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I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

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MINIWORKSHOP ON STRONG ELECTRON CORRELATIONS
"Disorder and Interaction in Quantum Systems and Their Classical Analogs"

(1 - 19 July 1996)

"Divide-and-Conquer Treatments of Correlated Electrons"

Shoudan Liang
Pennsylvania State University
Department of Physics
University Park, PA 16802
U.S.A.

These are preliminary lecture notes, intended only for distribution to participants.

Divide-and-Conquer Treatments of Correlated Electrons

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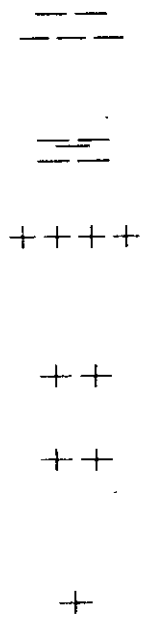
Outlines

- Introduction
  - Why electron correlations can usually be ignored
  - Importance of electron correlations, some examples
  - Why electron correlations are hard to treat
- The Divide-and-Conquer method: Renormalization
  - Hilbert space truncation
  - The importance of the energy scale hierarchy
- Adaptive Renormalization Group: a Generalization of Wilson's Method
  - Hartree-Fock theory
  - Making energy scale hierarchy
  - A test calculation for an exactly solvable model

Reasons for ignoring electron correlations at low energy
V. Weisskopf Science 113 101 (1951)

- In quantum mechanics, the effect of interaction is to scatter a particle from one state to another.
- Although the interactions are strong, at core level, because of Pauli principle, all states are occupied. There is no state to scatter to.
- Screening
- Only true at low energy



Well known models of independent particles

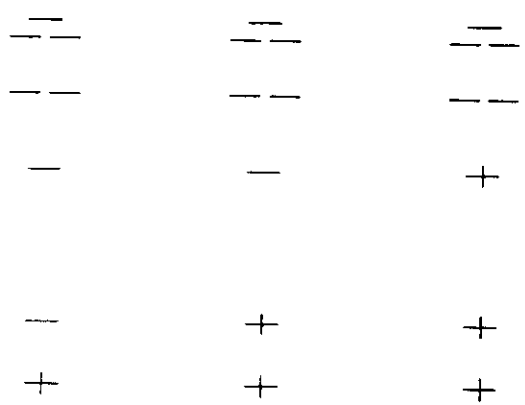
- Landau Fermi liquid theory
- Shell structure of nuclear properties

Examples where electron correlations are important

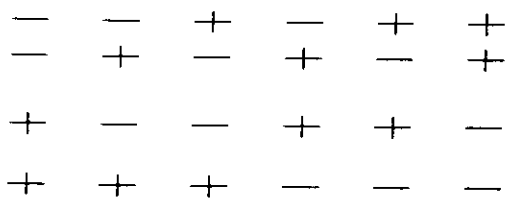
- Fractional quantum Hall effect: elementary excitations have fractional charge such as $e/3$.
- High T_c superconductors.
- Rare earth compounds.
- Mott insulator: insulator when the band is half filled.
- Magnetism, both ferromagnets and antiferromagnets.
- Catalysts involving transition metals, computer assisted catalyst design. $
- Quantum chemistry.

Why the problem of correlated electrons is hard?

- **Independent fermions:**



- **Interacting fermions:** all configurations needed.



