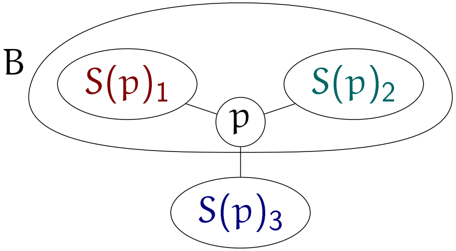


- *Ansatz:*

$$|\phi\rangle = a_1 |\psi(S(p)_1)\rangle + a_2 |\psi(S(p)_2)\rangle + a_3 |\psi(S(p)_3)\rangle + a_c |\delta_p\rangle$$

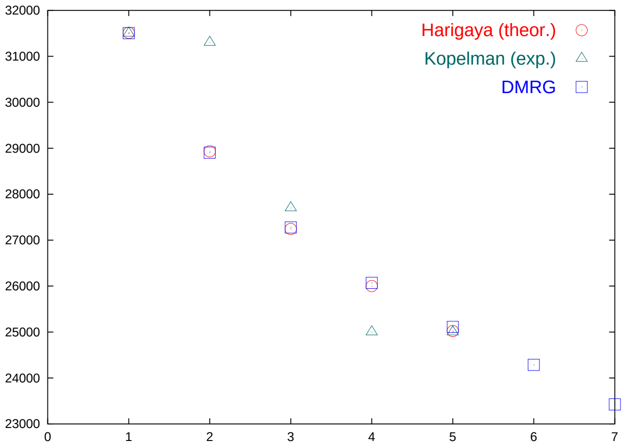
$$H_{Sb} = \begin{pmatrix} H[S(p)_1] & 0 & 0 & T[S(p)_1] \\ 0 & H[S(p)_2] & 0 & T[S(p)_2] \\ 0 & 0 & H[S(p)_3] & T[S(p)_3] \\ T^\dagger[S(p)_1] & T^\dagger[S(p)_2] & T^\dagger[S(p)_3] & H_{pp} \end{pmatrix}$$

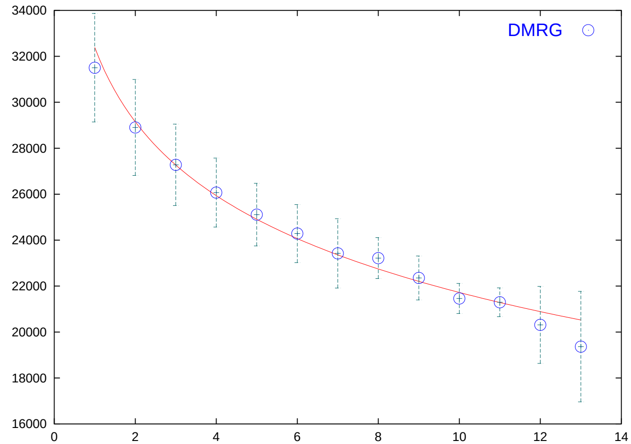
- *Block fusion:*



Some results

- **Extended Dendrimers.**





Experimental results (Kopelman et al.), Theoretical results (Harigaya's model via exact diagonalization and DMRG).

- **Compact Dendrimers.** Experimentally: OAE does not decrease. Numerically: Harigaya's model yields a power law dependence on generation.

Conclusions?

Regarding Dendrimers' Physics.

- Harigaya's model qualitatively explain the spectrum of extended dendrimers. Why does it not work for compact ones? Interaction?
- Linear cluster theory predicts correctly the spectrum, but is not justified!
- Although more measures should be done for exciton conductivity, extended dendrimers may serve as antennae.

Regarding the DMRG Application.

- Computational resources drastically reduced. Results are exact.
- Many exciton models may be tackled now.

◇ For more details, see Martín-Degado et al. PRB, 65, 155116 (2002) and J. Rodríguez-Laguna, `cond-mat/0207340`.