Richardson-Gaudin integrability in quantum many-body systems

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David Rowe Memorial
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mentorship

> *"First you try to solve the problem...*
> *Then, when you're stuck, you look into the literature . . . but not too much"*
>
> –david j rowe

mentorship

> *"Everything vibrates. . . and rotates a little."*
>
> –david j rowe

What I learned from David

- get the physics
- mathematical elegance

The quantum many-body problem

The mission of a quantum many-body theorist

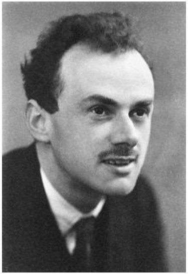
1. Construct the A-body Hamiltonian

$$\hat{H} = \sum_{i=1}^{A} -\frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i<j} V_2(r_i, r_j) + \sum_{i<j<k} V_3(r_i, r_j, r_k) + \dots$$

2. and solve the A-body Schrödinger equation

$$\langle r_1, r_2, \dots, r_A|\hat{H}|\Psi\rangle = E\langle r_1, r_2, \dots, r_A|\Psi\rangle$$

The unsolved problem



"The fundamental laws necessary for the mathematical treatment of large parts of physics and the whole of chemistry are thus fully known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved"

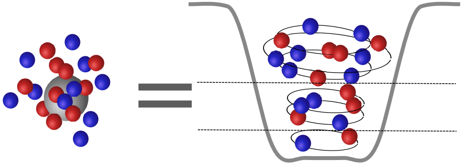
P. A. M. Dirac. Proc. Roy. Soc. 123, 714 (1929).

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



Size explosion of the Hilbert space

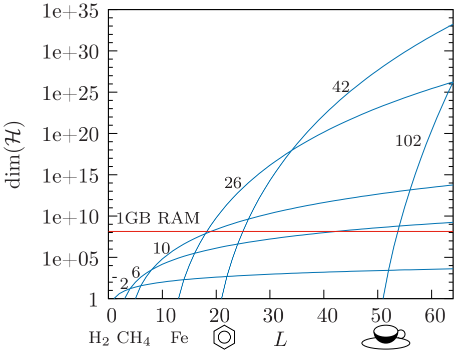
Hilbert space

- Basis of Slater determinants

$$|\psi\rangle = \sum_{i=1}^{\dim \mathcal{H}} c_i |\mathrm{SD}_i\rangle$$

- Combinatorial problem

$$\dim \mathcal{H} \sim e^N$$



Nuclear Pairing

pairing

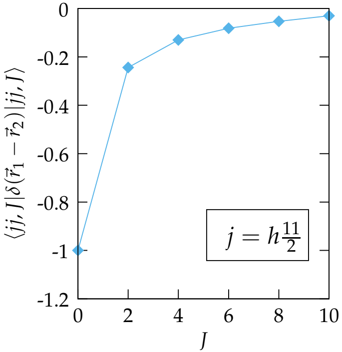
- Effective short-range interactions

$$\langle jj; J | V_{\text{res}} | jj; J \rangle \sim \delta_{0J}$$

- Pairing Hamiltonian

$$H = \sum_{i=1}^{L} \varepsilon_i \hat{n}_i + \sum_{ij}^{L} g_{ij} \hat{S}_i^\dagger \hat{S}_j$$

- $su(2)$ quasi-spin



Richardson's solution to the BCS Hamiltonian (i)

- The reduced BCS Hamiltonian

$$H_{\mathrm{BCS}} = \sum_{i=1}^{L} \varepsilon_i \hat{n}_i + g \sum_{ij}^{L} \hat{S}_i^\dagger \hat{S}_j$$

- is diagonalised by means of a Bethe Ansatz wavefunction

$$|\psi\rangle = \prod_{\alpha=1}^{N} S_\alpha^\dagger |\theta\rangle \qquad \text{with} \qquad S_\alpha^\dagger = \sum_{i=1}^{L} \frac{S_i^\dagger}{2\varepsilon_i - x_\alpha}$$

- provided the free Richardson variables x_α satisfy the

Richardson-Gaudin (RG) equations

$$\frac{1}{2g} + \sum_{i=1}^{L} \frac{d_i}{2\varepsilon_i - x_\alpha} - \sum_{\beta\neq\alpha}^{N} \frac{1}{x_\beta - x_\alpha} = 0 \qquad (\forall \alpha = 1 \dots N)$$

