

Peter Schuck (1940-2022)

Relativistic Equation of Motion Framework for Nuclear Physics

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Conference on Quantum Many-Body Correlations in memory of Peter Schuck IJCLab, Orsay, France, March 21-23, 2023

Hierarchy of energy scales and nuclear many-body problem



• The major conflict:

Separation of energy scales => effective field theories

vs

The physics on a certain scale is governed by the next higher-energy scale

Hamiltonian:

H = K + V



internal degrees of freedom: next energy scale

Standard Model: free propagation and interaction (input) String theory: merging strings NO "Interaction"





Possible solution:

- Keep/establish connections between the scales via emergent phenomena
- ↔ A universal approach to the strongly-coupled QMBP?

The underlying mechanism of NN-interaction:



A strongly-correlated many body system: single-fermion propagator, particle-hole propagator and related observables

$$H = \sum_{12} \bar{\psi}_1 (-i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + M)_{12} \psi_2 + \frac{1}{4} \sum_{1234} \bar{\psi}_1 \bar{\psi}_2 \bar{v}_{1234} \psi_4 \psi_3 = T + V^{(2)}$$

 $G_{11'}(t - t') = -i\langle T\psi(1)\bar{\psi}(1')\rangle \qquad 1 = \{\xi_1, t\}$

$$G_{11'}(\varepsilon) = \sum_{n} \frac{\eta_1^n \bar{\eta}_{1'}^{n*}}{\varepsilon - \varepsilon_n^+ + i\delta} + \sum_{m} \frac{\chi_1^m \bar{\chi}_{1'}^{m*}}{\varepsilon + \varepsilon_m^- - i\delta}$$

$$\eta_1^n = \langle 0^{(N)} | \psi_1 | n^{(N+1)} \rangle$$

$$\chi_1^m = \langle m^{(N-1)} | \psi_1 | 0^{(N)}
angle$$

Ground state of N particles (Excited) state of (N+1) particles

$$R_{12,1'2'}(t-t') = -i\langle T(\bar{\psi}_1\psi_2)(t)(\bar{\psi}_{2'}\psi_{1'})(t')\rangle$$

$$\begin{aligned} R_{12,1'2'}(\omega) &= \sum_{\nu > 0} \Big[\frac{\rho_{21}^{\nu} \bar{\rho}_{2'1'}^{\nu*}}{\omega - \omega_{\nu} + i\delta} - \frac{\bar{\rho}_{12}^{\nu*} \rho_{1'2'}^{\nu}}{\omega + \omega_{\nu} - i\delta} \Big] \\ \\ \xrightarrow{\text{Excitation}}_{\text{energies}} \rho_{12}^{\nu} &= \langle 0 | \bar{\psi}_2 \psi_1 | \nu \rangle \end{aligned}$$

Hamiltonian, extendable to 3-body etc.

Single-particle propagator

Fourier transform: Spectral expansion

Residues - spectroscopic (occupation) factors

Poles - single-particle energies

Particle-hole response function

Fourier transform: Spectral expansion

Residues - transition densities

Poles - excitation energies

Exact equations of motion (EOM) for binary interactions: one-body problem

One-fermion propagator

$$G_{11'}(t-t') = -i\langle T\psi(1)\bar{\psi}(1')\rangle$$

EOM: Dyson Eq. $G(\omega) = G^{(0)}(\omega) + G^{(0)}(\omega)\Sigma(\omega)G(\omega)$

$$\Sigma(\omega) = \Sigma^{(0)} + \Sigma^{(r)}(\omega)$$

Irreducible kernel (Self-energy, exact):

(*)

