

BETWEEN INTEGRABILITY

$$H = \sum_{\alpha\beta} \langle \alpha | H_0 | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} + \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta}$$

traditionally. build the Hilbert space from yr excitations
 remaining volume: go the other direction: paired states first

why: | nuclear: plot (E_n) neutron separation energies
 | chemical: kondo pairs. coffee.

In both cases, ~~pp~~ pairs are strongly correlated

$$H_{\text{non}} = \sum_i \langle i | H_0 | i \rangle (a_i^{\dagger} a_i + a_i^{-\dagger} a_i^{-}) + \sum_{i\neq j} \langle i | V | j \rangle a_i^{\dagger} a_i^{-} a_j^{-} a_j + \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} + \text{other} \dots$$

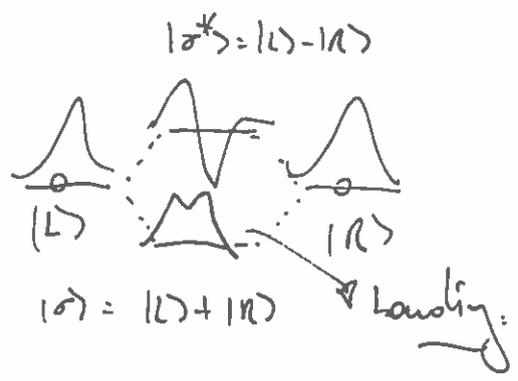
$$H_{\text{non}} = \sum_i \epsilon_i (M_i + M_i^{-}) + \sum_{ij} V_{ij} S_i^{\dagger} S_j + \sum_{\alpha\beta} W_{\alpha\beta} M_{\alpha} M_{\beta}$$

In both cases, pairs are strongly correlated.

nuclear: collective pair correlations \rightarrow Cooper pairs
chemistry: hard 'static' correlations: handing/unhanded around the Fermi surface

CHEMISTRY

H_2



$$|R\rangle = \alpha |\sigma\sigma\rangle + \beta |\sigma^*\sigma^*\rangle$$

when $R \sim R_0$: $|\alpha| \gg |\beta|$

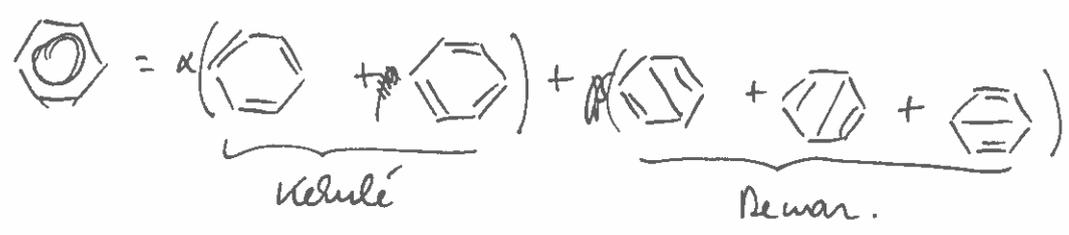
when $R \rightarrow \alpha$: $\beta = -\alpha$

→ chemists have been looking for the "mean-field" structure in terms of pairs instead of electrons.

→ GEMINALS

$$|G\rangle = \sum_{\alpha=1}^N \left(\sum_{\beta \neq \alpha} G_{\alpha\beta} s_{\alpha}^{\dagger} s_{\beta}^{\dagger} \right) |0\rangle$$

→ partially abandoned because of $\langle i, i \dots i | G \rangle = \text{per}(G)$.
 → partially recovered in valence bond theory.

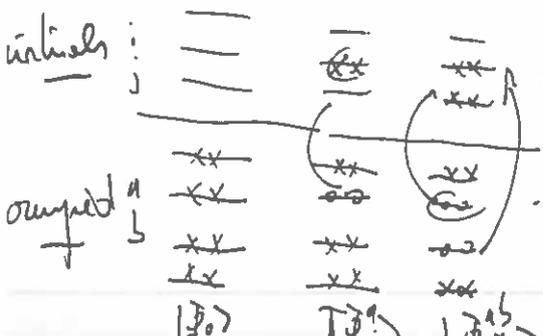


→ Inspired by Richardson: do we have ~~off~~ ~~more~~ horrible geminals?