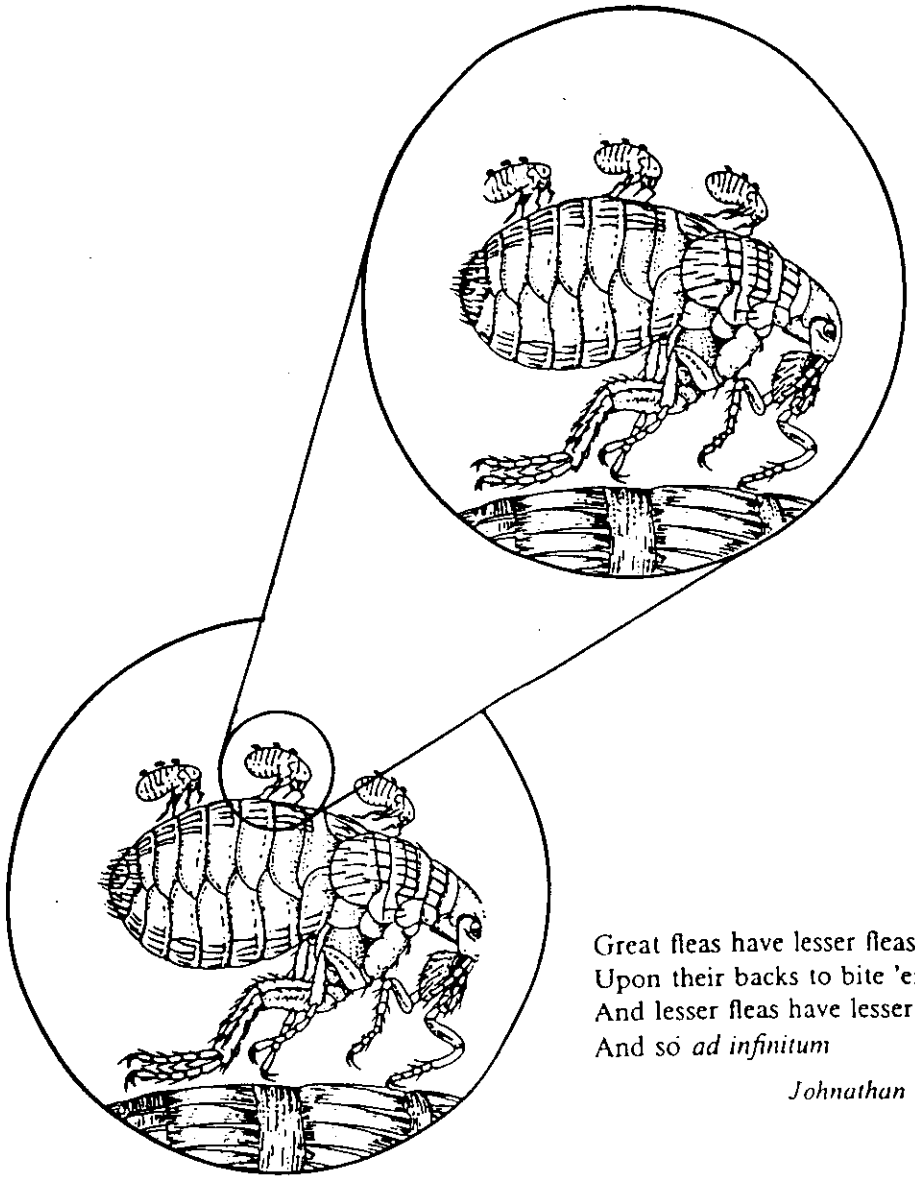
$$\begin{pmatrix} \text{The total number of} \\ \text{configurations for} \\ N \text{ levels and } M \text{ particles} \end{pmatrix} = \binom{N}{M} = \frac{N!}{(N-M)!M!}$$

Numerical methods for correlated electrons

- **Quantum Monte Carlo,**
  difficulty with the 'minus sign' problem.
- **Exact diagonalization,**
  limited to small systems.
- **Configuration interaction,**
  incomplete treatment of correlations.
- **Density functional theory,**
  unknown energy functional.

Divide and Conquer

renormalization group
Hilbert space pruning



Great fleas have lesser fleas
Upon their backs to bite 'em.
And lesser fleas have lesser still.
And so *ad infinitum*

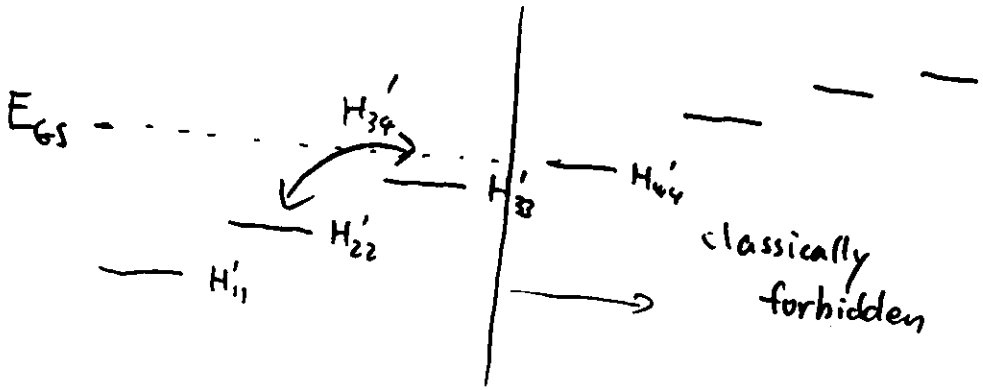
Johnathan Swift

$$U H U^{\dagger} = H' = \begin{pmatrix} \text{sub} \\ \text{matrix} \\ \hline \\ \\ \end{pmatrix}$$

Submatrix contains all low energy information to a good approximation

if $H' = \begin{pmatrix} & & 0 \\ & \ddots & \\ 0 & & \end{pmatrix}$ none-zero only near diagonal

