Natural Orbitals and the Equation of Motion Phonon Method

Jan Pokorný

Czech Technical University in Prague, Czechia (CTU)
Nuclear Physics Institute, Czech Academy of Sciences, Řež, Czechia (NPI CAS)

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Outline

- Nuclear Structure Theory
- Quantum Mechanics
  - Hilbert spaces, Hamiltonians, bra-ket formalism
- Second-Order Perturbation Theory

- Density Matrix
- Natural Orbitals
- Equation of Motion Phonon Method

- Results
- Conclusions
- Plans for 2020

Nuclear Structure Theory

What is inside the atomic nucleus?

- asked since the Rutherford experiment (19??)[1]
- to this day no exact answer, we need models
- the first model approaches – liquid drop, shell model
- collective vs. microscopic

What about the potential between nucleons?

- no answer from QCD
- potentials based on meson exchange (realistic)
- or just fit a function that satisfies all symmetries known in NN interaction (phenomenological, effective)
- what about many-body interactions?

Collective behaviour, excitations, transitions?

- we try to find a model that describes most nuclear phenomena

[1] Question for undergrad students.

Quantum Mechanics

Hilbert space $\mathcal{H}$

Vector space with scalar product that induces norm and metric and is complete.

I.e. every Cauchy series of its elements converges to its limit in the Hilbert space.

Hamiltonian $\hat{H}$

Sum of kinetic energy operators and potential energy operators acting on all particles in the given Hilbert space.

Schrödinger Equation

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = \hat{H}\psi(\vec{x},t) \tag{1}$$

Dirac Formalism

Bra- $\langle\psi|$ and ket- $|\psi\rangle$ vectors

Hermite conjugates

$$(|\psi\rangle)^+ = \langle\psi| \tag{2}$$

Scalar product example in $\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}x)$

$$\langle\psi|\phi\rangle = \int_{\mathbb{R}} \bar{\psi}(x)\phi(x)\mathrm{d}x \tag{3}$$

Obviously the norm gives

Norm

$$||\psi|| = \langle\psi|\psi\rangle^{\frac{1}{2}} \tag{4}$$

Second Quantization

- creation $(a^\dagger)$ and annihilation (a) operators, particle vacuum $|0\rangle$

One-particle state

$$|\psi\rangle = a^\dagger |0\rangle \tag{5}$$

N-particle state – fully antisymmetric – Slater determinant

$$|\psi\rangle = a_N^\dagger \dots a_2^\dagger a_1^\dagger |0\rangle \tag{6}$$

Pauli exclusion principle – antisymmetrization

$$\{a_i^\dagger, a_j^\dagger\} = a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0 \Rightarrow a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger \tag{7}$$

Isotropic Harmonic Oscillator

Hamiltonian of the HO

$$\hat{H} = \frac{\hat{P}^2}{2M} + \frac{1}{2}M\omega^2\hat{Q}^2 \tag{8}$$

- the eigenstates of $\hat{H}$ in Eq. (8) construct orthogonal basis of the Hilbert space $\mathcal{H}$
  - what are the eigenstates, what is the Hilbert space (?)
- we can parametrize the eigenstates by their quantum numbers

Eigenstates (coupled with spin, nucleons are spin-1/2 fermions)

$$|i\rangle = |n_i l_i j_i m_{j_i}\rangle = a_i^\dagger|0\rangle \tag{9}$$

$$\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}} \tag{10}$$

$$E_i = (2n_i + l_i + \frac{3}{2}) \cdot \hbar\omega \tag{11}$$

Perturbation Theory

Hamiltonian with a perturbation

$$\hat{H} = \hat{H}_0 + \hat{H}' \tag{12}$$

$\hat{H}_0$ – intrinsic, $\hat{H}'$ – perturbation

- let us suppose that we know the eigenstates of $\hat{H}_0$

$$\hat{H}_0 |\psi_m\rangle = E_m |\psi_m\rangle \tag{13}$$

- eigenstates form an orthonormal basis

$$\langle \psi_n | \psi_m \rangle = \delta_{nm}$$
$$\sum_m |\psi_m\rangle\langle\psi_m| = \mathbb{I} \tag{14}$$