Instantaneous term (Hartree-Fock incl. "tadpole") Short-range correlations

$$\Sigma_{11'}^{(0)} = -\langle \gamma^0 \Big\{ [V, \psi_1], \bar{\psi}_{1'} \Big\} \gamma^0 \rangle$$

$$= \sum_{22'} \overline{v}_{121'2'} \langle \overline{\psi}_2 \psi_{2'} \rangle = \overbrace{\overline{v}}_{1}^{\rho_{2'2}}$$

t-dependent (dynamical) term (symmetric version): Long-range correlations

$$\Sigma_{11'}^{(r)} = i \langle T\gamma^0 [V, \psi_1](t) [V, \bar{\psi}_{1'}](t') \gamma^0 \rangle^{irr}$$

$$= -\frac{1}{4} \sum_{234} \sum_{2'3'4'} \bar{v}_{1234} G^{(3)irr}_{432',23'4'}(t-t') \bar{v}_{4'3'2'1'}$$



 $E_0 = \frac{1}{2\pi} \int d\varepsilon \sum_{12} (T_{12} + \varepsilon \delta_{12}) \mathrm{Im} G_{21}(\varepsilon)$

Koltun-Migdal-Galitsky sum rule: the binding energy

$$\rho_{11'} = -i \lim_{t=t'-0} G_{11'}(t-t')$$

is the full solution of (*): includes the dynamical term!

"Ab-initio DFT":

Equation of motion (EOM) for the particle-hole response

Particle-hole propagator (response function):
$$R_{12,1'2'}(t-t') = -i\langle T(\bar{\psi}_1\psi_2)(t)(\bar{\psi}_{2'}\psi_{1'})(t')\rangle$$

spectra of excitations, masses, decays, ...

EOM: Bethe-Salpeter-Dyson Eq.

 $R(\omega) = R^{(0)}(\omega) + R^{(0)}(\omega)F(\omega)R(\omega) \qquad (**) \qquad F(t-t') = F^{(0)}\delta(t-t') + F^{(r)}(t-t')$

Irreducible kernel (exact):

Instantaneous term ("bosonic" mean field): Short-range correlations





Self-consistent mean field F⁽⁰⁾, where

$$\rho_{12,1'2'} = \delta_{22'}\rho_{11'} - i \lim_{t' \to t+0} R_{2'1,21'}(t-t')$$
contains the full solution of (**) including the dynamical term!

t-dependent (dynamical) term: Long-range correlations



Non-perturbative treatment of two-point G⁽ⁿ⁾ in the dynamical kernels

• Quantum many-body problem in a nutshell: Direct EOM for G⁽ⁿ⁾ generates G⁽ⁿ⁺²⁾ in the (symmetric) dynamical kernels and further high-rank correlation functions (CFs); an equivalent

of the BBGKY hierarchy. N_{Equations} = N_{Particles} & Coupled 🙀 !!!

Non-perturbative solution:
 Cluster decomposition

"Self-consistent GFs" This work $\bullet \mathbf{G}^{(3)} = \mathbf{G}^{(1)} \mathbf{G}^{(1)} \mathbf{G}^{(1)} + \mathbf{G}^{(2)} \mathbf{G}^{(1)} + \mathbf{\Xi}^{(3)}$

 $\mathbf{A} \mathbf{G}^{(4)} = \mathbf{G}^{(1)} \mathbf{G}^{(1)} \mathbf{G}^{(1)} \mathbf{G}^{(1)} + \mathbf{G}^{(2)} \mathbf{G}^{(2)} + \mathbf{G}^{(3)} \mathbf{G}^{(1)} + \mathbf{\Xi}^{(4)}$

Truncation on two-body level



Exact mapping: particle-hole (2q) quasibound states

Emergence of effective "particles" (phonons, vibrations):

Emergence of superfluidity:



