Targeting Real chemical accuracy at the EXascale

TREX e-school with TurboRVB

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Lecture II : Jastrow correlated variational wavefunctions

- The many body problem and Dirac’s dream Slater determinant, BCS, AGP
- Variational wavefunction: Jastrow-Mean field

- Parametrization and localized basis set
- Example on Hydrogen and Carbon molecules

Hamiltonian and Dirac’s challenge

$$H = -\sum_{I=1}^{N} \frac{\Delta_i}{2m} - \sum_{I,i} \frac{Z_I}{|\vec{r}_i - \vec{R}_I|} + \sum_{1 \le I < J \le M} \frac{Z_I Z_J}{|\vec{R}_I - \vec{R}_J|} + \sum_{1 \le i < j \le N} \frac{1}{|\vec{r}_i - \vec{r}_j|} - \cancel{\sum_{i=1}^{N} \frac{\Delta_I}{2m_I}}$$

After the invention of quantum mechanics, P. A. M. Dirac made the following observation:
"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that
the exact application of these laws leads to equations much too complicated to be soluble.
It therefore becomes desirable that *approximate practical methods* of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems…"

Born-Oppheneimer approximation m_I → ∞
The positions of the atoms are just input parameters

But it is not enough, after several attempts (e.g.DFT)

Some useful definition before starting:

Electron coordinates i,j

$$\begin{aligned} \vec{\xi} &= \vec{r}_i \sigma_i \\ x &= \{\xi_1, \xi_2 \cdots \xi_N\} \end{aligned}$$

Atomic coordinates a,b

$$\vec{R}_1, \vec{R}_2, \cdots$$

The random walk on x conserves the number $N_\uparrow$ of spin-up electrons and the number $N_\downarrow$ of spin down ones $N = N_\uparrow + N_\downarrow$

Therefore we set (TurboRVB conventions):

$$\begin{aligned} \sigma_i &= \uparrow \text{ for } i \leq N_\uparrow \\ \sigma_i &= \downarrow \text{ otherwise, i.e. } i = N_\uparrow + 1, N_\uparrow + 2, \cdots, N \end{aligned}$$

The wave function

$$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \cdots \vec{r}_{N_e}\sigma_{N_e})$$

satisfies (Pauli principle):

$$\Psi(\vec{r}_1, \sigma_1, \vec{r}_2\sigma_2, \cdots \overset{\longleftrightarrow}{\vec{r}_i\sigma_i \cdots \vec{r}_j\sigma_j} \cdots \vec{r}_{N_e}\sigma_{N_e}) = -\Psi(\vec{r}_1, \sigma_1, \cdots \overset{\longleftrightarrow}{\vec{r}_j\sigma_j \cdots \vec{r}_i\sigma_i} \cdots \vec{r}_{N_e}\sigma_{N_e})$$

And we have to find the one such that:

$$(H\Psi)(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \cdots, \vec{r}_{N_e}\sigma_{N_e}) = E\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \cdots, \vec{r}_{N_e}\sigma_{N_e})$$

…and the one with minimum eigenvalue E

Mean field

Within mean field the electrons do not interact

$$H = \sum_i -\frac{1}{2}\nabla_i + V_{\text{Selfconsistent}}(\vec{r}_i, \sigma_i)$$

One can diagonalize the mean-field Hamiltonian:

$$H_{MF} = -\frac{1}{2}\nabla + V_{\text{Selfconsistent}}(\vec{r}, \sigma)$$

$$H_{MF}\phi_i(\vec{r}, \sigma) = \epsilon_i \phi_i(\vec{r}, \sigma) \qquad \phi_i(\vec{r}, \sigma) = \begin{cases} \phi_i^{\uparrow}(\vec{r})\delta_{\sigma,\uparrow} & \mathrm{i} \leq \mathrm{N}_{\uparrow} \\ \phi_i^{\downarrow}(\vec{r})\delta_{\sigma,\downarrow} & \mathrm{i} > \mathrm{N}_{\uparrow} \end{cases}$$

$\phi_i(\vec{r}, \sigma)$ are called "molecular orbitals"
and ϵ_i are the single particle energies

Mean field

What are the eigenfunctions for N-electrons within mean-field?

Any product state of indipendent particles:

$$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2 \cdots, \vec{r}_N\sigma_N) = \phi_1(\vec{r}_1\sigma_1) \times \phi_2(\vec{r}_2\sigma_2) \times \cdots \phi_N(\vec{r}_N\sigma_N$$

with energy: $E = \sum_{i=1}^{N} \epsilon_i$

For bosons you can put all electrons in the same state $\epsilon_i = \epsilon_1 \forall i$
And this will be an allowed symmetric wf but fermions?

How to satisfy antisymmetry?

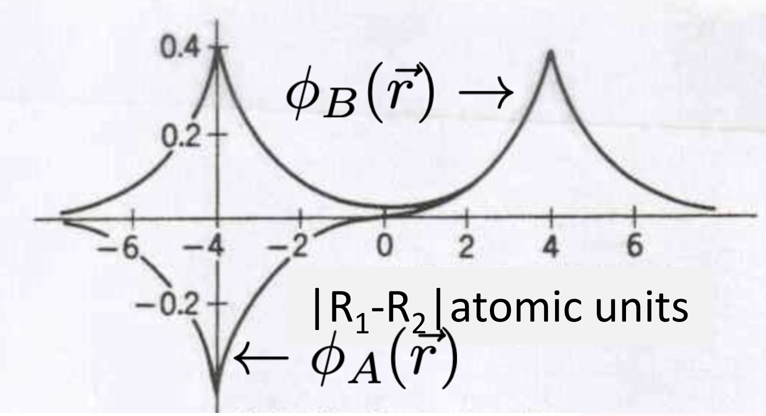
Mean-Field Slater determinant: Apply antisymmetrization to a product state

$$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2 \cdots, \vec{r}_N\sigma_N) = \mathcal{A}\,\phi_1(\vec{r}_1\sigma_1) \times \phi_2(\vec{r}_2\sigma_2) \times \cdots \phi_N(\vec{r}_N\sigma_N) \quad \rightarrow \quad E = \sum_{i=1}^{N} \epsilon_i$$

$$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2, \cdots, \vec{r}_{N_e}\sigma_{N_e}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\vec{r}_1\sigma_1) & \phi_2(\vec{r}_1, \sigma_1) & \cdots & \phi_{N_e}(\vec{r}_1, \sigma_1) \\ \phi_1(\vec{r}_2\sigma_2) & \phi_2(\vec{r}_2, \sigma_2) & \cdots & \phi_{N_e}(\vec{r}_2, \sigma_2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(\vec{r}_{N_e}\sigma_{N_e}) & \phi_2(\vec{r}_{N_e}, \sigma_{N_e}) & \cdots & \phi_{N_e}(\vec{r}_{N_e}, \sigma_{N_e}) \end{vmatrix}$$

Hydrogen molecule

$$
\begin{aligned}
\phi_1(\vec{r},\sigma) &= \delta_{\sigma,\uparrow}\phi_B(\vec{r}) \\
\phi_2(\vec{r},\sigma) &= \delta_{\sigma,\downarrow}\phi_B(\vec{r})
\end{aligned}
$$