Perturbation Theory

First-order correction

$$E_m^{[1]} = \langle \psi_m | \hat{H}' | \psi_m \rangle$$
$$|\psi_m^{[1]}\rangle = \sum_{n \neq m} \frac{\langle \psi_m | \hat{H}' | \psi_m \rangle}{E_m - E_n} |\psi_n\rangle \tag{15}$$

Second-order correction

$$E_m^{[2]} = \sum_{n \neq m} \frac{|\langle \psi_n | \hat{H}' | \psi_m \rangle|^2}{E_m - E_n}$$
$$|\psi_m^{[2]}\rangle = \sum_{k \neq m} \sum_{n \neq m} \frac{\langle \psi_n | \hat{H}' | \psi_m \rangle}{E_m - E_n} \frac{\langle \psi_k | \hat{H}' | \psi_m \rangle}{E_m - E_k} |\psi_k\rangle \tag{16}$$

Hartree-Fock Method

Nuclear Hamiltonian ⇒ Mean Field + Residual Interaction

$$\hat{H} = \sum_{a=1}^{A} \frac{\hat{P}_a^2}{2M_a} + \frac{1}{2} \sum_{a \neq b}^{A} \hat{V}(\vec{r}_a, \vec{r}_b) \Rightarrow \hat{H}_{\mathrm{MF}} + \hat{V}_{\mathrm{res.}} \tag{17}$$

- Nobel prize winning question #1

  What is $\hat{V}(\vec{r}_a, \vec{r}_b)$?

- Nobel prize winning question #2

  How to solve the Schrödinger equation with the Hamiltonian (17)?

- let us now focus on the second (many-body problem) which we can approximatively solve with variational method – Hartree-Fock
- Hilbert's space – set of Slater determinants
- we calculate the minimum of energy: $\langle\psi|\hat{H}|\psi\rangle$ - what is $|\psi\rangle$?

Hartree-Fock Basis

- unitary transformation between two bases – matrix U_{ij}
- we change the HO basis and look for the change in energy

$$E_{\psi'} = \langle \psi' | \hat{H} | \psi' \rangle$$

- iterative method $\psi' \to \psi$ (new basis as an input for the next step)
- we stop when $|E_\psi - E_{\psi'}| < \delta$, where δ is a given precision parameter
- the new basis is called the Hartree-Fock basis and the ground state is called the Hartree-Fock state denoted as $|\mathrm{HF}\rangle$

Hartree-Fock State

$$|\mathrm{HF}\rangle = \prod_{i=1}^{Z} a_i'^{\dagger} |0\rangle_{\mathrm{p}} \otimes \prod_{i=1}^{N} b_i'^{\dagger} |0\rangle_{\mathrm{n}} \tag{18}$$

One-Body Density Matrix

One-Body Density Matrix

$$\rho_{ji} = \langle \mathrm{HF} | a_i^\dagger a_j | \mathrm{HF} \rangle \tag{19}$$

- construction of Natural Orbitals (NO) basis – perturbation theory up to 2^{nd} order

Correlated Wave Function

$$|\Psi_{\mathrm{corr.},m}^{\mathrm{MBPT(2)}}\rangle = |\psi_m^{[0]}\rangle + |\psi_m^{[1]}\rangle + |\psi_m^{[2]}\rangle \tag{20}$$

Correlated One-Body Density Matrix

$$\rho_{ji}^{\mathrm{corr.}} = \langle \Psi_{\mathrm{corr.}}^{\mathrm{MBPT(2)}} | : a_i^\dagger a_j : | \Psi_{\mathrm{corr.}}^{\mathrm{MBPT(2)}} \rangle \tag{21}$$