Emergence of effective degrees of freedom



Emergent phonon vertices and propagators: calculable from the underlying H, which does not contain phonon degrees of freedom

$$H = \sum_{12} h_{12} \psi_1^{\dagger} \psi_2 + \frac{1}{4} \sum_{1234} \bar{v}_{1234} \psi_1^{\dagger} \psi_2^{\dagger} \psi_4 \psi_3 \qquad \text{``Ab-initio''}$$
$$H = \sum_{12} \tilde{h}_{12} \psi_1^{\dagger} \psi_2 + \sum_{\lambda\lambda'} \mathcal{W}_{\lambda\lambda'} Q_{\lambda}^{\dagger} Q_{\lambda'} + \sum_{12\lambda} \left[\Theta_{12}^{\lambda} \psi_1^{\dagger} Q_{\lambda}^{\dagger} \psi_2 + h.c. \right] \qquad \text{Effective QVC}$$

Cf.: The Standard Model elementary interaction vertices: boson-exchange interaction is the input:

 γ, g, W^{\pm}, Z^0

Possibly derivable?

E.L., P. Schuck, PRC 100, 064320 (2019) E.L., Y. Zhang, PRC 104, 044303 (2021)

Problems with approximate treatments: poles "mismatch", (non)-positivity and optical theorem



Superfluid dynamical kernel: adding particle-number violating contributions Mapping on the QVC in the canonical basis



Quasiparticle dynamical self-energy (matrix): normal and pairing phonons are unified





Cf.: Quasiparticle static self-energy (matrix) in HFB

 $\hat{\Sigma}^0 = \begin{pmatrix} \Sigma_{11'} & \Delta_{11'} \\ -\Delta_{11'}^* & -\tilde{\Sigma}_{11'}^T \end{pmatrix}$

Bogoliubov transformation

E.L., Y. Zhang, PRC 104, 044303 (2021) Y. Zhang et al., PRC 105, 044326 (2022)

Nuclear response: toward a complete theory



RQTBA³ with correlated 3p3h configurations: 2q+2phonon



- The new complex configurations 2q+2phonon included for the first time enforce fragmentation and spreading toward higher and lower energies, thus, modifying both giant and pygmy dipole resonances;
- Exp. Data: V.A. Erokhova et al., Bull. Rus. Acad. Phys. 67, 1636 (2003)
- RQTBA³ demonstrates an overall systematic improvement of the description of nuclear excited states heading toward spectroscopic accuracy without strong limitations on masses and excitation energies.

E.L., P. Schuck, PRC 100, 064320 (2019)



Low-Energy dipole strength distribution: IS vs EM



Spin-isospin excitations (Gamow-Teller resonance) 2q+phonon configurations in the dynamical kernel (pn-RQTBA)



More correlations: Emergent "time machine"

Ground state correlations induced by QVC: backward-going diagrams (V. Tselyaev, 1989)

New unblocking mechanism:





Gamow-Teller strength in 90-Zr:



The backward-going diagrams are solely responsible for the β + strength in neutron-rich nuclei



C. Robin, E.L., Phys. Rev. Lett. 123, 202501 (2019)

Finite-temperature response: the phaphonon dynamical kernel

$$R_{12,1'2'}(t-t') = -i\langle \mathcal{T}(\bar{\psi}_1\psi_2)(t)(\bar{\psi}_{2'}\psi_{1'})(t')\rangle \to -i\langle \mathcal{T}(\bar{\psi}_1\psi_2)(t)(\bar{\psi}_{2'}\psi_{1'})(t')\rangle_T$$

$$< \dots > \equiv < 0|\dots|0> \to < \dots >_T \equiv \sum_n exp\Big(\frac{\Omega - E_n - \mu N}{T}\Big) < n|\dots|n>$$

Method: EOM for Matsubara Green's functions

$$\begin{array}{c} \text{averages} & \begin{array}{c} & \begin{array}{c} \text{thermal averages} \\ \\ \mathcal{R}_{14,23}(\omega,T) = \tilde{\mathcal{R}}_{14,23}^{0}(\omega,T) + \\ & + \sum_{1'2'3'4'} \tilde{\mathcal{R}}_{12',21'}^{0}(\omega,T) \left[\tilde{V}_{1'4',2'3'}(T) + \delta \Phi_{1'4',2'3'}(\omega,T) \right] \mathcal{R}_{3'4,4'3}(\omega,T) \\ & \delta \Phi_{1'4',2'3'}(\omega,T) = \Phi_{1'4',2'3'}(\omega,T) - \Phi_{1'4',2'3'}(0,T) \end{array}$$