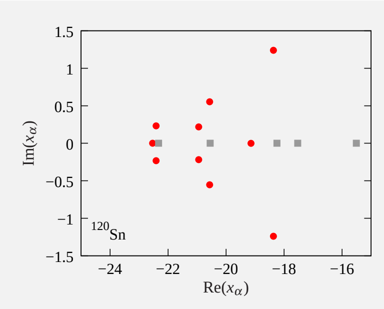
Richardson's solution for the BCS Hamiltonian (ii)

- Bethe Ansatz eigenstate(s)

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

- Richardson-Gaudin equations

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



Where's the magic?

Integrability (loose definition)

A quantum system is integrable when its Hamiltonian supports as many conserved quantities as degrees of freedom in the system.

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http://www2.unb.ca/~sde6/saclaylectures.html

Richardson-Gaudin integrability

Special case: the Hamiltonian is built from conserved charges

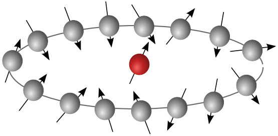
$$\hat{H} = \sum_{i=1}^{L} \varepsilon_i \hat{R}_i, \qquad \text{with} \qquad [\hat{R}_i, \hat{R}_j] = 0, \quad \forall i,j = 1..L$$

- Conserved charges of $\bigoplus_{i=1}^{L} su(2)_i$ problem

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

- Integrability gives Yang-Baxter-Gaudin algebra

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



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

Richardson-Gaudin Integrability

1. Challenges
2. Opportunities

WhyBotherson-EtAlors Integrability

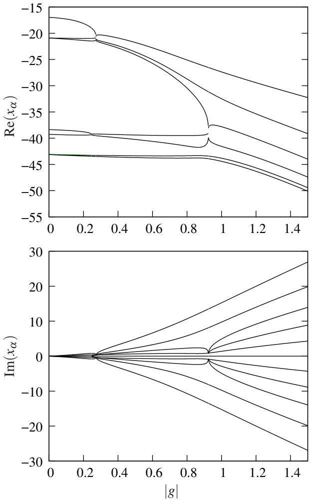
1. Challenges
2. Opportunities

Challenges: numerical solutions

- Numerical singularities

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

- electrostatic analog: attractive and repulsive



Tamm-Dancoff Approximation (RPA)

- Assumption: bosonic character

$$\hat{H}(b^\dagger)^n|\theta\rangle = n\hbar\omega(b^\dagger)^n|\theta\rangle$$

- Generalised boson

$$b_i^\dagger = \sum_{j=1}^{L} c_{ij} S_j^\dagger, \quad \forall i$$

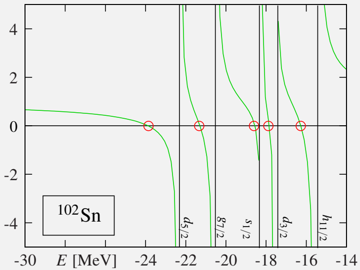
- We can construct the n-boson state from the 1-boson operators

$$|n_1, n_2, \ldots, n_m\rangle = \prod_{i=1}^{L} \frac{1}{\sqrt{n_i!}}(b_i^\dagger)^{n_i}|\theta\rangle$$

TDA secular equation

The 1-boson eigenvalue equation

$$1 + 2g\sum_{i=1}^{L}\frac{d_i}{2\varepsilon_i - \hbar\omega} = 0,$$

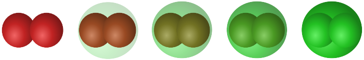


A pseudo-deformed algebra

- We can construct the following pseudo-deformed algebra

$$[S_i^0, S_i^\dagger] = S_i^\dagger, \quad [S_i^0, S_i] = -S_i, \quad [S_i^\dagger, S_i] = 2(\xi S_i^0 + (\xi - 1)d_i)$$

