Integrable Richardson-Gaudin bases for pairing Hamiltonians

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Computational Challenges in Nuclear and Many-Body Physics
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The collaboration

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  (Department of Physics & Astronomy, Ghent University)
- Patrick Bultinck
  (Department of Inorganic and Physical chemistry, Ghent University)
- Paul Johnson, Peter Limacher, Paul Ayers, Katharina Boguslawski, PawełTecmer
  (Department of Chemistry, McMaster University)
- Jean-Sébastien Caux, Rianne van den Berg
  (Institute for Theoretical Physics, University of Amsterdam)
- Veerle Hellemans (Department of Physics, Université Libre de Bruxelles)

1 Pairing
- The quantum many-body problem
- Pairing

2 Integrability
- Richardson
- for Sn isotopes
- Gaudin

3 ...& beyond
- The quantum many-body problem revisited
- Richardson-Gaudin basis
- inspired by integrability

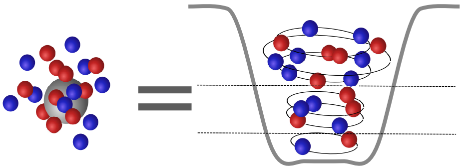
4 Outlook and conclusions
- Conclusions
- Acknowledgments

Configuration Interaction

- Bound systems can be embedded within a mean field

$$\hat{H} = \sum_{i=1}^{N} [\hat{T}_i + V_m(r_i)] + [\sum_{i<j}^{N} V(r_i, r_j) - \sum_{i=1}^{N} V_m(r_i)] = \sum_{i=1}^{N} \hat{H}_i + \sum_{i<j}^{N} V_{res}(r_i, r_j)$$

- The Hilbert space is spanned by all possible single-particle Slater determinants
- Residual interactions are treated in active valence space



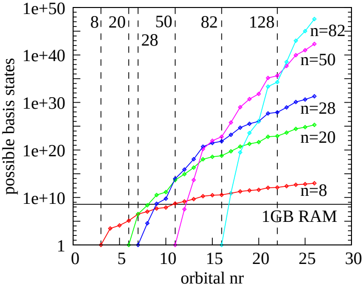
Dimensions of the Configuration Interaction

dimensions

- Full Space calculations are extremely resource demanding
- Dimensions scale exponential at half filling

$$\dim \sim e^n$$

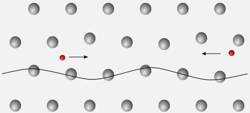
- Truncations are necessary



Origin of pairing

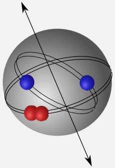
- Capture the dominant correlations in the system
- Pairing correlations are ubiquitous

Superconductivity



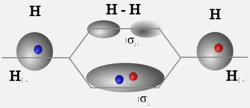
electron-phonon coupling

Nuclear Structure



short-range interactions

Molecular Structure



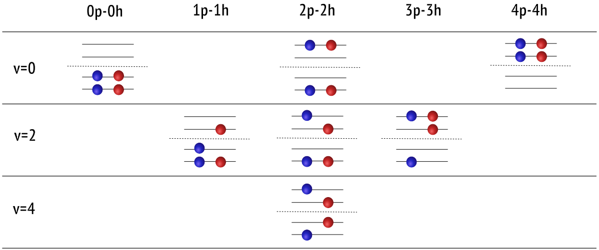
bonding-antibonding

Hierarchy by Seniority

- Hamiltonian can be reordered wrt seniority ($v = 0, 2, 4$)

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{ik}^{v=0} V_{i\bar{i}k\bar{k}} a_i^\dagger a_{\bar{i}}^\dagger \tilde{a}_k \tilde{a}_{\bar{k}} + \sum_{i \neq j, k}^{v=2} V_{ijk\bar{k}} (a_i^\dagger a_j^\dagger \tilde{a}_k \tilde{a}_{\bar{k}} + h.c.) + \ldots$$

- seniority : number of particles *not* coupled pairwize together
- $\{S_i^\dagger, S_i, S_i^0\} = \{a_i^\dagger a_{\bar{i}}^\dagger, \tilde{a}_i \tilde{a}_{\bar{i}}, \frac{1}{2}(n_i + n_{\bar{i}} - 1)\}$ span $su(2)$ quasi-spin algebra