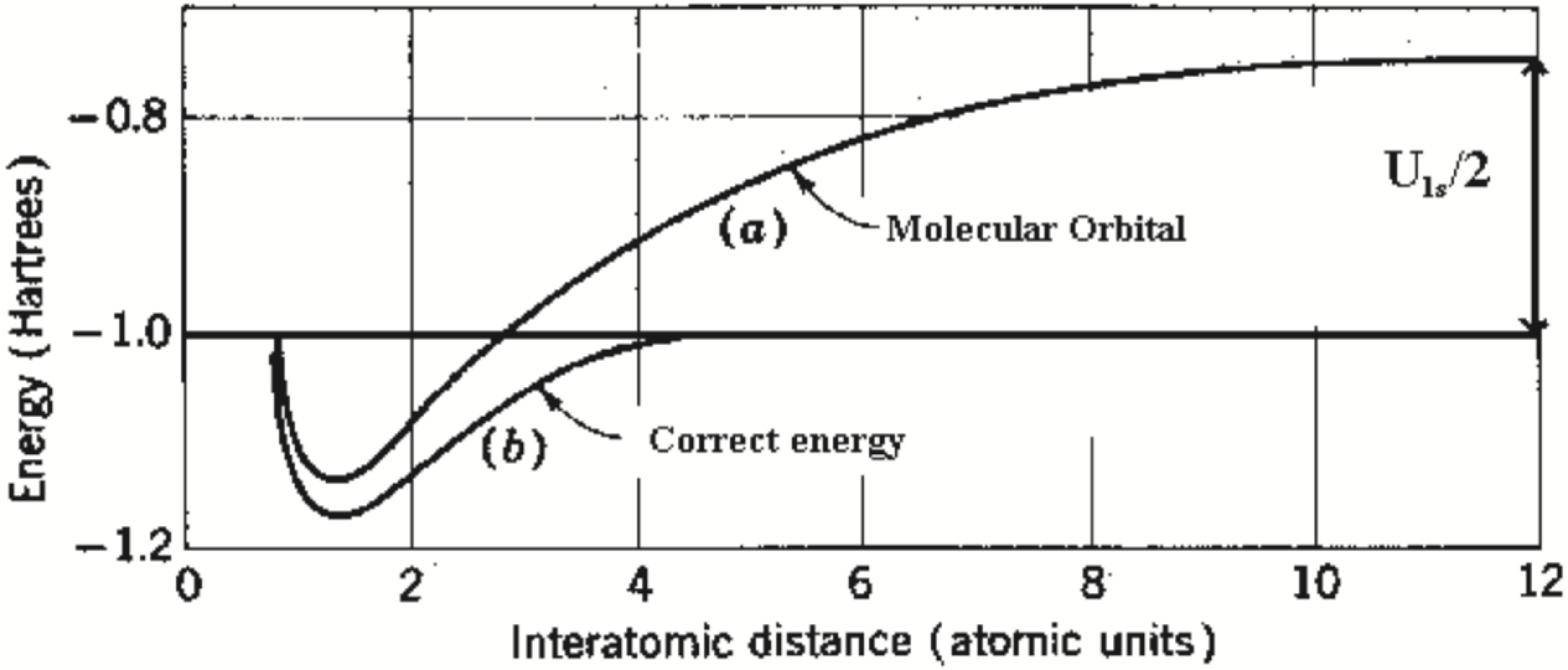


$$\Psi(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \phi_1(\vec{r}_1\sigma_1) & \phi_2(\vec{r}_1,\sigma_1) \\ \phi_1(\vec{r}_2\sigma_2) & \phi_2(\vec{r}_2,\sigma_2) \end{vmatrix} = \frac{1}{\sqrt{2}}(\delta_{\sigma_1,\uparrow}\delta_{\sigma_2,\downarrow} - \uparrow\leftrightarrow\downarrow)\phi_B(\vec{r}_1)\phi_B(\vec{r}_2)$$

Hartree-Fock: $H_{MF} = -\frac{1}{2}\nabla + V_{\text{Selfconsistent}}(\vec{r},\sigma)$ $\quad E = 2\epsilon_B - V_{Hartree} + \frac{1}{|\vec{R}_1 - \vec{R}_2|}$

$$V_{\text{Selfconsistent}}(\vec{r},\sigma) = -\frac{1}{|\vec{r}-\vec{R}_1|} - \frac{1}{|\vec{r}-\vec{R}_2|} + \int d^3\vec{r}'\,\frac{1}{|\vec{r}-\vec{r}'|}\phi_B(\vec{r}')^2$$

Disaster of Mean-Field (HF) for H_2



Why is that?

Absence of correlation for large distance $\phi_{1s}(\vec{r}) = \frac{1}{\sqrt{\pi}} \exp(-r)$

$$\phi_B(\vec{r}) = \frac{1}{\sqrt{2}} \left[\phi_{1s}(|\vec{r} - \vec{R}_1|) + \phi_{1s}(|\vec{r} - \vec{R}_2|) \right]$$

Thus the orbital part is > 0 even when both electrons are on R_1 or R_2

$$\phi_B(\vec{r}_1) \times \phi_B(\vec{r}_2) \simeq \frac{1}{2\pi} \rightarrow \text{Wrong atomic contribution}$$

How we can get a better Slater determinant?

Take the Hydrogen Hamiltonian (Slater basis) at R_a: $H_{R_a} = -\frac{1}{2}\nabla - \frac{1}{|\vec{r} - \vec{R}_a|}$

The eigenstates of H_{Ra} form a complete set and a fortiori for a=1,2, →

$$\phi_B(\vec{r}) = \sum_{i,a} c_{i,a}\phi_{i,a}(\vec{r})$$

Thus, by optimizing the coefficients c_{ia}, one can reach the best HF by large enough basis on a single atom, e.g.: 1s2s2p3s3p3d….

Similar arguments hold for Gaussian (GTO) basis:

$$\phi_{ia}(\vec{r}) = \begin{cases} Y_{l_i m_i}(\vec{n}) \; \exp(-Z_i|\vec{r}-\vec{R}_a|) & STO \\ Y_{l_i m_i}(\vec{n}) \; \exp(-Z_i|\vec{r}-\vec{R}_a|^2) & GTO \end{cases}$$

where $\vec{n} = (\vec{r}-\vec{R}_a)/|\vec{r}-\vec{R}_a|$ and Y_{lm} are spherical harmonics (in their standard real form adopted in TurboRVB)

But the same problem remains … clearly.

Better than mean field for H_2?