- So, with ξ, we can control the bosonic character of the fermion pair



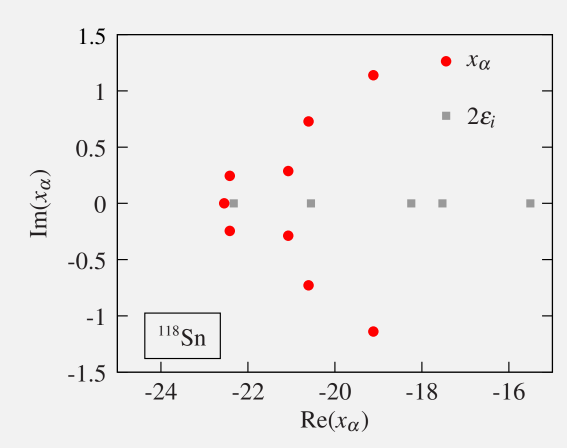
- The deformed pairing Hamiltonian remains exactly solvable with the

deformed Richardson Gaudin equations

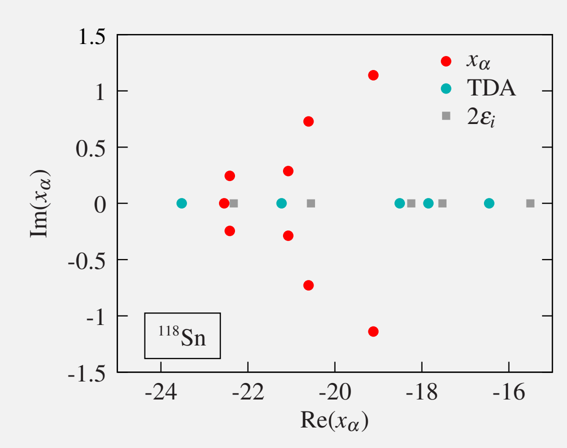
$$\frac{1}{2g} + \sum_{i=1}^{L} \frac{d_i}{2\varepsilon_i - x_\alpha} - \xi \sum_{\beta \neq \alpha}^{N} \frac{1}{x_\beta - x_\alpha} = 0 \qquad (\forall \alpha = 1 \ldots N)$$

- $\xi = 1$: we obtain the standard RG equations
- $\xi = 0$: we obtain N seniority-free copies of the TDA equation

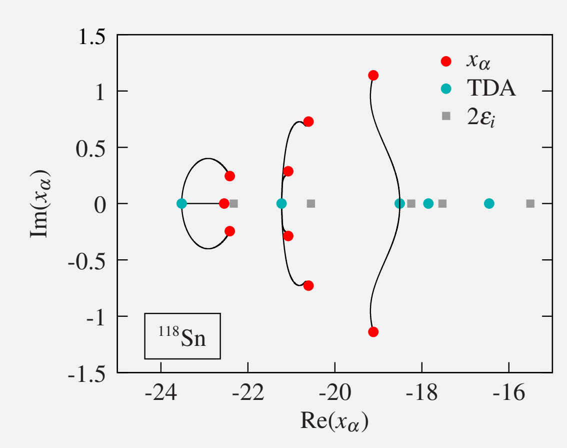
Pseudo deformation as a numerical solver



Pseudo deformation as a numerical solver



Pseudo deformation as a numerical solver



Eigenvalue-based method

Recall the conserved charges

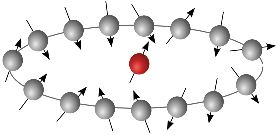
$$\hat{R}_i = (S_i^0 + \tfrac{1}{2}) + g \sum_{j \neq i}^{L} \tfrac{1}{2} X_{ij} (S_i^\dagger S_j + S_i S_j^\dagger) + Z_{ij} (S_i^0 S_j^0 - \tfrac{1}{4})$$

- Operator identity ($\forall i = 1 \dots L$)

$$\hat{R}_i^2 = \hat{R}_i - \tfrac{1}{2} g \sum_{j \neq i} Z_{ij} (\hat{R}_i - \hat{R}_j) + \tfrac{1}{4} g^2 N(L-N)\Gamma$$