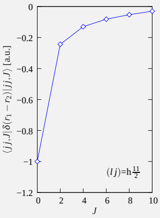


Pairing for spherical nuclei

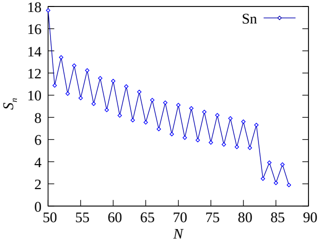
The interaction can be developed in a total angular momentum J expansion

$$\hat{H} = \sum_a \varepsilon_a \hat{n}_a + \frac{1}{4}\sum_J \sum_{abcd} \langle ab, JM|V|cd, JM\rangle [a^\dagger_{j_a} a^\dagger_{j_b}]^{(J)} \cdot [\tilde{a}_{j_c}\tilde{a}_{j_d}]^{(J)}$$

short-range interaction



- $J = 0$ dominance
- DOCI : keep only $v = 0$
  Doubly Occupied CI
- $\dim \mathcal{H}(v=0) \sim e^{N/2}$
- separation energies



DOCI in molecular systems

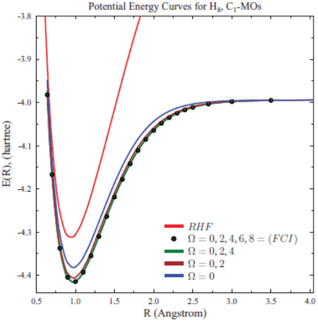
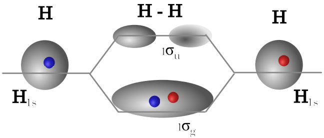


FIG. 3. Potential energy curves ([1]A-ground state) for the symmetric dissociation of H_8 molecule using CAS[8/8] active space and cc-pVDZ basis sets with symmetry-broken molecular orbitals. The $\Omega = 0,2,4,6,8$ case represents FCI≡CASSCF[8/8].



- seniority scheme is beneficial for *strong static* correlations. ✎
- DOCI : keep only $v = 0$
- orbital optimizations are crucial ✍
- $\dim \mathcal{H}(v = 0) \sim e^{N/2}$

✎ L. Bytautas, T. M. Henderson, C. A. Jiménez-Hoyos, J. K. Ellis, and G. E. Scuseria (2011) J. Chem. Phys. 135, 0441199

✍ P. A. Limacher, T. D. Kim , P. W. Ayers, P. A. Johnson, sdb, D. Van Neck, and P. Bultinck (2013) Mol. Phys. 112, 853

Richardson Hamiltonian

- schizophrenic Hamiltonian: *reduced* BCS, *Richardson*, *rational*, *s-wave* pairing, *level-independent* pairing, *simplified* pairing, *pure* pairing, etc. ... Hamiltonian
- (over)simplified & schematic

$$H = \sum_{i=1}^{m} 2\varepsilon_i S_i^0 + g \sum_{ij=1}^{m} S_i^\dagger S_j$$

- m mutually independent $su(2)$ quasi-spin algebras

$$\{S_i^\dagger, S_i, S_i^0\} = \{a_i^\dagger a_{\bar{i}}^\dagger, a_{\bar{i}} a_i, \tfrac{1}{2}(n_i + n_{\bar{i}} - 1)\}$$

- m free parameters, plus scale.

Richardson's solution for the pairing problem

- The reduced BCS Hamiltonian is known to be exactly solvably
- The Hamiltonian can be diagonalised using a Bethe Ansatz wavefunction

$$|\psi\rangle = \prod_{\alpha=1}^{N} S^\dagger_\alpha |\theta\rangle \qquad \text{with} \qquad S^\dagger_\alpha = \sum_i \frac{S^\dagger_i}{2\varepsilon_i - E_\alpha}$$

- provided the parameters E_α fullfill the

Richardson-Gaudin (RG) equations

$$1 - 2g \sum_{i=1}^{m} \frac{\frac{1}{2}v_i - \frac{1}{4}\Omega_i}{2\varepsilon_i - E_\alpha} - 2g \sum_{\beta\neq\alpha}^{N} \frac{1}{E_\beta - E_\alpha} = 0 \qquad (\forall\alpha = 1\ldots N)$$