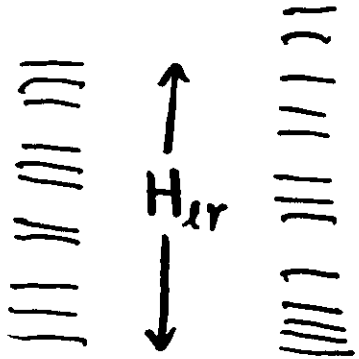
H' describes one-dimensional hoping



Density Matrix Renormalization Group

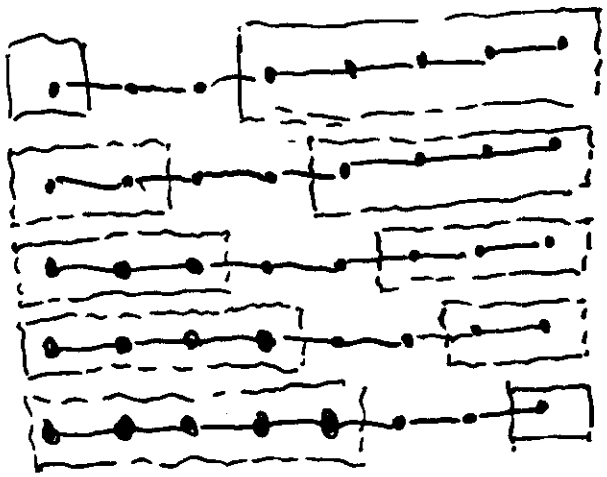
S. Wh

$$\Phi_{GS} = \sum_{lr} \psi_{lr} |l\rangle |r\rangle$$



$$\frac{H_{lr}^2}{E_i - E_0}$$

By using density matrix eigenstate, H_{lr} is large only between a small number of states. i.e. boundary states.



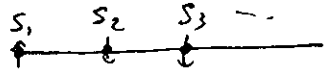
Improve the groung state by a self-consistent iteration.

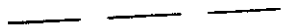
Wilson's paradigm

A hierarchy of energy scales in the hamiltonian

$$H = \mathbf{s}_1 \cdot \mathbf{s}_2 + 0.1\ \mathbf{s}_2 \cdot \mathbf{s}_3 + 0.01\ \mathbf{s}_3 \cdot \mathbf{s}_4 + 10^{-3}\ \mathbf{s}_4 \cdot \mathbf{s}_5 + \ldots$$

We are only interested in the low energy excitations





- For a general hamiltonian, the hierarchy of energy scales required is unfortunately not apparent. In fact, for the Hubbard model we have discussed, all the interactions have the same strength.

$$\boldsymbol{H} = -t \sum_{\langle ij\rangle\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

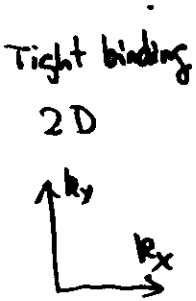
- Can we make an energy hierarchy by suitably choosing single particle orbitals?

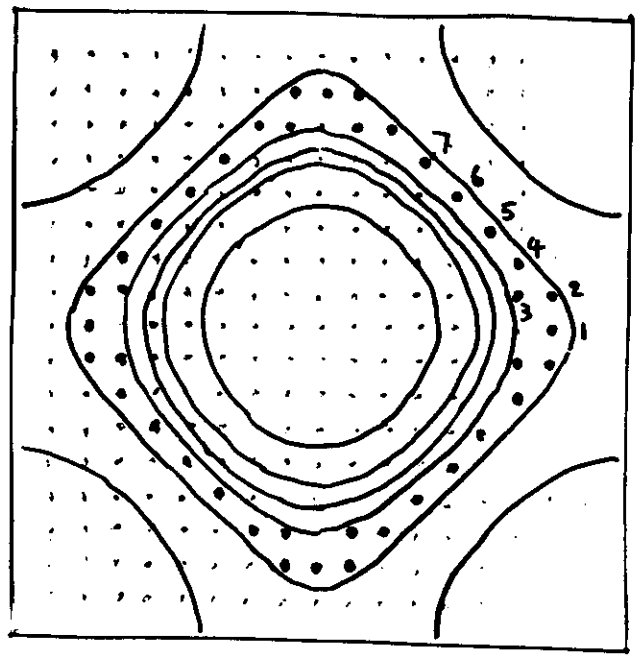
- For the two dimensional Hubbard model, an explicit construction can be made. The hamiltonian displays an exponentially distributed hierarchy of energy scales. (S. Liang, *J. Phys. Chem. Solids*, ~~in press~~ 56 1729).