The exact ground state of H_2 is a singlet:

$$\Psi(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2) = \frac{1}{\sqrt{2}}(\delta_{\sigma_1,\uparrow}\delta_{\sigma_2,\downarrow} - \uparrow\leftrightarrow\downarrow)g(\vec{r}_1,\vec{r}_2)$$

where g is the so called "geminal function" $g(\mathbf{r}_1,\mathbf{r}_2)=g(\mathbf{r}_2,\mathbf{r}_1)$

if $g(\vec{r}_1,\vec{r}_2) = \phi_B(\vec{r}_1)\times\phi_B(\vec{r}_2)$ we have the HF, but we can do much better

Geminal power

Basis :

$$\phi_{1,1} = \frac{1}{\sqrt{\pi}} \exp(-|\vec{r} - \vec{R}_1|)$$

$$\phi_{1,2} = \frac{1}{\sqrt{\pi}} \exp(-|\vec{r} - \vec{R}_2|)$$

Bonding: $\phi_B = \frac{1}{\sqrt{2}}(\phi_{11} + \phi_{1,2})$

Antibonding: $\phi_A = \frac{1}{\sqrt{2}}(\phi_{11} - \phi_{1,2})$

$$\begin{aligned} g_{HF}(\vec{r}_1, \vec{r}_2) &= \frac{1}{2}(\phi_{1,1} + \phi_{1,2})(\vec{r}_1) \times (\phi_{1,1} + \phi_{1,2})(\vec{r}_2) \\ &= \frac{1}{2}(\phi_{1,1}(\vec{r}_1)\phi_{1,2}(\vec{r}_2) + \vec{r}_1 \leftrightarrow \vec{r}_2) \\ &+ \xcancel{\frac{1}{2}(\phi_{1,1}(\vec{r}_1)\phi_{1,1}(\vec{r}_2) + \phi_{1,1}(\vec{r}_2)\phi_{1,2}(\vec{r}_2))} \end{aligned}$$

← Heitler-London

← Unwanted atomic

What does it mean?

We have the freedom to change each coefficient in the atomic basis expansion:

$$g(\vec{r}_1, \vec{r}_2) = \sum_{ia,jb} \lambda_{ia,jb} \phi_{ia}(\vec{r}_1) \phi_{jb}(\vec{r}_2)$$ ← Localized STO/GTO exp.

Provided the matrix λ is symmetric, i.e. by diagonalizing it:

$$g(\vec{r}, \vec{r}') = \sum_{I} \lambda_I \phi_I(\vec{r}) \phi_I(\vec{r}')$$

Molecular orbital expansion:

$$\phi_I = \sum_{ia} c^I_{ia} \phi_{ia}$$

e.g. For Heitler-London $\lambda_1 = \lambda_2 = 1 \ \phi_1 = \phi_A \ \phi_2 = \phi_B$

Hydrogen: one electron problem

$$\Psi(\vec{r}\sigma) = R_{nl}(r)Y_{lm}(\theta,\phi)$$

$$R_{nl} = \frac{\chi_{nl}(r)}{r}$$

$$\begin{aligned} H_l &= -\frac{1}{2m}\partial_r^2 - Z/r + \frac{l(l+1)}{2mr^2} \\ (H_l\chi_{nl})(r) &= E_n\chi_{nl}(r) \end{aligned}$$

Exact solution for small r distance

$$H_l = -\frac{1}{2m}\partial_r^2 - Z/r + \frac{l(l+1)}{2mr^2} + U(r)$$

$$\chi_{nl}(r) = Cr^{l+1}(1 + Ar + O(r^2))$$

$$A = -\frac{Zm}{1+l}$$

Universal independent of U(r), if $\lim rU(r) \to 0$

Cusp conditions (exact for any eigenstate)

Electron-ion:

$$\frac{\Psi(\cdots \vec{r}_i \simeq \vec{R}_J \cdots)}{\Psi(\cdots \vec{r}_i = \vec{R}_J \cdots)} = 1 - Z_J|\vec{r}_i - \vec{R}_J| + O(|\vec{r}_i - \vec{R}_j|^2)$$

Electron-electron:

$$\frac{\Psi(\cdots \vec{r}_i \simeq \vec{r}_j \;\sigma_i = -\sigma_j \cdots)}{\Psi(\cdots \vec{r}_i = \vec{r}_j \;\sigma_i = -\sigma_j \cdots)} = 1 + \frac{1}{2}|\vec{r}_i - \vec{r}_j| + O(|\vec{r}_i - \vec{r}_j|^2)$$

The Jastrow factor

$$J(\vec{r}_1,\sigma_1,\vec{r}_2\sigma_2,\cdots\vec{r}_i\sigma_i\cdots\vec{r}_j\sigma_j\cdots\vec{r}_{N_e}\sigma_{N_e}) = +J(\vec{r}_1,\sigma_1,\cdots\vec{r}_j\sigma_j\cdots\vec{r}_i\sigma_i\cdots\vec{r}_{N_e}\sigma_{N_e})$$

$$\begin{aligned}\Psi(\vec{x}) &= J(\vec{x}) \times \Psi_{MF}(\vec{x}) \\ \vec{x} &= (\vec{r}_1\sigma_1,\vec{r}_2\sigma_2,\cdots,\vec{r}_{N_e}\sigma_{N_e})\end{aligned}$$

The simplest Jastrow

$$
\begin{aligned}
J(\vec{x}) &= J_1(\vec{x})J_2(\vec{x}) \\
J_1(\vec{x}) &= \exp\left[\sum_{I=1}^{N} u_{ei}(\vec{r}_i)\right] \\
J_2(\vec{x}) &= \exp\left[\sum_{i<j} u_{ee}(|\vec{r}_i - \vec{r}_j|)\right] \\
u_{ei}(\vec{r}) &= -\sum_{I} Z_I \frac{|\vec{r} - \vec{R}_I|}{1 + a|\vec{r} - \vec{R}_I|} \\
u_{ee}(r) &= \frac{r}{2(1 + br)}
\end{aligned}
$$

How to compute the expectation value on $J|\Psi_{MF}\rangle$?

$$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2) = \frac{1}{\sqrt{2}}(\delta_{\sigma_1,\uparrow}\delta_{\sigma_2,\downarrow} - \delta_{\sigma_1,\downarrow}\delta_{\sigma_2,\uparrow})J_1(\vec{x})J_2(\vec{x})g(\vec{r}_1, \vec{r}_2$$

$$g(\vec{r}_1, \vec{r}_2) = \phi_B(\vec{r}_1)\phi_B(\vec{r}_2) \quad \text{Slater determinant}$$

$$g(\vec{r}_1, \vec{r}_2) = \sum_{ia,jb} \lambda_{ia,jb}\phi_{ia}(\vec{r}_1)\phi_{jb}(\vec{r}_2) \quad \text{better than above}$$

On a mesh already impossible for N=2, e.g
on a mesh 512^3 we have 512^6=144Pbyte (!)