- with the eigenstate energy given by

$$E = \sum_{\alpha=1}^{N} E_\alpha + \sum_{i=1}^{k} \varepsilon_i v_i .$$

Correlated pairs

- Richardson product state

$$|\psi\rangle = \prod_{\alpha=1}^{N} \sum_{i=1}^{m} \frac{S_i^\dagger}{2\varepsilon_i - x_\alpha} |\theta\rangle$$

- Neutron superfluidity in Sn

  woods-saxon ε_j

  $g = -2.5\text{MeV}/\sqrt{A}$

Level (i)	(Ω_i)	Energy (ε_i)
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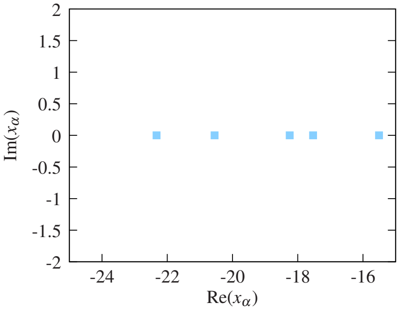

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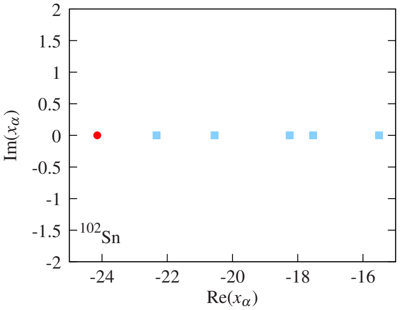

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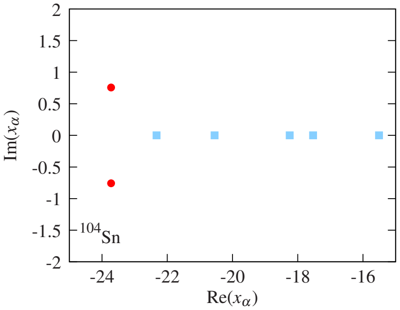

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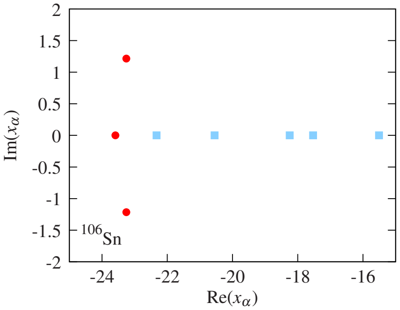

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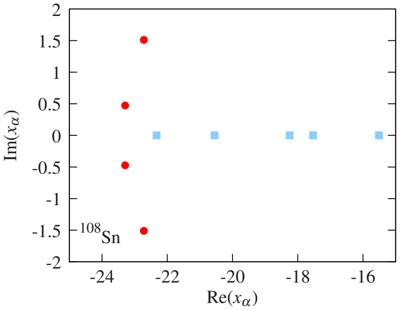

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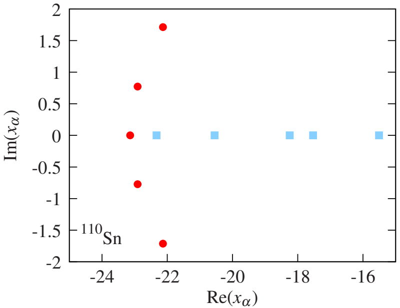

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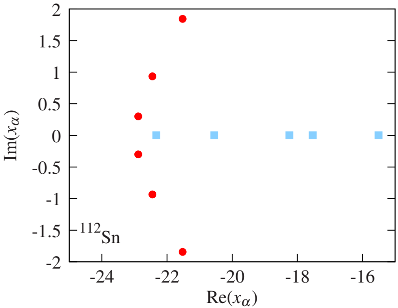

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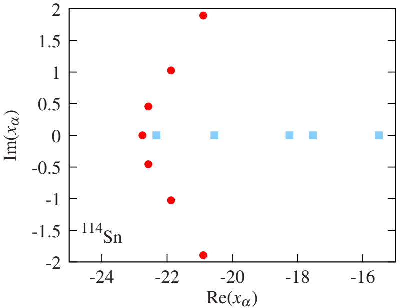