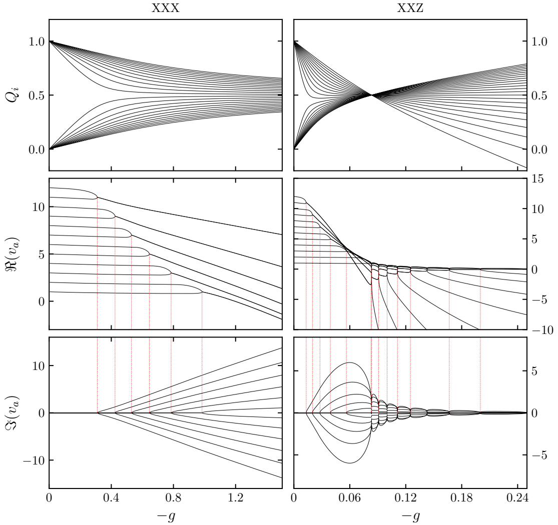
- Acting on the eigenstates

$$Q_i^2 = Q_i - \tfrac{1}{2} g \sum_{j \neq i} Z_{ij} (Q_i - Q_j) + \tfrac{1}{4} g^2 N(L-N)\Gamma$$



P Claeys, sdb, Van Raemdonck & Van Neck, Phys Rev B91, 155102 (2015

Eigenvalue-based method

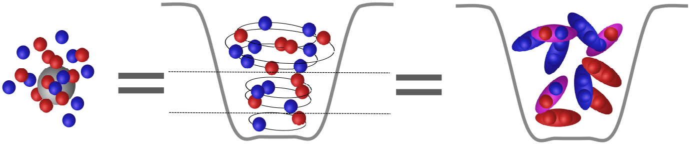


Opportunities: quantum many-body theory

- 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

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

- overlap with slater states

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

- factorial scaling

A Faribault & D Schuricht (2012) J Phys A45 485202
P Claeys, SDB, M Van Raemdonck, D Van Neck (2015) Phys. Rev. B91, 155102
P Claeys, D Van Neck & SDB (2017) SciPost Phys. 3, 028

Richardson states

- special geminal states

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

- overlap with slater states (Borchardt)

$$\langle \mathrm{Slater}|\mathrm{RG}\rangle = \frac{\det(RG * RG)}{\det(RG)}$$

- overlap with off-shell RG states (Slavnov)

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

variational Richardson-Gaudin (varRG)

- *non*-integrable pairing Hamiltonian

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

- RG as variational ansatz

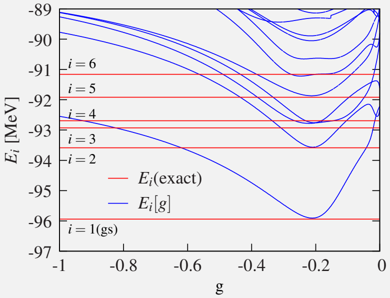
$$E[g] = \langle RG(g) | H | RG(g) \rangle$$

- $\min_g E[g]$ on integrable manifold

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

- g defines a RG integrable model

Nuclear ^{116}Sn



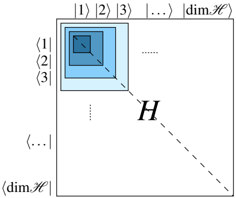
sdb, P Claeys, JS Caux, D Van Neck & PW Ayers, arxiv:1712.01673

Richardson-Gaudin Configuration Interaction

- Correlated basis from varRG
- Isospectral flow

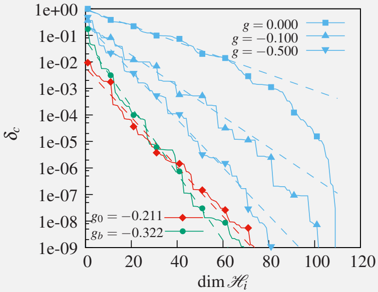
$$H(g) = U^{\dagger}(g)H(0)U(g)$$

- Configuration Interaction



→ Optimized convergence

Nuclear ^{116}Sn

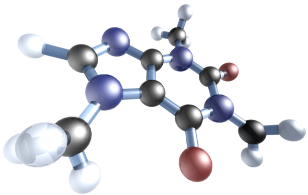


SDB, P Claeys, JS Caux, D Van Neck & PW Ayers, arxiv:1712.01673

Quantum Chemistry: Geminals

geminal states

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



- mean field state for pairs
- G is the Geminal matrix
- Lewis structures

1953 Proposed by Hurley, Lennard-Jones & Pople

- Computationally intractable

Proc. Roy. Soc. A220, 446 (1953)

QuNB group

quantum chemistry/
electronic structure theory

- geminal theory
- symmetry breaking
- tensor network methods
- machine learning
- out-of-equilibrium
- quantum computing

Thanks David!

Thanks David!