Instead of taking the product of single particle function (leading to the Slater determinant) take the most generic two spin-1/2 fermion wf:

$$g(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2) = -g(\vec{r}_2\sigma_2,\vec{r}_1\sigma_1)$$

Consider the product of N/2 electron pairs :

$$\Psi(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2,\cdots\vec{r}_N\sigma_N) = \mathcal{A}\prod_{i=1}^{N/2} g(\vec{r}_i\sigma_i,\vec{r}_{i+N/2}\sigma_{i+N/2})$$

= The Pfaffian of the NxN skew matrix: $M_{ij} = g(\vec{r}_1\sigma_i,\vec{r}_j\sigma_j)$ i.e. N^3 flops

[1] M. Bajdich, L. Mitas et. al. PRB 77, 115112 2008

In most cases the Pfaffian → Determinant

AGPs:

$$g(\vec{r}_i\sigma_i, \vec{r}_j\sigma_j) = g_S(\vec{r}_i, \vec{r}_j)\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

AGPu:

$$g(\vec{r}_i\sigma_i, \vec{r}_j\sigma_j) = g_S(\vec{r}_i, \vec{r}_j)\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} + g_T(\vec{r}_i, \vec{r}_j)\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$$

The ''unavoidable Pfaffian''

$$\begin{aligned} g(\vec{r}_i\sigma_i,\vec{r}_j\sigma_j) &= g_S(\vec{r}_i,\vec{r}_j)\frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}+g_T(\vec{r}_i,\vec{r}_j)\frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}} \\ &+ g_{T\uparrow}(\vec{r}_i,\vec{r}_j)|\uparrow\uparrow\rangle+g_{T\downarrow}(\vec{r}_i,\vec{r}_j)|\downarrow\downarrow\rangle \end{aligned}$$

When parallel spins correlations matter → Pfaffian is necessary

We will see that in C_2 these correlations are unexpectedly important

And this applies to the realistic electronic Hamiltonian…:

$$H = -\sum_i \frac{\Delta_i}{2} - \sum_{ij} \frac{Z_j}{|\vec{r}_i - \vec{R}_j|} + \sum_{i<j} \frac{1}{|\vec{r}_i - \vec{r}_j|} + \frac{Z_i Z_j}{|\vec{R}_i - \vec{R}_j|}$$

All mean-field states can be written in terms of a pairing function g and Pfaffian (antisym)

$\{R_i\}$ are atomic classical coordinates within the Born-Oppenheimer approximation

$$\langle \vec{r}_1, \vec{r}_2, \vec{r}_3 \cdots \vec{r}_N | J | \mathrm{MF} \rangle = \exp\left[\sum_{i<j} u(\vec{r}_i, \vec{r}_k)\right] Pf[g(\vec{r}_i, \vec{r}_j)]$$

Two-el. Jastrow (symmetric)

Given that, one can apply **Variational Monte Carlo** and compute all correlation functions by a statistical method

The general J|MF>

No further approximation required fully ab-initio (no U, no double counting)

We use a localized basis set for both u and g

$$g(\vec{r}\sigma,\vec{r}'\sigma') = \sum_{ia,jb} \lambda^{\sigma,\sigma'}_{ia,jb}\phi_{ia}(\vec{r})\phi_{ib}(\vec{r}')$$

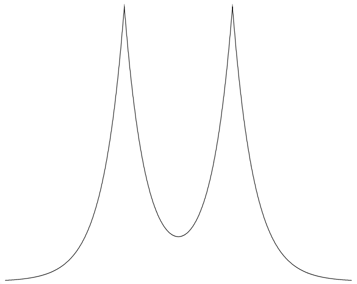
$$u(\vec{r}\sigma,\vec{r}'\sigma') = \sum_{ia,jb} J^{\sigma,\sigma'}_{ia,jb}\phi_{ia}(\vec{r})\phi_{ib}(\vec{r}') + u^{\sigma,\sigma'}_{ee}(|\vec{r}-\vec{r}'|) + u_{ei}$$

A huge number of parameters such that:

$$\begin{aligned} J^{\sigma,\sigma'}_{ia,jb} &= J^{\sigma',\sigma}_{jb,ia} \\ \lambda^{\sigma,\sigma'}_{ia,jb} &= -\lambda^{\sigma',\sigma}_{jb,ia} \end{aligned}$$

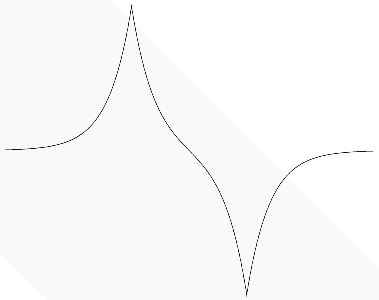
Consider the H dimer in a gas of many ones:

$1\sigma_g$



Bonding orbital

$1\sigma_u$



Antibonding orbital

The pairing function is $1\sigma_g(r)1\sigma_g(r') - 0.25 \;\; 1\sigma_u(r)1\sigma_u(r')$

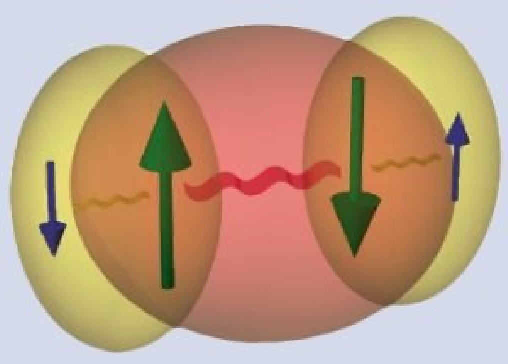
But can accommodate 4 electrons per dimer!

The Jastrow can remove these crazy charge +4

Resonating valence bond (RVB)

In this theory the chemical valence bond is described as a singlet pair of electrons

$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)\left[\Psi_a(r)\Psi_b(r') + a \leftrightarrow b\right]$$



spin up and spin down electrons in a spin singlet state
a and *b* are nuclear indexes