- A variational procedure has been formulated to select optimal orbitals with energy hierarchy. (S. Liang, *Phys. Rev. Lett.*, **75**, 3493 (1995)).

Tight binding

2D





Fermi surfa

Equal ener

partition

$$f_{0s} = \frac{1}{\sqrt{N_s}} \sum_j C_{kj} \qquad s\text{-wave}$$

$$f_{1s} = \frac{1}{\sqrt{N_s}} \sum_j a_{1j} C_{kj} \qquad p\text{-wave} \qquad a_{1j} = e^{i\frac{2\pi}{N_s}}$$

$$f_{2s} = \frac{1}{\sqrt{N_s}} \sum_j a_{2j} C_{kj} \qquad d\text{-wave}$$

$$\vdots$$

Hubbard model

$$H = \sum_{k\sigma} \epsilon(k) c^\dagger_{k\sigma} c_{k\sigma} + \frac{U}{N} \sum_{kk'q} c^\dagger_{k\uparrow} c^\dagger_{k'\downarrow} c_{k'+q\downarrow} c_{k-q\uparrow}$$

For k_j **within** shell s

$$c_{k_1} = \frac{1}{\sqrt{N_s}}(f_{0s} + b_{11} f_{1s} + b_{12} f_{2s} + \ldots)$$

$$c_{k_2} = \frac{1}{\sqrt{N_s}}(f_{0s} + b_{21} f_{1s} + b_{22} f_{2s} + \ldots)$$

$$\vdots$$

The U-term becomes

$$\frac{U}{N} \sum_{\{s_i, m_i\}} C\{s_i, m_i\} f^\dagger_{m_1 s_1 \uparrow} f^\dagger_{m_2 s_2 \downarrow} f_{m_3 s_3 \downarrow} f_{m_4 s_4 \uparrow}$$

Consider $\frac{C(\{s_i\}, m_i = m)}{C(\{s_i\}, m_i = 0)}$

$\{s_1\ s_2\ s_3\ s_4\}$ all combinations

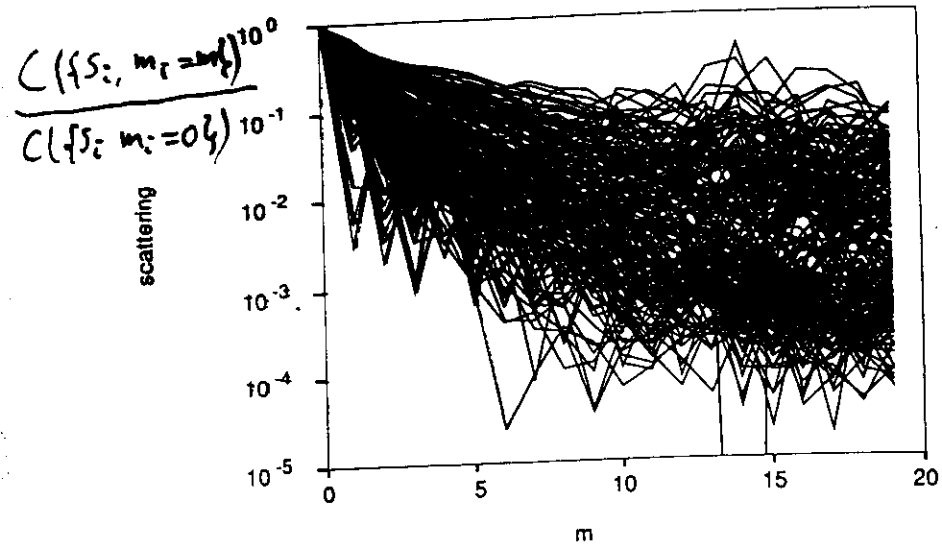
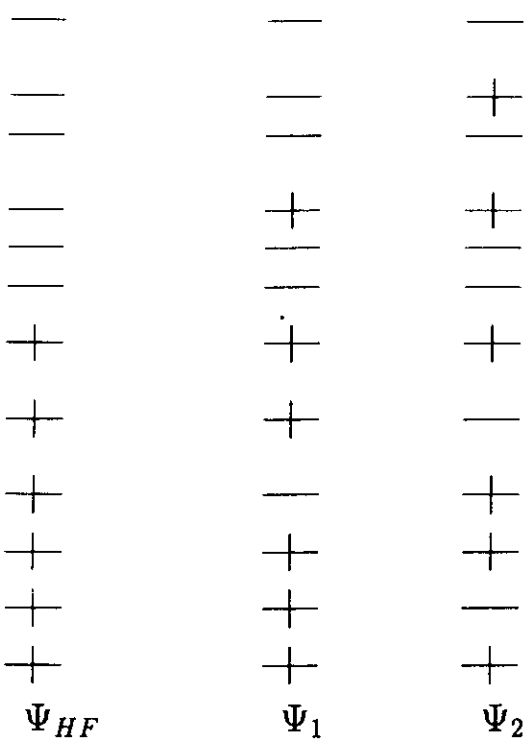