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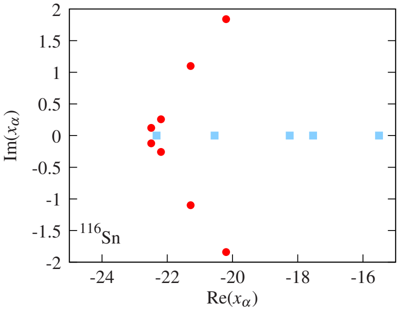

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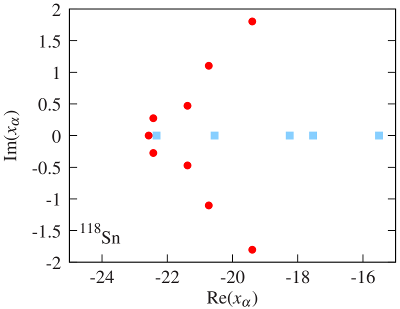

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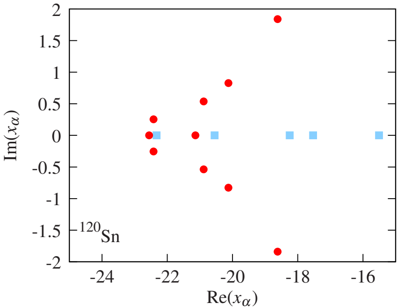

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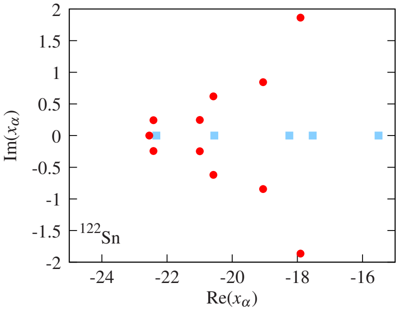

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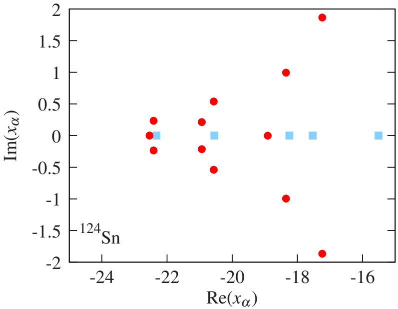

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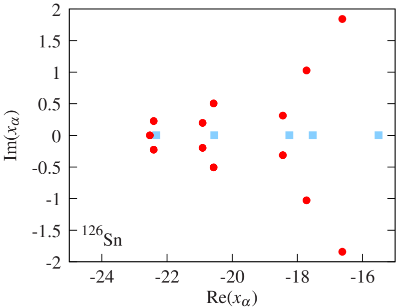

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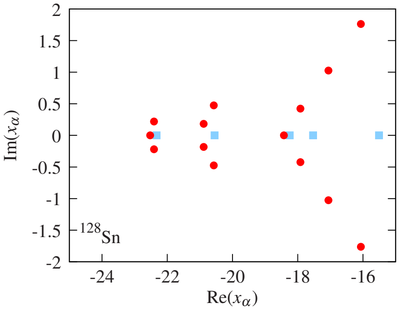

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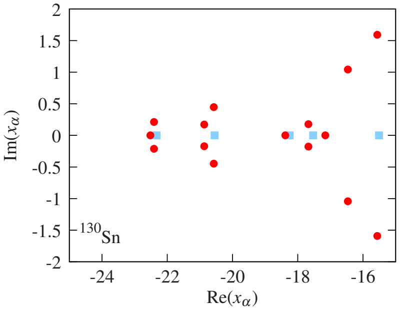

Energy observables

Eigen Energy

$$E = \sum_{\alpha=1}^{N} x_\alpha + \sum_{i=1}^{m} \varepsilon_i v_i$$

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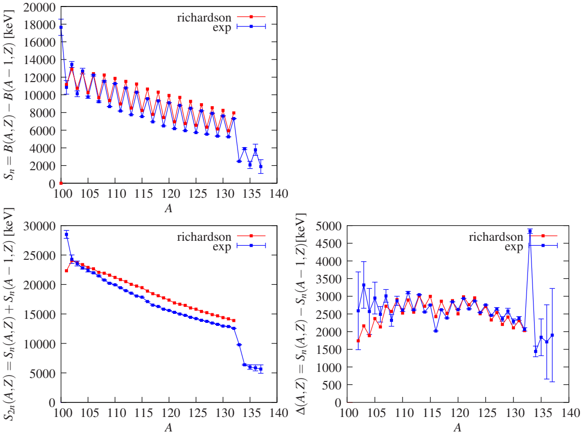