Richardson: for chemistry? ~~no~~ ~~not~~ The Richardson GS is made for collective pairing, not $(s_{\alpha}^{\dagger} - s_{\alpha'}^{\dagger}) |0\rangle$.

other methods? pSE: projected Schrödinger equation: solve w/ ss configurations that are important

define: $|T_0\rangle = \prod_{j=1}^N s_j^{\dagger} |0\rangle$ (filling up the vacuum).



$$|T_1^a\rangle = s_a^{\dagger} \prod_{j \neq i} s_j^{\dagger} |0\rangle$$

$$|T_2^{ab}\rangle = s_a^{\dagger} s_b^{\dagger} \prod_{j \neq i, a} s_j^{\dagger} |0\rangle$$

NUCLEAR:

Richardson is approximately good

Sm isotopes: Woods Saxon + $g = - \frac{2.5 \text{ MeV}}{A}$

What about more realistic interactions?

→ ~~the~~ G-matrix pairing interactions \hat{H} Zeldovich ^{PAN} Phys. At. Nucl. 66 1281 (2003)

$$H = \sum_k \epsilon_k n_k - \sum_{jk} G_{jk} S_j^\dagger S_k$$

↳ non-integrable

$$G_{jk} = -V_0(jk) \frac{1}{((2j+1)(2k+1))}$$

(*) we RG state as variational input:

$$E[g] = \langle RG(g) | H | RG(g) \rangle$$

$$\rightarrow E = \min_g E[g]$$

$\overset{116}{S_M}$

→ (*) we G-matrix for ϵ_j

(*) we $|RG(g)\rangle$ from solution of

$$H_{\text{res}} = \sum_j \epsilon_j n_j + g \sum_j S_j^\dagger S_j$$

(*) minimise $E[g]$ under constraint of on the manifold of integrable systems

$$E = \langle \psi_{\alpha} | H | \psi_{\alpha} \rangle - \sum_{\alpha=1}^N \lambda_{\alpha} R_{\alpha}(\psi_{\alpha}) (\psi_{\alpha})$$

$$\frac{\partial E}{\partial \lambda_{\alpha}} = 0 \quad \frac{\partial E}{\partial g} = 0 \quad \frac{\partial E}{\partial \alpha} = 0$$

(*1) In practice, sleep at descent

(*1) It is also possible to take ϵ_j as variational parameters

(*1) Add basis states $|RG_i\rangle$ $i=2 \dots$ dim of \mathcal{R} until convergence

find energy at $\epsilon_1, \epsilon_2, \dots$

$$\begin{pmatrix} \langle RG_1 | H | RG_1 \rangle & \langle RG_1 | H | RG_2 \rangle & \dots \\ \langle RG_2 | H | RG_1 \rangle & \langle RG_2 | H | RG_2 \rangle & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Q: what about gem shells? (minimally broken states?)

→ PT (MRPT ~~!!!!~~): you only have one?

→ Include refined sensitivity states?

- CC? (power are pCCD)

- higher order alphas? : $so(5)$

$$so(5) \begin{cases} S_{\pi}^{\pm} = \tilde{p}^{\pm} p^{\pm} & S_{\eta} = pp & S_{\eta}^0 = \frac{1}{2} pp \\ S_{\nu}^{\pm} = m^{\pm} m^{\pm} & S_{\nu} = mm & S_{\eta}^0 = \frac{1}{2} mm \\ T_{\pm}^{\pm} = m^{\pm} p & T^{\pm} = p^{\pm} m & S_{\pi\nu}^{\pm} = p^{\pm} m^{\pm} & S_{\pi\nu} = mp \end{cases}$$