FIG. 2. Plotted are the ratios of Hubbard U scattering terms for $m_i = m$ over the corresponding terms for $m_i = 0$. The curves are for different (s_1, s_2, s_3, s_4) configurations. Only the terms with $m < 20$ are shown. A system of 30×30 lattices is divided into 6 momentum shells with $\epsilon_F = -1.3t$ and separation energies between shells at $|\epsilon - \epsilon_F| = 0.25t, t$. The upper panel is for terms of the form $n_{sm\uparrow} n_{s'm\downarrow}$(with $n_{sm\sigma} = f^\dagger_{sm\sigma} f_{sm\sigma}$) that involve density only. The lower panel is for all the rest.

Hartree-Fock theory

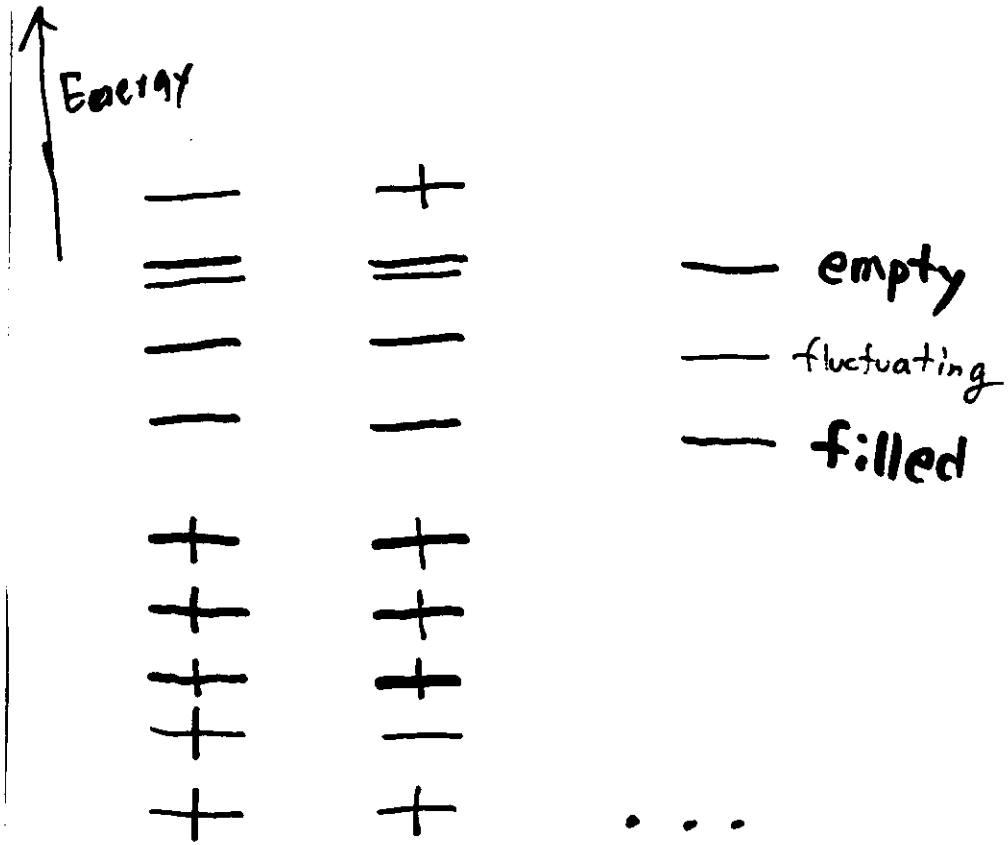
$$\Psi_{HF} = \frac{1}{\sqrt{M!}} \det(\psi_j(r_i))$$