Significance of Richardson's solution

Diagonalisation

- Exact results
- Exponential scaling
- General interaction

Richardson

- Exact results
- Linear scaling
- Integrable systems

BCS

- Variational
- Linear scaling
- General interaction

What's the magic?

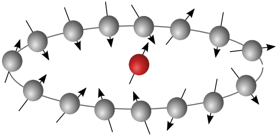
Integrable system (loose definition)

A system with m degrees of freedom is called integrable if the Hamiltonian can be written as a sum of m mutually commuting operators

$$\hat{H} = \sum_{i=1}^{m} \varepsilon_i \hat{R}_i, \qquad \text{with} \qquad [\hat{R}_i, \hat{R}_j] = 0, \quad \forall i, j = 1..m$$

- Conserved charges of the pairing problem

$$R_i = S_i^0 + \sum_{j \neq i}^{m} \frac{1}{2} X_{ij} (S_i^\dagger S_j + S_i S_j^\dagger) + Z_{ij} S_i^0 S_j^0$$



- Integrability defines Gaudin algebra ✍

$$X_{ij} X_{jk} + X_{ki} Z_{ij} + X_{ki} Z_{jk} = 0, \quad \forall ijk$$

✍ M. Gaudin, J. Phys. (Paris) **37** 1087 (1976)

What's the magic?

- Conserved charges & XXZ Gaudin algebra

$$R_i = S_i^0 + \sum_{j\neq i}^{m} \tfrac{1}{2} X_{ij}(S_i^\dagger S_j + S_i S_j^\dagger) + Z_{ij} S_i^0 S_j^0, \quad X_{ij}X_{jk} + X_{ki}Z_{ij} + X_{ki}Z_{jk} = 0$$

rational model (XXX)

- reduced BCS (Richardson)

$$X_{ij} = Z_{ij} = \frac{1}{\varepsilon_i - \varepsilon_j}$$

hyperbolic model (XXZ) ✎

- factorisable interactions

$$X_{ij} = \frac{\sqrt{\varepsilon_i \varepsilon_j}}{\varepsilon_i - \varepsilon_j}, \quad Z_{ij} = \frac{1}{2}\frac{\varepsilon_i + \varepsilon_j}{\varepsilon_i - \varepsilon_j}$$

✍ G. Ortiz, R. Somma, J. Dukelsky & S. Rombouts (2005) Nucl. Phys. B707, 421
✎ S. Rombouts, J. Dukelsky & G. Ortiz (2010) Phys. Rev. B82 224510
✎ J. Dukelsky, S. Lerma, L. Robledo, R. Rodriguez-Guzman, & S. Rombouts (2011) PRC84, 061301(R)
✎ M. Van Raemdonck, sdb, & D. Van Neck (2014), Phys. Rev. B89, 155136

A gallery of integrable systems

- Nearest-neighbour Heisenberg spin chains for quantum state transfer
  ✍ H. Bethe, Z. Phys. **71** 205 (1931)
- 1D Fermi-Hubbard model
  ✍ E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20** 1445 (1968)
- Pairing Hamiltonian
  ✍ R. W. Richardson, Phys. Lett. **3** 277 (1963)
- Jaynes-Cummings and Dicke Hamiltonians for photon-ion interactions
  ✍ M. Gaudin, J. Phys. (Paris) **37** 1087 (1976)
- *p*-wave interactions in Fermi gases
  ✍ S. Rombouts, *et. al.*, Phys. Rev. **B82** 224510 (2010)
- Proton-neutron pairing in the $SO(5)$ isovector and $SO(8)$ isoscalar channel
  ✍ J. Dukelsky, *et. al.*, Phys. Rev. Lett. **96** 072503 (2006)
- Kondo-like impurity model
  ✍ G. Ortiz, *et. al.* Nucl. Phys. **B707**, 421 (2005)
- ...