T > 0:

1p1h+phonon dynamical kernel:

T = 0:

$$\begin{split} \Phi_{14,23}^{(ph)}(\omega,T) &= \frac{1}{n_{43}(T)} \sum_{\mu,\mu=\pm 1} \eta_{\mu} \Big[\delta_{13} \sum_{6} \gamma_{\mu;62}^{\eta_{\mu}} \gamma_{\mu;64}^{\eta_{\mu}*} \times \\ &\times \frac{\left(N(\eta_{\mu}\Omega_{\mu}) + n_{6}(T) \right) \left(n(\varepsilon_{6} - \eta_{\mu}\Omega_{\mu}, T) - n_{1}(T) \right)}{\omega - \varepsilon_{1} + \varepsilon_{6} - \eta_{\mu}\Omega_{\mu}} + \\ &+ \delta_{24} \sum_{5} \gamma_{\mu;15}^{\eta_{\mu}} \gamma_{\mu;35}^{\eta_{\mu}*} \times \\ &\times \frac{\left(N(\eta_{\mu}\Omega_{\mu}) + n_{2}(T) \right) \left(n(\varepsilon_{2} - \eta_{\mu}\Omega_{\mu}, T) - n_{5}(T) \right)}{\omega - \varepsilon_{5} + \varepsilon_{2} - \eta_{\mu}\Omega_{\mu}} - \\ &- \gamma_{\mu;13}^{\eta_{\mu}} \gamma_{\mu;42}^{\eta_{\mu}*} \times \\ &\times \frac{\left(N(\eta_{\mu}\Omega_{\mu}) + n_{2}(T) \right) \left(n(\varepsilon_{2} - \eta_{\mu}\Omega_{\mu}, T) - n_{3}(T) \right)}{\omega - \varepsilon_{3} + \varepsilon_{2} - \eta_{\mu}\Omega_{\mu}} - \\ &- \gamma_{\mu;31}^{\eta_{\mu}} \gamma_{\mu;42}^{\eta_{\mu}} \times \\ &\times \frac{\left(N(\eta_{\mu}\Omega_{\mu}) + n_{4}(T) \right) \left(n(\varepsilon_{4} - \eta_{\mu}\Omega_{\mu}, T) - n_{1}(T) \right)}{\omega - \varepsilon_{1} + \varepsilon_{4} - \eta_{\mu}\Omega_{\mu}} \Big], \end{split}$$



GT+ response and electron capture (EC) rates at T>0: the neighborhood of ⁷⁸Ni

GT+ response

Electron capture rates around 78Ni





E.L., C. Robin, H. Wibowo, PLB 800, 135134 (2020)

E.L., P. Schuck, PRC 104, 044330 (2021) E.L., C. Robin, PRC 103, 024326 (2021)



Interplay of superfluidity and collective effects in core-collapse supernovae:

- -> Amplifies the EC rates and, consequently,
- Reduces the electron-to-baryon ratio leading to lower pressure
- · Promotes the gravitational collapse
- ✤ Increases the neutrino flux and effective cooling
- Allows heavy nuclei to survive the collapse

Formalism at T>0: the pairing channel

$$\begin{aligned} \text{Averages redefined:} \\ G_{12,1'2'}(t-t') &= -i\langle \mathcal{T}(\psi_1\psi_2)(t)(\bar{\psi}_{2'}\bar{\psi}_{1'})(t')\rangle \rightarrow -i\langle \mathcal{T}(\psi_1\psi_2)(t)(\bar{\psi}_{2'}\bar{\psi}_{1'})(t')\rangle_T \\ \text{Grand Canonical average:} \quad < \ldots > \equiv < 0|\ldots|0 > \rightarrow \quad < \ldots >_T \equiv \sum_n exp\Big(\frac{\Omega - E_n - \mu N}{T}\Big) < n|\ldots|n > 0|\ldots|n > 0|\ldots|n > 0 \end{aligned}$$