One-Body Density Matrix

- we need to construct density matrix ρ so that

$$\mathrm{Tr}\rho = A \tag{22}$$

- after a lengthy discussion over occupied and unoccopied single-particle states we arrive at

Total Density Matrix

$$\rho_{ji}^{\mathrm{tot}} = \langle \mathrm{HF}|a_i^{\dagger} a_j|\mathrm{HF}\rangle + \rho_{ji}^{\mathrm{corr.}} \tag{23}$$

- the correlated density matrix is a correction to the total ground-state density matrix

Natural Orbitals

- correlated one-body density matrix is decomposed into 9 terms

$$\rho_{ji}^{\text{tot.}} \approx \rho_{ji}^{00} + \rho_{ji}^{11} + \rho_{ji}^{20} + \rho_{ji}^{02} + (\rho_{ji}^{10} + \rho_{ji}^{01} + \rho_{ji}^{12} + \rho_{ji}^{21} + \rho_{ji}^{22}) \qquad (24)$$

- ρ_{ji}^{10} and ρ_{ji}^{01} are equal to zero[2], $\rho_{ji}^{12}, \rho_{ji}^{21}$, and ρ_{ji}^{22} get neglected
- terms in decomposition (24) are defined as follows:

$$\begin{aligned}
\rho_{ji}^{00} &= \langle \psi_m^{[0]} | a_i^\dagger a_j | \psi_m^{[0]} \rangle \equiv \langle \mathrm{HF} | a_i^\dagger a_j | \mathrm{HF} \rangle \\
\rho_{ji}^{11} &= \langle \psi_m^{[1]} | : a_i^\dagger a_j : | \psi_m^{[1]} \rangle \\
\rho_{ji}^{20} &= \langle \psi_m^{[2]} | : a_i^\dagger a_j : | \psi_m^{[0]} \rangle \\
\rho_{ji}^{02} &= \langle \psi_m^{[0]} | : a_i^\dagger a_j : | \psi_m^{[2]} \rangle \\
&\vdots
\end{aligned} \qquad (25)$$

[2] Brillouin Theorem

Natural Orbitals

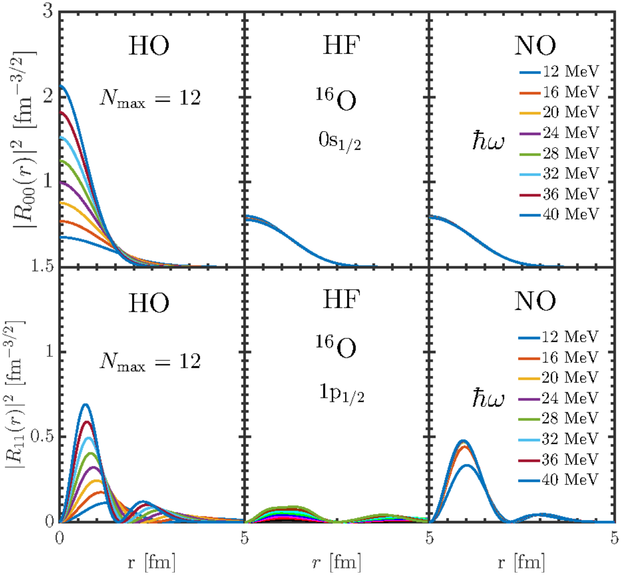
- the diagonalization of the one-body density matrix $\rho^{\text{tot.}}$ yields the basis of natural orbitals (unitary transformation)
- we define new creation and annihilation operators that are linear combinations of the corresponding HF operators – $\tilde{a}_i^\dagger, \tilde{a}_i$ and $\tilde{b}_i^\dagger, \tilde{b}_i$
- new wave function of the ground state (in NO basis)

$$|\mathrm{NAT}\rangle = \prod_h \tilde{a}_h^\dagger |0\rangle_{\mathrm{p}}^{\mathrm{NAT}} \otimes \prod_h \tilde{b}_h^\dagger |0\rangle_{\mathrm{n}}^{\mathrm{NAT}}, \tag{26}$$