1 Pairing
- The quantum many-body problem
- Pairing

2 Integrability
- Richardson
- for Sn isotopes
- Gaudin

3 ...& beyond
- The quantum many-body problem revisited
- Richardson-Gaudin basis
- inspired by integrability

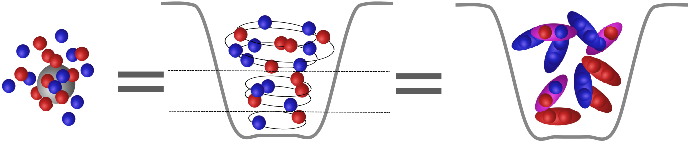
4 Outlook and conclusions
- Conclusions
- Acknowledgments

Integrable systems for non-integrable systems

- Beyond mean-field correlations are described exactly in integrable systems

$$\hat{H} = \sum_{i=1}^{N} \hat{H}_i + \sum_{i<j}^{N} [V_{res}(r_i, r_j) + V_{int}(r_i, r_j) - V_{int}(r_i, r_j)] = \hat{H}_{int} + \sum_{i<j}^{N} v_{res}(r_i, r_j)$$

- Use Bethe Ansatz wavefunctions as improved basis over Slater determinants.
- fCI, perturbation theory, Kohn-Sham DFT, projected Schrödinger formalism, coupled cluster...
- . . .



Correlation functions

Geminal states

- generalized richardson states

$$|\text{APG}\rangle = \prod_{\alpha=1}^{N} \sum_{i=1}^{m} G_{\alpha i} S_i^\dagger |\theta\rangle$$

- overlap with slater states

$$\langle \text{Slater}|\text{APG}\rangle = \text{Per}(G)$$

- factorial scaling

Richardson states

- special geminal states

$$|\text{RG}\rangle = \prod_{\alpha=1}^{N} \sum_{i=1}^{m} \frac{S_i^\dagger}{2\varepsilon_i - x_\alpha} |\theta\rangle$$

- overlap with slater states (Borchardt)

$$\langle \text{Slater}|\text{RG}\rangle = \frac{\det(RG * RG)}{\det(RG)^2}$$

- overlap with off-shell RG states (Slavnov)

$$\langle \text{off-RG}|\text{RG}\rangle = \det(\text{Slavnov})$$

Richardson-Gaudin states as variational ansatz

- *non*-integrable DOCI Hamiltonian

$$H = \sum_{i=1}^{m} \varepsilon_i n_i + \sum_{ik} V_{ik} S_i^\dagger S_k$$

- RG as variational ansatz

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

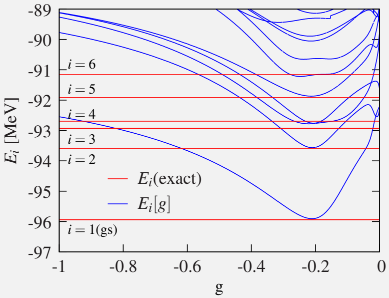
- $\min_g E[g]$ with integrability constraint

$$1 + \sum_{i=1}^{k} \frac{2 g d_i}{2\varepsilon_i - x_\alpha} - \sum_{\beta \neq \alpha}^{N} \frac{2g}{x_\beta - x_\alpha} = 0$$

- g defines a RG integrable model

example: ^{116}Sn

- realistic DOCI Hamiltonian with *G*-matrix formalism
- collective pair



Richardson-Gaudin bases as optimal active space

- non-integrable DOCI Hamiltonian

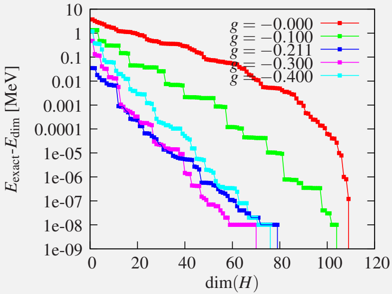
$$H = \sum_{i=1}^{m} \varepsilon_i n_i + \sum_{ik} V_{ik} S_i^\dagger S_k$$

- g defines a RG integrable model

$$H_{\text{int}} = \sum_{i=1}^{m} \varepsilon_i n_i + g \sum_{ik} S_i^\dagger S_k$$