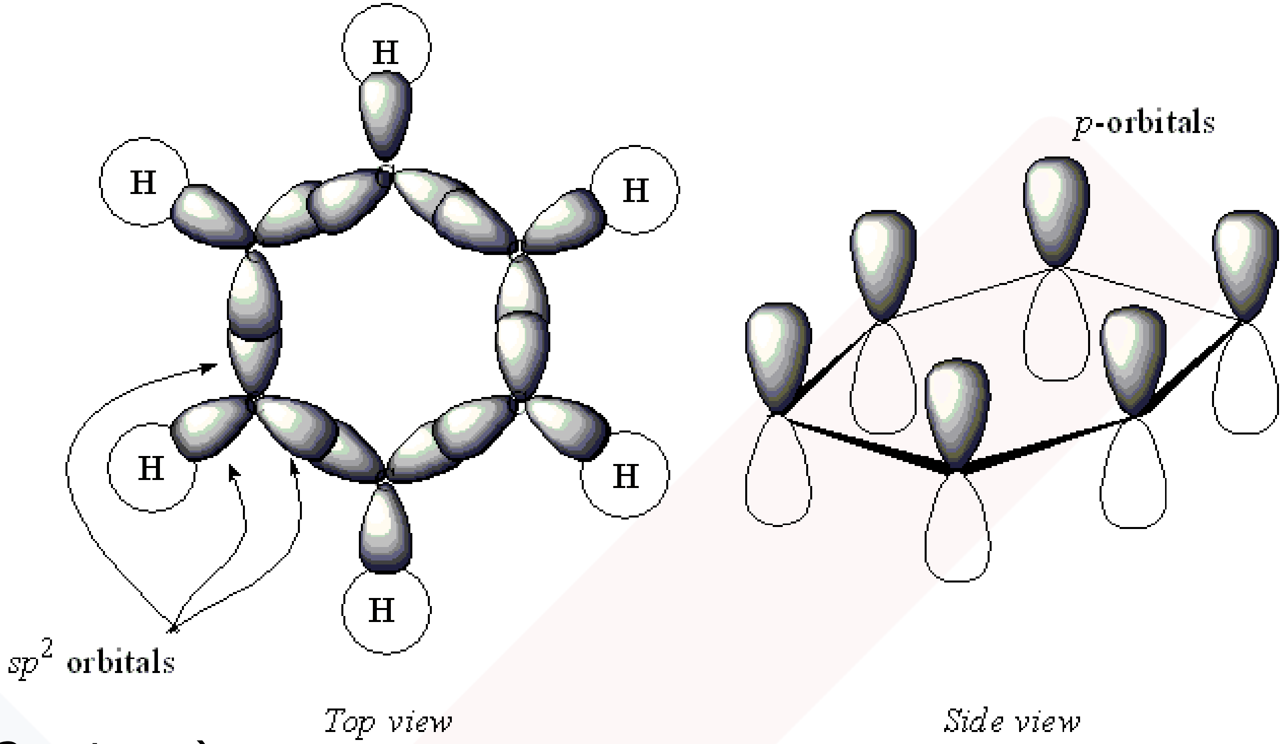
Linus Pauling

The true quantum state of a compound is a superposition or resonance of many valence bond states. The superposition usually improves the variational energy of the state.

L. Pauling, Phys. Rev. **54**, 899 (1938)

Example of RVB

Benzene C_6H_6



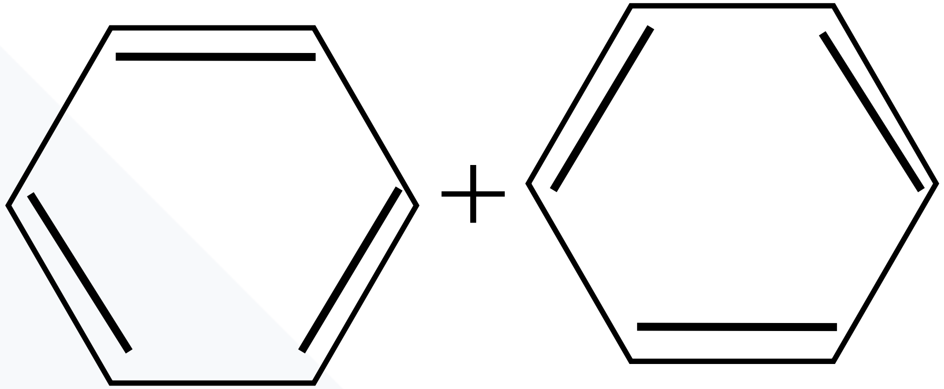
6 valence electrons in 6 sites ($2p_z$ type)
two ways to arrange nearest neighbor bonds (Kekule' states)

The rule: two singlet bonds cannot overlap on the same Carbon atom otherwise two electrons feel a too large Coulomb repulsion.

The Jastrow can make this job as a generic u can satisfy the RVB rule

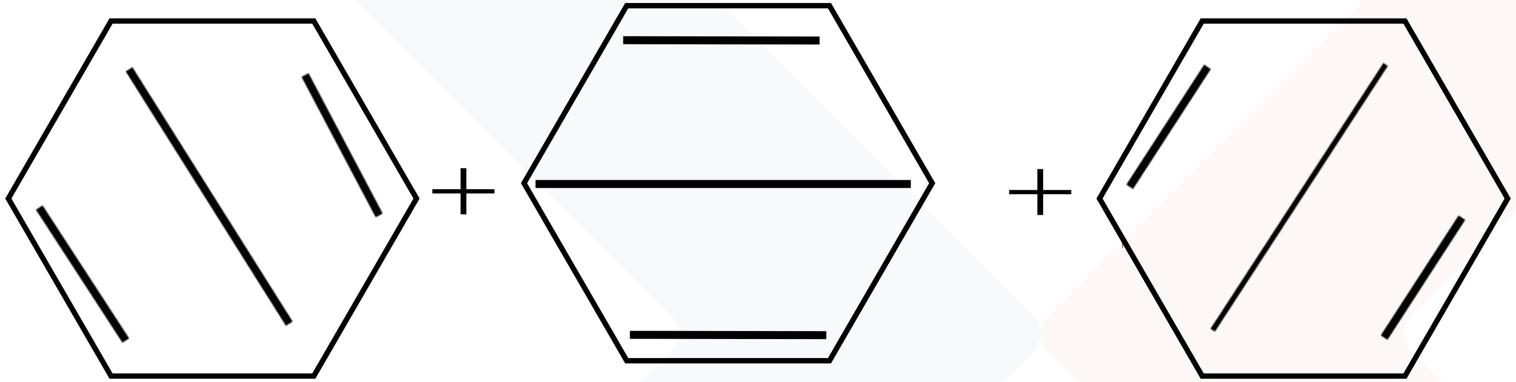
Resonating Valence Bonds in the benzene molecule

Kekule’ valence bonds



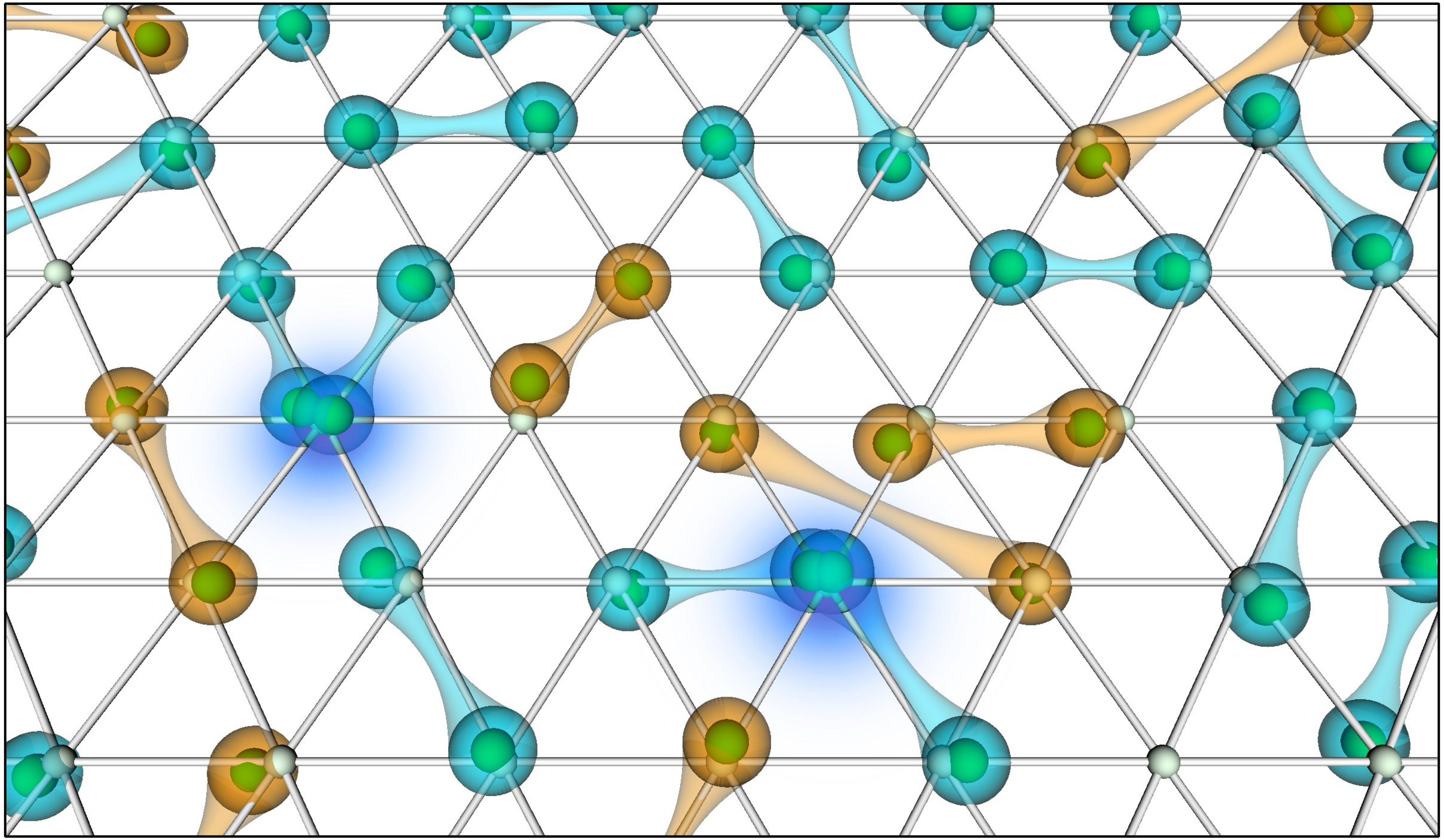
$$\rule{2em}{1pt} \;=\; \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle-\left|\downarrow\uparrow\right\rangle\right)\left[\Psi_a(r)\Psi_b(r')+a\leftrightarrow b\right]$$