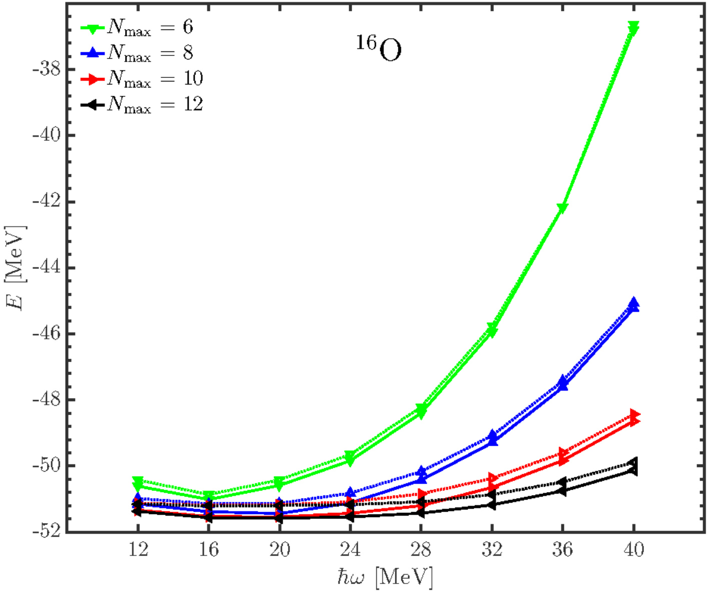
where h runs over first A occupied states

- we define occupied states by "occupation numbers"
- in HF basis occupation numbers are strictly 0 or 1
- in NAT basis the occupation numbers are ≈ 0 or ≈ 1
  - there is a well-defined gap between numbers close to 0 and those close to 1

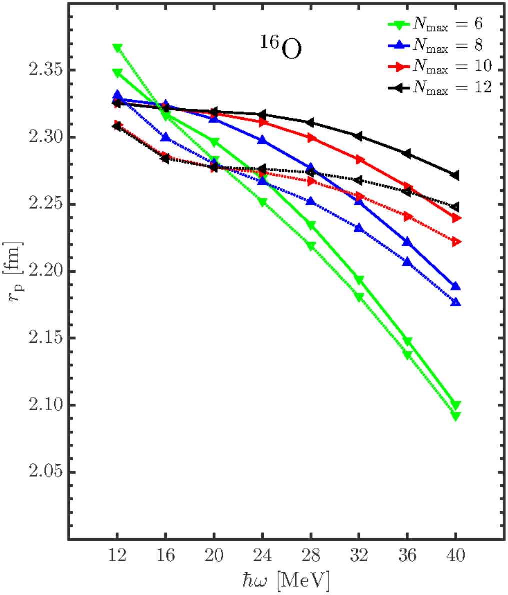
Radial Parts of Wave Functions



Energy of the Ground State of ^{16}O



Point Proton Radius of ^{16}O



Excitations – phonons – Tamm-Dancoff Approximation

- can be used in HF or NAT basis
  - NAT basis improves drastically the convergence of the correlation energy
- particle-hole excitations – phonons – linear combinations of p-h states

TDA Phonon

$$Q_\lambda^\dagger = \sum_{ph} c_{ph}^{\lambda,\mathrm{p}} a_p^\dagger a_h + \sum_{ph} c_{ph}^{\lambda,\mathrm{n}} b_p^\dagger b_h \tag{27}$$

- $c_{ph}^{\lambda,\mathrm{p}}, c_{ph}^{\lambda,\mathrm{n}}$ – linear combination coeff., $a_p^\dagger, b_p^\dagger$ – particle state p, a_h, b_h – hole state h
- particle states – unoccupied (HF basis occ. number 0, NAT basis occ. number ≈ 0)
- hole states – occupied (HF basis occ. number 1, NAT basis occ. number ≈ 1)