- complete basis set with hierarchy
- diagonalise H in increasing basis set $\{|RG_1\rangle, |RG_2\rangle, |RG_3\rangle, \ldots, |RG_i\rangle\}$
- correlation coefficients

example: ^{116}Sn



- quick convergence at optimal $g = -0.211$
- "flat" $g = 0$ flags collectivity

Richardson-Gaudin bases as optimal active space

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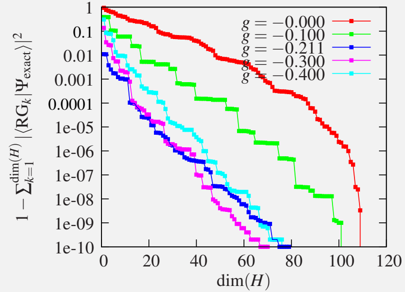

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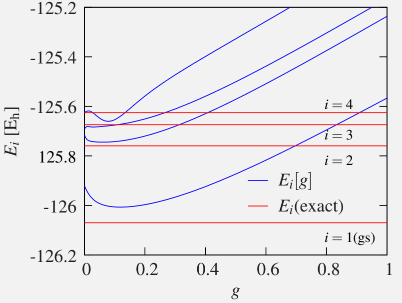
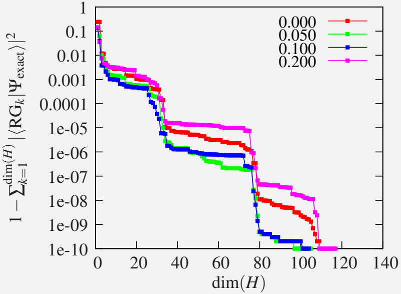
Another example: Ne (preliminary)

variational



active basis overlaps



- optimal repulsive g
- space restriction
  variation over $\{\varepsilon_i\}$

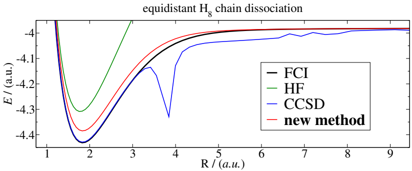
AP1roG (i)

- AP$n$roG picks n occupied orbitals and leaves virtual orbitals free

$$|\text{AP1roG}\rangle = \prod_{\alpha=1}^{N}\left(S_\alpha^\dagger + \sum_{i=N+1}^{m} G_{\alpha i} S_i^\dagger\right)|\theta\rangle$$

- projected Schrödinger approach: reference states

$$\langle\psi_{\text{ref}}|H|\text{AP1rog}\rangle = E\langle\psi_{\text{ref}}|\text{AP1rog}\rangle$$

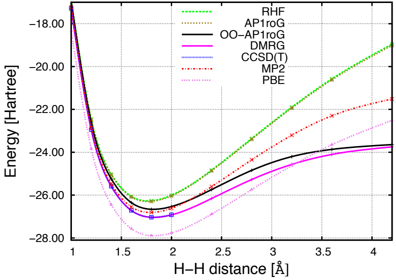


✎ P. A. Limacher, P. W. Ayers, P. A. Johnson, sdb, D. Van Neck, P. Bultinck (2013) JCTC 9, 1394

AP1roG (ii)

features

- equivalent to pCCD ✎
- sufficiently flexible (GVB-PP)
- static correlations from weak residual interactions
- orbital optimization ✍
- ? collective pairs? ✎ superconductivity/fluidity
- ? DOCI limit?



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✍ K. Boguslawski, P. Tecmer, P. W. Ayers, P. Bultinck, sdb, and D. Van Neck (2014) PRB89, 201106(R)
✍ P. Tecmer, K. Boguslawski, P. A. Johnson, P. A. Limacher, M. Chan, T. Verstraelen & P. W. Ayers (2014) JPCA, published online

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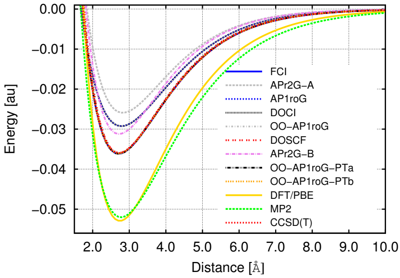