Matsubara imaginary-time formalism: temperature-dependent dynamical kernel

Direct:

Exchange:

E.L., P.Schuck, Phys. Rev. C 104, 044330 (2021)

BCS-like gap Eq., but with non-trivial T-dependence in $K^{(r)}$:

$$\Delta_1(T) = -\sum_2 \mathcal{V}_{1\bar{1}2\bar{2}} \frac{\Delta_2(T)(1-2f_2(T))}{2E_2}$$

$$f_1(T) = \frac{1}{\exp(E_1/T) + 1}$$
$$\mathcal{V}_{121'2'} = \frac{1}{2} \Big(K^{(0)}_{121'2'} + K^{(r)}_{121'2'}(2\lambda) \Big)$$

Pairing gap at T = 0, T>0 and critical temperature



E.L., P.Schuck, Phys. Rev. C 104, 044330 (2021)

Lipkin Hamiltonian on quantum computer

The algorithm: Variational Quantum Eigensolver (VQE) + quantum EOM (qEOM)

- VQE: a minimal encoding scheme is found ("J-scheme") and implemented, based on the symmetry of the LMG Hamiltonian. Yields an accurate ground state |0>.
- → qEOM generates efficiently the EOM matrix:

Two-level Lipkin Hamiltonian: **exactly solvable**

$$\hat{H} = \epsilon \hat{J}_z - \frac{v}{2} \left(\hat{J}_+^2 + \hat{J}_-^2 \right)$$



Generalized eigenvalue equation:

$$\begin{bmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{A}^* \end{bmatrix} \begin{bmatrix} X^n \\ Y^n \end{bmatrix} = E_{0n} \begin{bmatrix} \mathcal{C} & \mathcal{D} \\ -\mathcal{D}^* & -\mathcal{C}^* \end{bmatrix} \begin{bmatrix} X^n \\ Y^n \end{bmatrix}$$

$$\begin{aligned} \mathcal{A}_{\mu_{\alpha}\nu_{\beta}} &= \langle 0| \left[\left(\hat{K}_{\mu_{\alpha}}^{\alpha} \right)^{\dagger}, \left[\hat{H}, \hat{K}_{\nu_{\beta}}^{\beta} \right] \right] |0\rangle \\ \mathcal{B}_{\mu_{\alpha}\nu_{\beta}} &= - \langle 0| \left[\left(\hat{K}_{\mu_{\alpha}}^{\alpha} \right)^{\dagger}, \left[\hat{H}, \left(\hat{K}_{\nu_{\beta}}^{\beta} \right)^{\dagger} \right] \right] |0\rangle \\ \mathcal{C}_{\mu_{\alpha}\nu_{\beta}} &= \langle 0| \left[\left(\hat{K}_{\mu_{\alpha}}^{\alpha} \right)^{\dagger}, \hat{K}_{\nu_{\beta}}^{\beta} \right] |0\rangle \\ \mathcal{D}_{\mu_{\alpha}\nu_{\beta}} &= - \langle 0| \left[\left(\hat{K}_{\mu_{\alpha}}^{\alpha} \right)^{\dagger}, \left(\hat{K}_{\nu_{\beta}}^{\beta} \right)^{\dagger} \right] |0\rangle . \end{aligned}$$

Excitation operator: complexity a, K^a

. . .

$$\hat{K}^{1}_{\mu_{1}} = a^{\dagger}_{i}a_{j'} \qquad \qquad \hat{K}^{2}_{\mu_{2}} = a^{\dagger}_{i}a^{\dagger}_{j}a_{j'}a_{i'}$$