Dewar valence bond (believed less important)

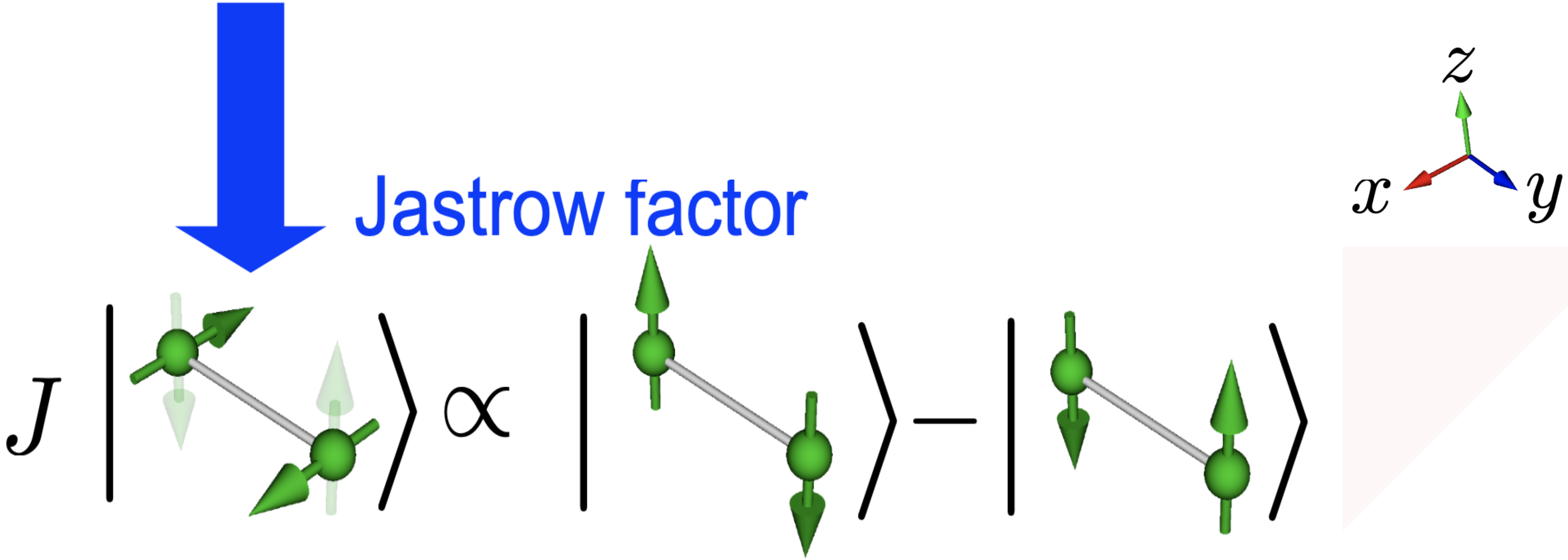


NB no next-neighbor valence bonds (frustrated)