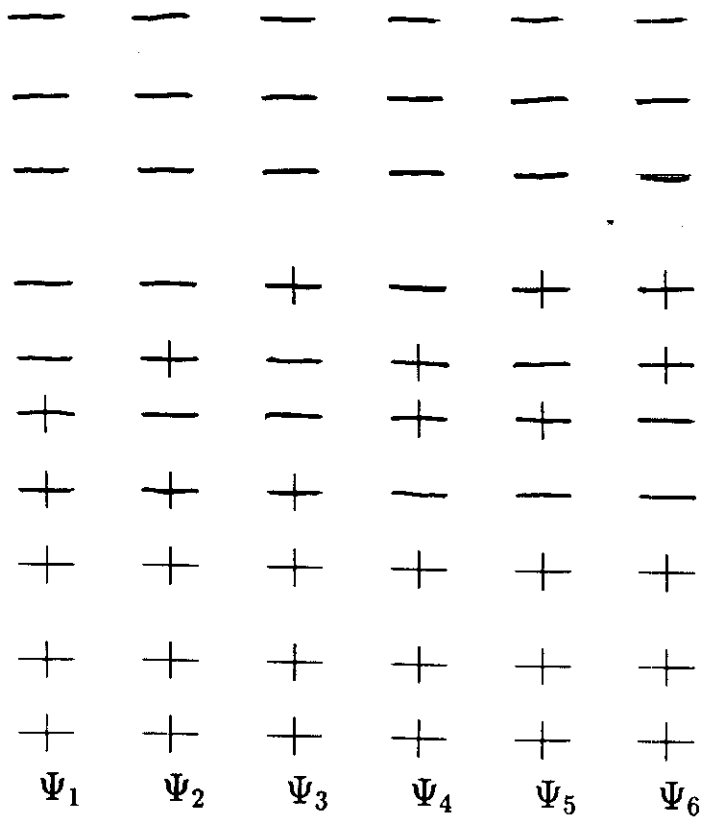
$$\psi_j(r) = \sum_\alpha T_{j\alpha} \phi_\alpha^{atom}(r)$$



- Complete set of $\binom{N}{M}$ states from HF orbitals
- However, they are not the eigenstates of H since

$$\langle \Psi_2 | H | \Psi_{HF} \rangle \neq 0$$



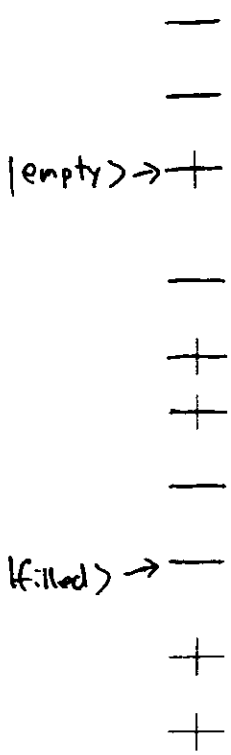


- There are 5 particles, three of them fill 3 core levels the other two are allowed to fluctuate among 4 valence levels and the remaining 3 levels are empty.

$$|1\rangle = \sum_{i=1}^{6} C_i |\Psi_i\rangle$$

- Optimize this wave function with respect to C_i
- Optimize the single particle orbitals $\psi_\alpha, \alpha = 1, ..., 10$ to take into account the largest correlation energy ignored in the HF theory.

After optimizing the single particle orbitals, diagonalize the hamiltonian $\langle \Psi_i | H | \Psi_j \rangle$ within the 6 dimensional Hilbert space, $|1\rangle$ is the **ground** state.



$$|2\rangle = \sum_{i=1}^{20} C_i |\Psi_i\rangle$$

$$\binom{6}{3} = \frac{6!}{3!3!} = 20$$

$$|\text{valence } 2\rangle = \left| \begin{matrix} \text{important states} \\ \text{from step 1} \end{matrix} \right\rangle \otimes |\text{empty}\rangle \otimes |\text{filled}\rangle$$

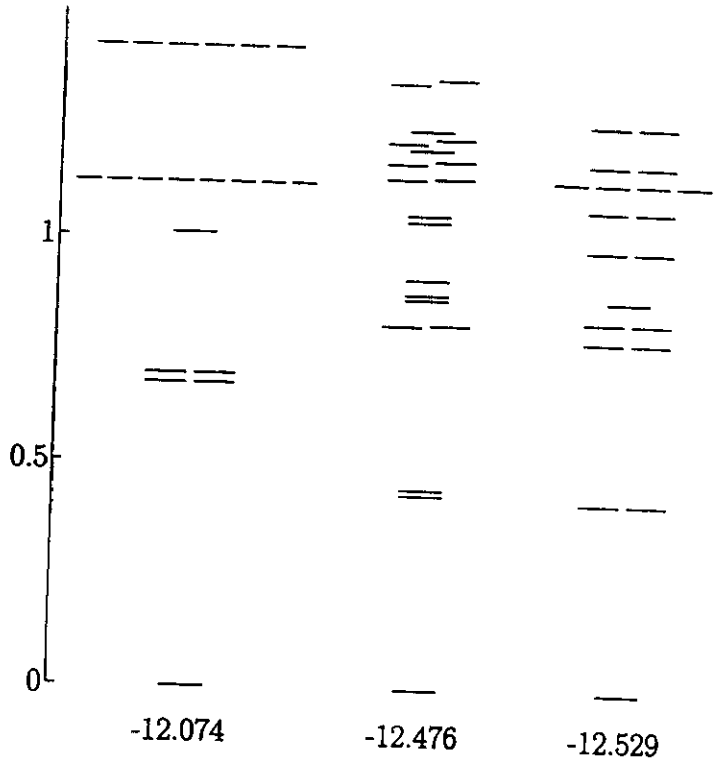
Optimize |empty⟩ among the remaining three orbitals (and the same with |filled⟩) to take into account the next largest correlation energy.