M. Hlatshwayo, et al., Phys. Rev. C 106, 024319 (2022)

Lipkin Hamiltonian on quantum computer: hardware results





M. Hlatshwayo, et al., Phys. Rev. C 106, 024319 (2022)

Conventions:

- $rac{h}{h} n_q = number of states$
- $\cdot \geq N = number of particles$
- $v = v / \varepsilon$ effective interaction strength
- * **I-scheme:** individual spin basis, $n_q = 2^N$
- J-scheme: total spin basis (coupled form), symmetry: n_q = N/2 + 1

Observations:

- ✤ Higher-rank excitation ~ higher accuracy
- Stronger coupling ~ lower accuracy
- More particles ~ lower accuracy
- Less qubits ~ higher accuracy

More particles, higher complexity (preliminary; simulator)



Quantum advantage: The same Pauli strings $\langle XYZ \rangle$ are to be measured for a = 1,2,3 Second RPA vs RPA: RPA breaks down early in the strong-coupling regime "Third" RPA and higher: More accurate solutions, tbd on a device



Summary:

Outlook

- Relativistic NFT is generalized to finite temperature and applied to nuclear superfluidity.
- Weak rates at astrophysical conditions are extracted: the correlations beyond mean field are found significant.

Current and future developments:

- Deformed nuclei: correlations vs shapes; first results just released (Yinu Zhang et al.);
- Efficient algorithms; quantum computing (Manqoba Hlatshwayo et al.);
- · ⊱ Implementation of the EC rates into the core-collapse supernovae simulations;
- Toward an "ab initio" description: implementations with bare NN-interactions;
- Superfluid pairing at T>0 to extend the application range (r-process);
- *Relativistic EOM's, bosonic EOM's, beyond Standard Model, …*

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Study Edition

P. Ring P. Schuck

The Nuclear Many-Body Problem



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NPD - 2018 Lise Meitner Prize Winners

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The Nuclear Physics Division of the EPS awards the prestigious Lise Meitner Prize every second year to one or several individuals for outstanding work in the fields of experimental, theoretical or applied nuclear science.



A short article about the life of Lise Meitner can be found here

Prize Winners 2018

The European Physical Society, through its Nuclear Physics Division, has awarded the 2018 Lise Prof. Dr. Peter Rin Meltner Prize to

ref. Peter Ring (Technische Universität München) and Prof. Peter Schuck (institut Physics uckaino Orasy auto Laboratorio de Physica) et dis Modificiation des Millaux Condense renobile) for their enormous impact on both theoretical and experimental many-body nuclei hysics. In particular. Piling developed new investigations in high-sing hebenomes, collectibrations and retail/visit nuclear energy density functionals while PSchuck: Introduced ne and retail was matter in connection with nucleas superfluidly auto alpha-partic contensation.

is prize consists of a Medal and a Diploma, in addition to a cash award. It will be presented during a ecial session at the $4^{\rm th}$ European Nuclear Physics Conference of the European Physical Society, ich will be held in Bologn=Hally on 2-7 September this year.

The 2018 Lise Meitner Prize was sponsored by GSI Heimholtzzentrum für Schwerionenforschung GmbH, Jamstadt, KVI Centre for Advanced Radiation Technology, Groningen, Forschungszentrum GmbH, Jülich, Laboratori Nazionali dei Sud, INFN, Catania, Laboratori Nazionali di Legnaro, nIVFN, Legnaro, and by Institut de Physique Nucléaire, Orsay.

Prize Winners Previous Years

A list of previous winners of the Lise Meitner Prize can be found here.