Cartoon picture of the J|MF> wave function

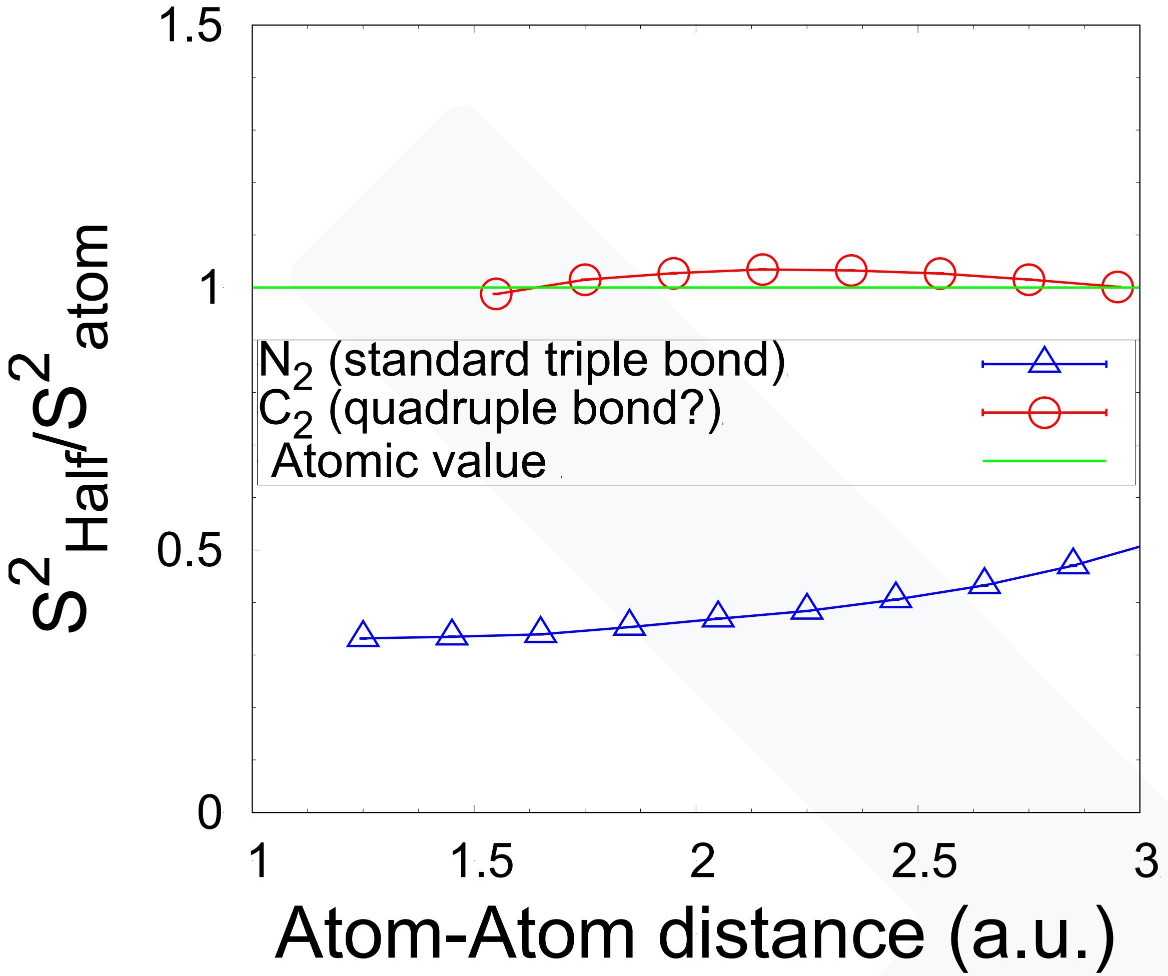


Importance of the spin Jastrow factor



Only when the spin-quantization direction of the Jastrow is not parallel to the order parameter direction spin-wave fluctuations are possible, and the correct singlet is recovered.
The exact solution of the Heisenberg model for large spin (spin-wave theory) has exactly the above form F.Franjic and S.S. Prog. Thor. Phys. **97** 399 (1997).

Atomic spin at bond distance: a key fingerprint of C_2



The atomic spin in a standard molecule Is screened and strongly reduced

In C_2 this does not occur. An extra binding is due to spin fluctuations interaction of atoms. It is hardly explained with a 4th bond picture.

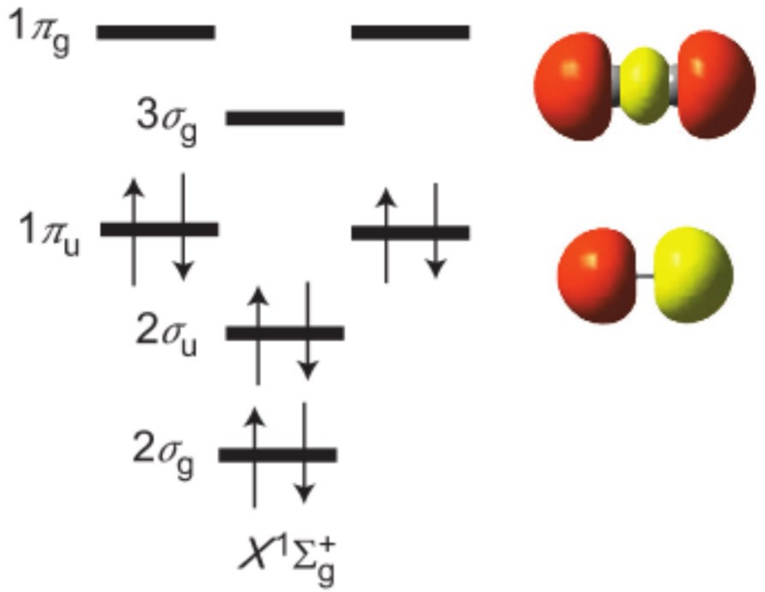
The total spin square $<S^2> \sim 0.03 \rightarrow$ small spin contamination

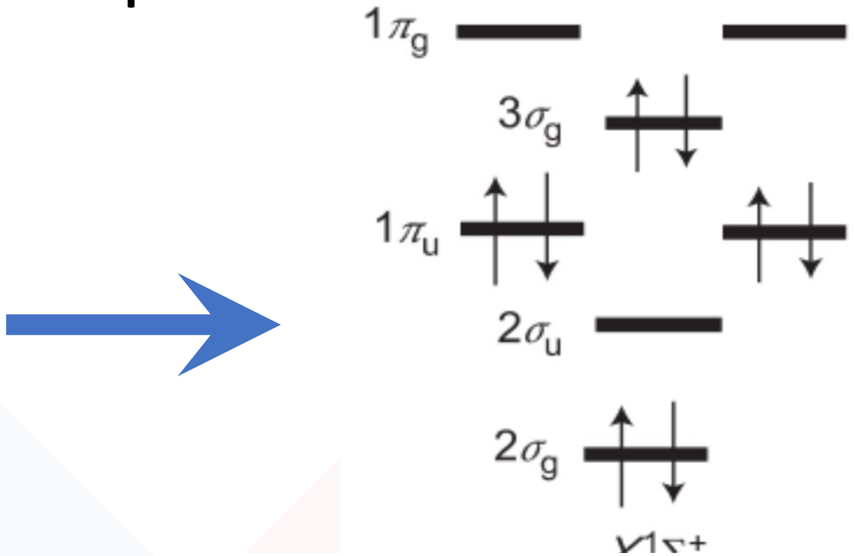
The C_2 is the smallest Néel state in nature

The proposed quadruple bond picture

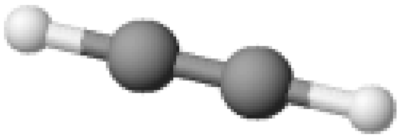
Standard double bond
π-orbitals occupied

Quadruple bond picture Shaik & al.Nat. Chem’12 ~ $3\boldsymbol{\sigma}_g$ ’’RVB’’ occupied