Testing the procedure on an exactly solvable model

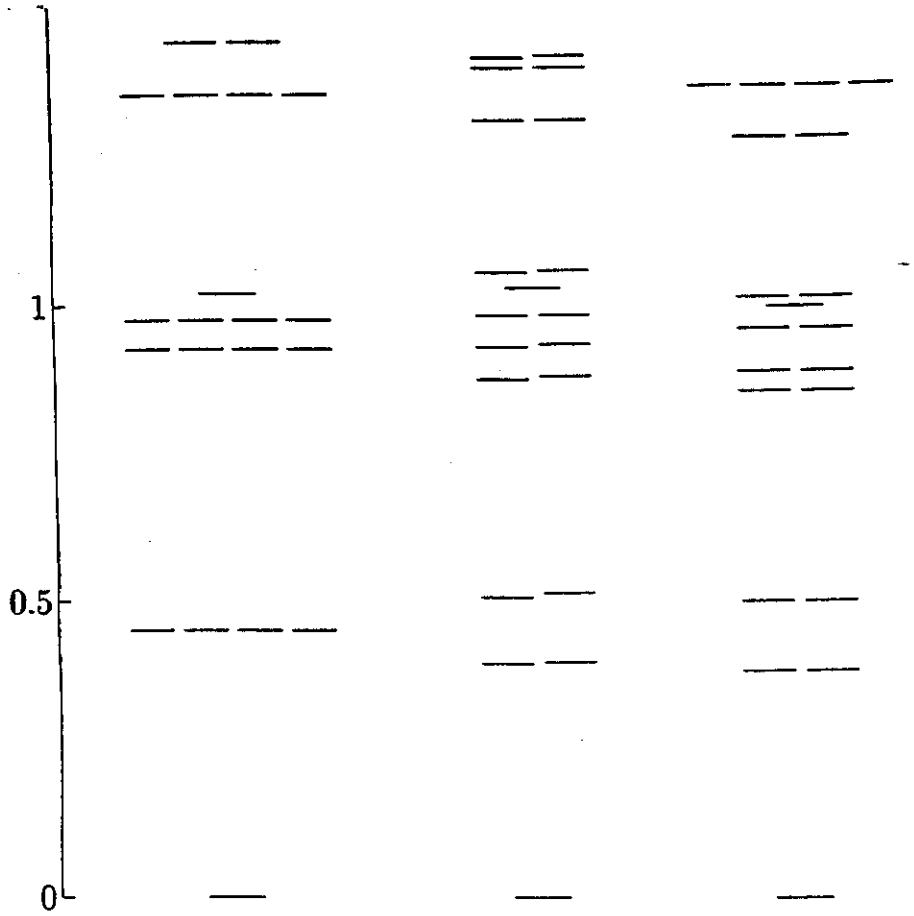
$$H = -t\sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + V\sum_i n_i n_{i+1}$$

H can be diagonalized using Bethe Ansatz(C. N. Yang and C. P. Yang, *Phys. Rev.* **150** 321 (1966)).

Mott Insulator for $V > 2t$ at half filling.