Springer





Finite amplitude method extended beyond QRPA (preliminary):

$$\delta \mathcal{R}_{\mu\nu}^{(20)}(\omega) = \frac{\delta \mathcal{H}_{\mu\nu}^{20}(\omega) + \sum_{\mu'\nu'} \Phi_{\mu\nu'\nu\mu'}^{(+)}(\omega) \delta \mathcal{R}_{\mu'\nu'}^{(20)}(\omega) + F_{\mu\nu}^{20}}{\omega - E_{\mu} - E_{\nu}}}{\delta \mathcal{H}_{\mu\nu}^{02}(\omega) + \sum_{\mu'\nu'} \Phi_{\mu\nu'\nu\mu'}^{(-)}(\omega) \delta \mathcal{R}_{\mu'\nu'}^{(02)}(\omega) + F_{\mu\nu}^{02}}{-\omega - E_{\mu} - E_{\nu}}.$$

 $\Phi_{\mu\mu'\nu\nu'}^{(+)}(\omega) = \left[\delta_{\mu'\nu'}\sum_{\gamma n} \frac{\Gamma_{\mu\gamma}^{(11)n}\Gamma_{\nu\gamma}^{(11)n*}}{\omega - \omega_n - E_{\mu'\gamma}} + \delta_{\mu\nu}\sum_{\gamma n} \frac{\Gamma_{\mu'\gamma}^{(11)n}\Gamma_{\nu'\gamma}^{(11)n*}}{\omega - \omega_n - E_{\mu\gamma}} + \sum_{n} \frac{\Gamma_{\mu\nu}^{(11)n}\Gamma_{\nu'\mu'}^{(11)n*}}{\omega - \omega_n - E_{\mu'\nu}} + \sum_{n} \frac{\Gamma_{\mu'\nu'}^{(11)n}\Gamma_{\nu\mu}^{(11)n*}}{\omega - \omega_n - E_{\mu\nu'}}\right]$ (leading approximation):

E.L., Y. Zhang, Phys. Rev. C 106, 064316 (2022)

Proof of principle: IVGMR in 24-Mg in a restricted model space

Generalized FAM (FAM-QVC)

Ongoing:

- Convergence improvement
- Optimization
- Cross-check routines



Are there theoretical limits on accuracy?

- Higher-rank configurations = higher accuracy? Can we quantify this? How accurately we can describe the observed spectra, in principle?
- Spectroscopic accuracy in nuclear structure: experiment (laser spectroscopy [eV], nuclear resonance fluorescence [keV]) ... no standards for theory. ~100 keV?
- Chemical accuracy 1 kcal/mol = 0.043 eV is possible with the gold standard for quantum chemistry calculations, namely the canonical coupled cluster (CC) expansion truncated at the second order in the electronic excitation operator and including an approximate treatment of the triple excitations (CCSD(T), where S stands for single, D for double, and (T) for non-iterative triple) [P.J. Ollitrault et al, Phys. Rev. Res. 2, 043140, 2020]
- ✤ CCSD(T) includes up to (correlated) 3p3h configurations and scales as O(N⁷) with the number of degrees of freedom N of the model Hamiltonian.
- In nuclear structure, there are relatively rare calculations with (correlated) 3p3h configurations for medium-heavy nuclei (QPM, EOM/RQTBA³, CC). The results are still not ideal.
- Is the problem in the underlying strong "forces", which are not weak and known with limited accuracy? Or the many-body methods? Likely both.
- Working with model (solvable) Hamiltonians allows one to solely focus on the manybody problem. Can be studied with quantum and hybrid algorithms on NISQ devices.

Mean field approximation and beyond



Mean field approximation (density functional theory, DFT)



Beyond mean field: particle-vibration coupling (PVC), leading approximation:



Single-(quasi)particle states. New implementation: FAM-QRPA+QVC

(i) Relativistic meson-nucleon Lagrangian + (ii) Relativistic Hartree-Bogoliubov (RHB) + (iii) Quasiparticle random phase approximation (QRPA): $J = 2^+ - 5^-$, K = [0,J]. Finite amplitude method (FAM): A. Bjelčić et al., CPC 253, 107184 (2020). Relativistic DD-PC1 interaction.