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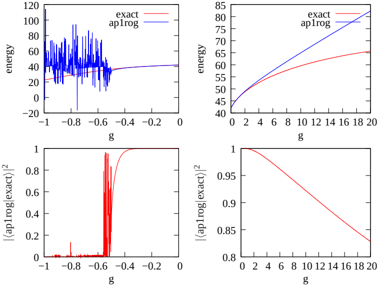

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beyond closed-shell singlet pair excitations: PT

- Static correlations can be captured by closed-shell geminals
- Dynamic correlations are missing
- MultiConfiguration Perturbation Theory (MCPT) brings them back✎

$$|\psi\rangle = |\psi_{\text{ref}}\rangle + \sum_L |L\rangle, \qquad \langle L|\psi_{\text{ref}}\rangle \neq 0$$

- Put static correlations in $|\psi_{\text{ref}}\rangle = |\text{AP1roG}\rangle$, dynamic in $|L\rangle$ ✍

	MP2	CCSD	DOCI	AP1roG	PTa	PTb
Ne	97.87%	98.45%	31.76%	31.75%	99.34%	97.17%

✎ M. Kobayashi, A. Szabados, H. Nakai & P. Surján (2010) JCTC 6, 2024
✍ P. A. Limacher, P. W. Ayers, P. A. Johnson, sdb, D. Van Neck & P Bultinck (2014) PCCP 16, 561

beyond closed-shell singlet pair excitations: algebras

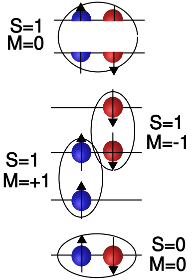
Lie algebras underpinning integrability

$$[G^\alpha, G^\beta] = \sum_\gamma c_\gamma^{\alpha\beta} G^\gamma, \quad R_i = \sum_\alpha H_i^\alpha + \sum_{j\neq i}\sum_\alpha X_{ij}^\alpha G_i^\alpha G_j^{-\alpha}$$

- Closed-shell singlet pairing: SU(2)

$$[S_i^\dagger, S_i] = 2S_i^0, \quad [S_i^0, S_i^\dagger] = S_i^\dagger, \quad [S^0, S_i] = -S_i$$

- Open-shell singlet pairing: SO(5)
- Open-shell triplet pairing: SO(5)
- Singlet+triplet: SO(8)



✍ J. Dukelsky, *et. al.*, Phys. Rev. Lett. **96** 072503 (2006)
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Remarks and Conclusions

Richardson

Schematic (pairing) correlations

Correlation functions

Slavnov/Borchardt theorem

Integrability

Complete basis set

theory (beyond integrability)

fCI, coupled-cluster, variational, perturbation theory, Kohn-Sham DFT, ...

The collaboration

- Dimitri Van Neck, Mario Van Raemdonck, Kris Heyde, Patrick Bultinck
  (Ghent University)
- Paul Ayers, Paul Johnson, Peter Limacher, Katharina Boguslawski, PawełTecmer
  (McMaster University)
- Jean-Sébastien Caux, Rianne van den Berg
  (University of Amsterdam)
- Veerle Hellemans
  (Université Libre de Bruxelles)

thanks

thanks & some references

Thank you for your attention!

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  J. Dukelsky, S. Pittel, G. Sierra (2004) Rev. Mod. Phys. 76, 643
- ✎ Richardson-Gaudin integrability in the contraction limit of the quasispin
  sdb (2012) Phys. Rev. C86, 044332
- ✎ A size-consistent approach to strongly correlated systems using a generalized antisymmetrized product of nonorthogonal geminals
  P. A. Johnson, P. W. Ayers, P. A. Limacher, sdb, D. Van Neck, P. Bultinck (2013) Comp. Theor. Chem. 1003, 101
- ✎ A New Mean-Field Method Suitable for Strongly Correlated Electrons: Computationally Facile Antisymmetric Products of Nonorthogonal Geminals
  P. A. Limacher, P. W. Ayers, P. A. Johnson, sdb, D. Van Neck, P. Bultinck (2013) J. Chem. Theor. Comp. 9, 1394
- ✎ Efficient description of strongly correlated electrons with mean-field cost
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