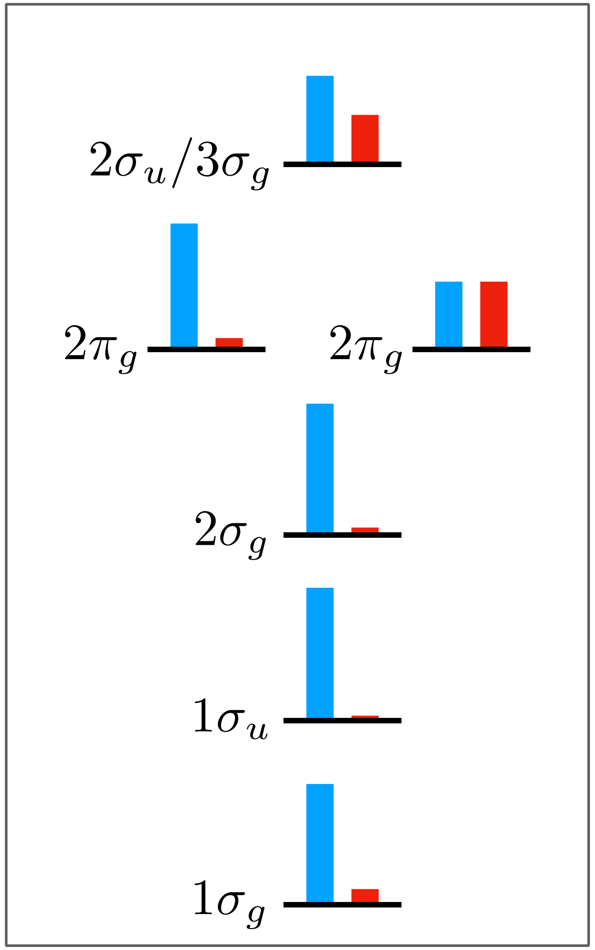


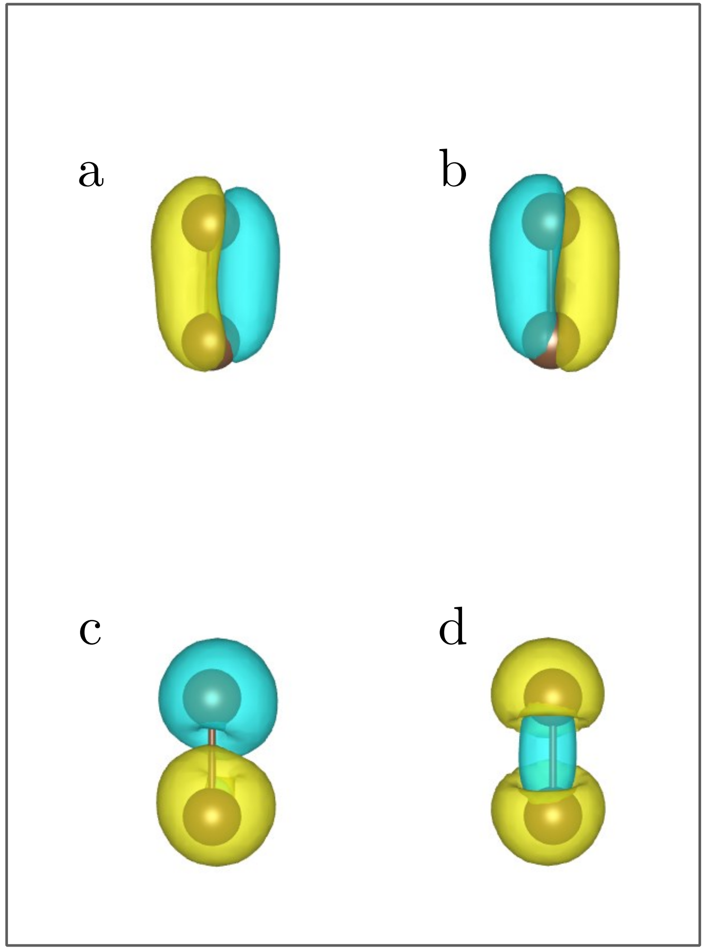
This could explain why acetilene $HC{\equiv}CH$



has smaller binding energy, but C_2 has a longer bond length.

Our molecular orbitals, by ab-initio optimization





In our picture $2\boldsymbol{\sigma}_u/3\boldsymbol{\sigma}_g$ is 65% /35% occupied→ double bond picture is ''more correct''.

The extra binding is just a correlated effect due to spin fluctuations.

This explains also why bond length is larger vs HCCH

The C_2 is the smallest Néel state in nature [C. Genovese & S. Sorella JCP **153**, 164301 (2020)]

TurboRVB

- **TurboRVB Quantum Monte Carlo package**

(just google search, or: https://people.sissa.it/~sorella)

main developers:

Sandro Sorella
Kousuke Nakano
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Leonardo Spanu

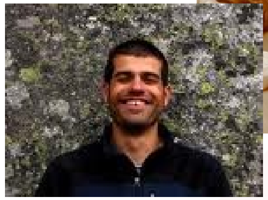
- **Funding:**

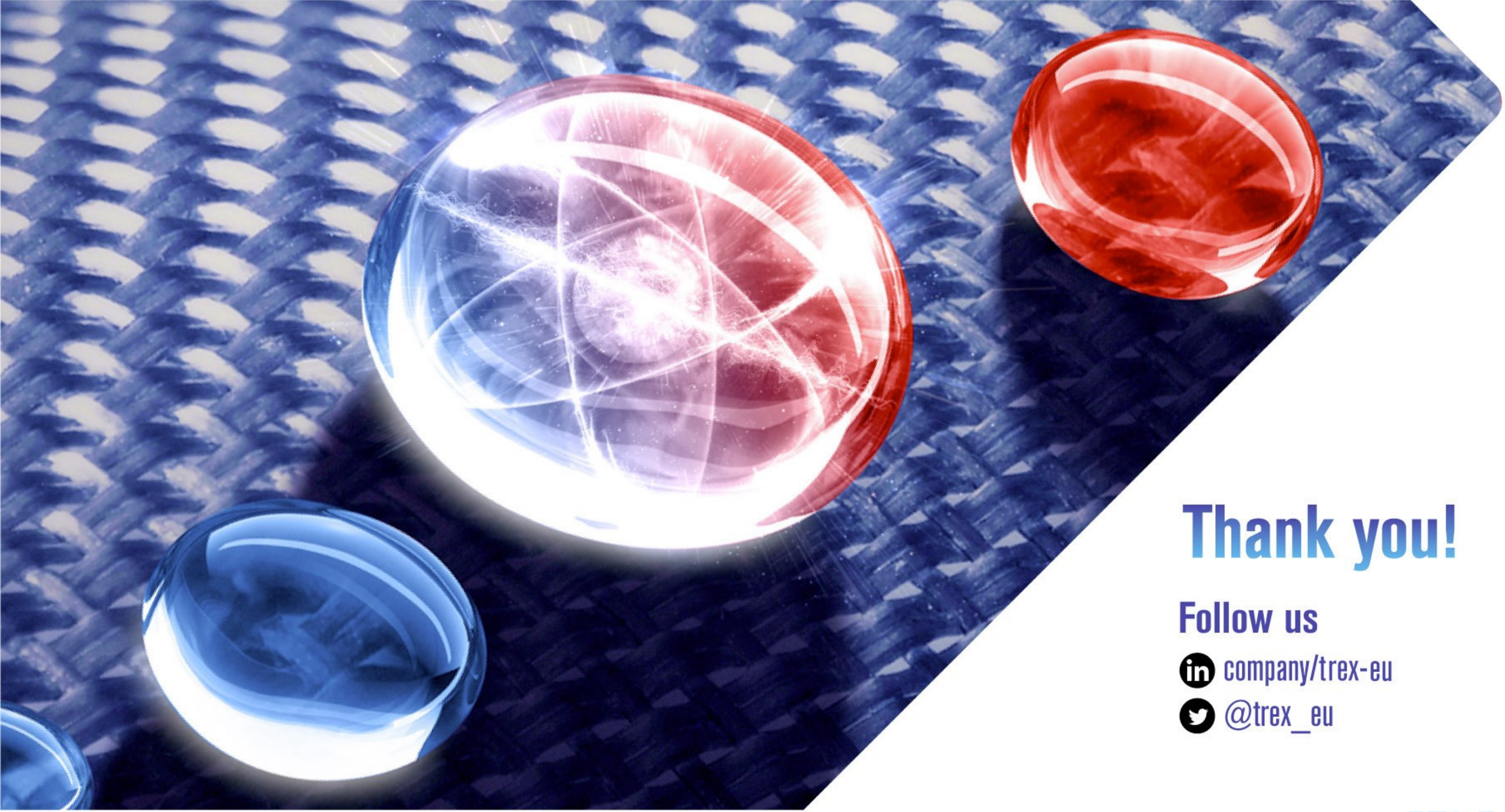
TREX, PRIN, JSPS

- **Computational support**

PRACE, CINECA Bologna
Fugaku Japan
SISSA





Thank you!

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