Single-(quasi)particle states in 38S

Fragmentation of quasiparticle states: RHB vs RHB+QVC



Fragmentation mechanism: schematic



Y. Zhang et al., PRC 105, 044326 (2022)



Nilsson diagram: RHB+QVC (dominant only)



Single-(quasi)particle states in 249,251 Cf

A. Afanasjev et al.: Long-standing problem of the description of single-particle states in deformed nuclei.

Systematic studies for ²⁴⁹Bk and ²⁵¹Cf in the mean-field approximation:

²⁵¹Cf

3.5

2.5

2

1.5

0.5

0

-0.5

-1

3

 $1/2^{-1}$

 $3/2^{-1}$

11/2

7/2

 $1/2^{+}$

3/2

RHB

²⁵⁰Cf

 $\beta_2 = 0.29$

RHB: DD-PC1

RQRPA phonon subspace:

(b)

K = [0, J]

 $7/2^{+}$

 $1/2^{-1}$

 $5/2^{+}$

9/2

RHB

²⁴⁹Cf

 $\frac{1/2^{+}}{7/2^{+}}$

 $5/2^+$

 $9/2^{-1}$

Exp

RHB+PVC

(a)

J = [2,5]

(1/2)

(3/2)

 $3/2^{-1}$

11/2

3/2

 $7/2^{+}$

 $1/2^{+}$

Exp

RHB+PVC

Deformed one-quasiparticle states: covariant and nonrelativistic mean-field calculations vs experiment:



Beyond mean field: RHB+QVC calculations. Dominant fragments in ²⁵¹Cf and ²⁴⁹Cf.

The spectroscopic factors are quenched even stronger than in spherical nuclei. Can this be measured?

Two-level Lipkin (Meshkov-Glick), LMG, Hamiltonian:

$$\hat{H} = \epsilon \hat{J}_z - \frac{v}{2} \left(\hat{J}_+^2 + \hat{J}_-^2 \right) - \frac{w}{2} \left(\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ \right)$$

Quasispin operators:

$$\hat{J}_{z} = \frac{1}{2} \sum_{p=1}^{N} \left(\hat{a}_{p,+}^{\dagger} \hat{a}_{p,+} - \hat{a}_{p,-}^{\dagger} \hat{a}_{p,-} \right), \qquad N = 2j+1$$
$$\hat{J}_{+} = \sum_{p=1}^{N} \hat{a}_{p,+}^{\dagger} \hat{a}_{p,-} \text{ and } \hat{J}_{-} = \left(\hat{J}_{+} \right)^{\dagger}$$

Excitation operator:

Configuration complexity:

3

$$\hat{O}_{n}^{\dagger} = \sum_{\alpha} \sum_{\mu_{\alpha}} \left[X_{\mu_{\alpha}}^{\alpha}(n) \hat{K}_{\mu_{\alpha}}^{\alpha} - Y_{\mu_{\alpha}}^{\alpha}(n) \left(\hat{K}_{\mu_{\alpha}}^{\alpha} \right)^{\dagger} \right]$$

$$\hat{K}^1_{\mu_1} = a^{\dagger}_i a_{j'} \qquad \qquad \hat{K}^2_{\mu_2} = a^{\dagger}_i a^{\dagger}_j a_{j'} a_{i'}$$

M. Hlatshwayo, et al., Phys. Rev. C 106, 024319 (2022)

Atomic nuclei on quantum computer: accessing emergence via entanglement

Variational Quantum Eigensolver (VQE) + Quantum Equation of Motion (qEOM):



Implementation for N = 4 (IBM-Q): RPA vs SRPA vs exact



Beyond SRPA, toward quantum advantage [in progress]

Two-level Lipkin Hamiltonian: **exactly solvable** $\hat{H} = \epsilon \hat{J}_z - \frac{v}{2} \left(\hat{J}_+^2 + \hat{J}_-^2 \right)$ $\epsilon \hat{J}_z = \frac{v}{2} \left(\hat{J}_+^2 + \hat{J}_-^2 \right)$

M. Hlatshwayo et al., Phys. Rev. C 106, 024319 (2022)