$V = -1.5t$

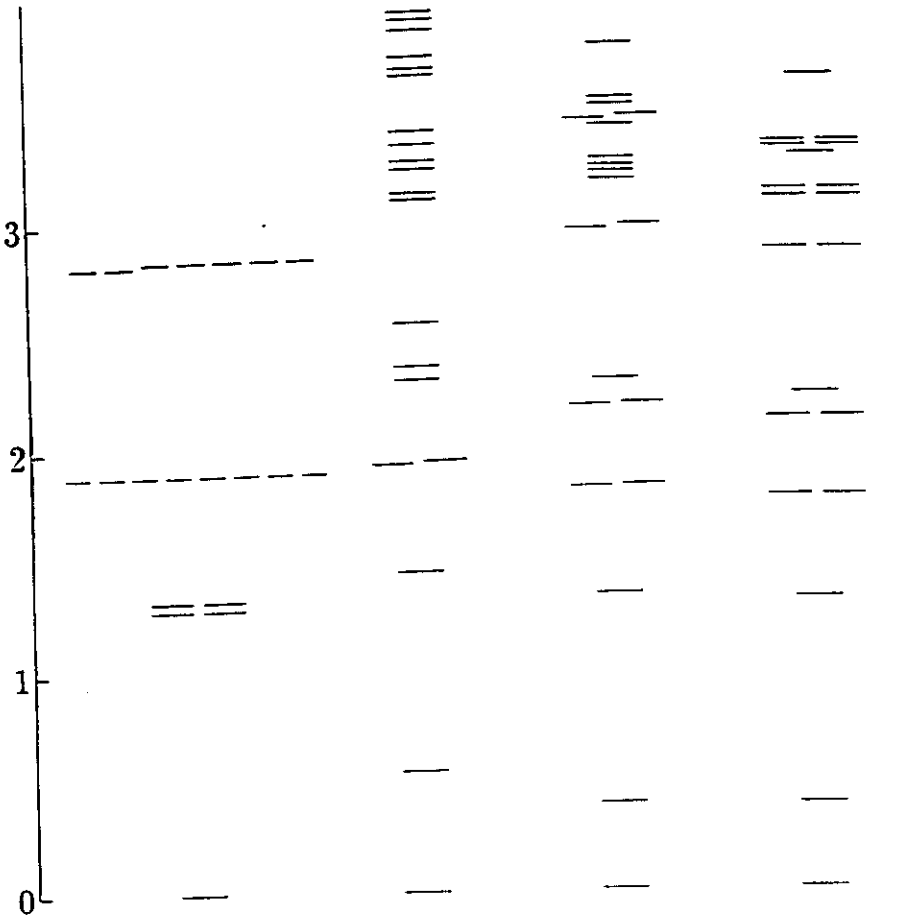


-16.640 (a) HF

-16.745 (b) ARG

-16.959 (c) EXACT

V=t, 13 particles, 31 levels, $\binom{31}{13} = 2 \times 10^8$, 100 states kept



-2.816 (a) HF

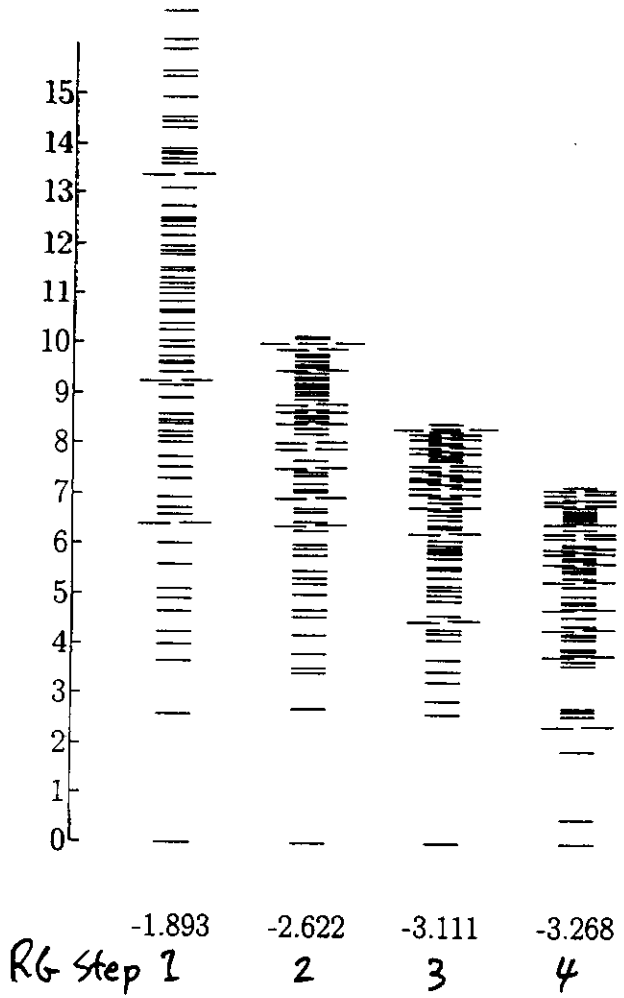
-4.143 (b) 100 states

-4.255 (c) 200 states

-4.280 (d) EXACT

V=2t

7 particles



V = 4

: 14 sites 7 particles, starting

Adaptive Renormalization Group

- The process of selecting new orbitals is quite similar to the Hartree-Fock theory
- The effects of correlation ignored in Hartree-Fock theory are systematically included.
- The method is completely general, applicable to atoms and molecules.
- Our new method can become an enabling technology useful to other scientists.