Tamm-Dancoff Equation

- 1 phonon excitation

TDA Equation in HF basis

$$\langle \mathrm{HF} | Q_{\lambda'} [\hat{H}, Q_\lambda^\dagger] | \mathrm{HF} \rangle = (E_\lambda - E_{\mathrm{HF}}) \delta_{\lambda' \lambda} \tag{28}$$

- TDA can be used on NAT basis too

2 Phonons – Plan for 2020

- Equation of Motion Phonon Method
  - construction of n-phonon basis from knowledge of $n-1$ phonon basis
  - mean field (HF or NAT) – 0 phonons – known
  - TDA – 1 phonon

Phonon Basis States

$$|\alpha_n\rangle = \sum_{\lambda\alpha_{n-1}} |(Q^\dagger_\lambda \times \alpha_{n-1})^{\alpha_n}\rangle \tag{29}$$

Equation of Motion

$$\langle\beta||[\hat{H}, Q^\dagger_\lambda]^\lambda||\alpha\rangle = (E_\beta - E_\alpha)\langle\beta||Q^\dagger_\lambda||\alpha\rangle \tag{30}$$

- so far – 2 phonon calculations – plan for 2020
  - improvement of the EMPM code

EMPM Calculations

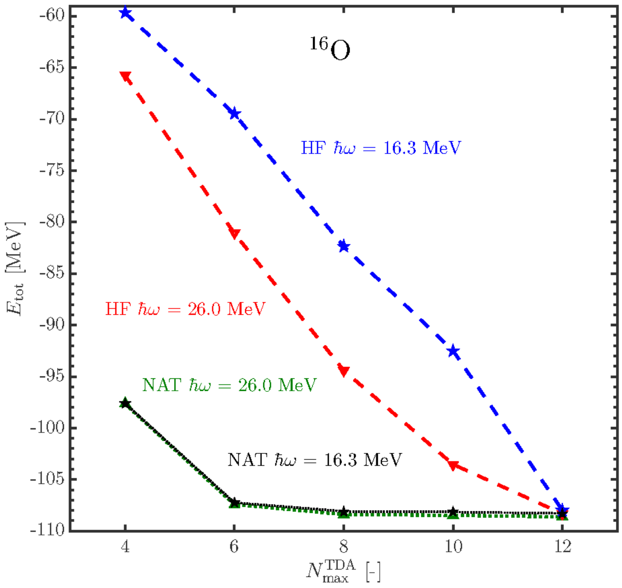
Equation of Motion – expanded

$$\sum_{\lambda'\alpha'\lambda''\alpha''} \left[(E_\lambda + E_\alpha - E_\beta)\delta_{\lambda\lambda'}\delta_{\alpha\alpha'} + \mathcal{V}^{\beta}_{\lambda\alpha\lambda'\alpha'}\right] \mathcal{D}^{\beta}_{\lambda'\alpha'\lambda''\alpha''} C^{\beta}_{\lambda''\alpha''} = 0 \quad (31)$$

- E_β – correlation energy
- $\mathcal{D}^{\beta}_{\lambda'\alpha'\lambda''\alpha''}$ – overlap matrix
- $\mathcal{V}^{\beta}_{\lambda\alpha\lambda'\alpha'}$ – phonon-phonon interaction matrix

- technical difficulties – the dimensions of the matrices

EMPM Calculations in HF and NAT Bases



Summary

- we introduced construction of the basis of natural orbitals (NAT)
  - second-order many-body perturbation theory
- wave functions in NAT basis are more stable than in HF even for the unoccupied states
- energy of the ground state less dependent on $\hbar\omega$, as well as point proton radii
- we document significant improvement of the convergence of correlation energy in 2-phonon calculations