From the NN Interaction to Nuclear Structure and Reactions

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Abstract. We present a novel approach for the treatment of realistic nucleon-nucleon interactions in nuclear many-body systems. A unitary correlation operator is used to explicitly introduce short-range central and tensor correlations in many-body states. The correlated interaction is used as an effective interaction in nuclear structure calculations. Results for Lithium isotopes including proton and neutron distributions, radii as well as magnetic moments and quadrupole moments are shown. Molecular resonances in the ^{16}O-^{16}O system are given as a first application in reaction theory.

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1. Nucleon-Nucleon Interaction

Realistic interactions that fit the nucleon-nucleon scattering data like the Argonne and Bonn interactions possess a strong repulsive core and a strong tensor force that lead to strong short-range correlations in the many-body wave function. These correlations can not be described with the simple many-body states of a mean-field or shell model approach. An explicit treatment of the short-range correlations is necessary. Well known methods are the G-matrix as used for example with the Coupled-Cluster Model or the Lee-Suzuki transformation as used in the No-Core Shell Model (see contributions in these proceedings). Another recent approach is the V_{lowk} [1] that uses renormalization group arguments to derive a low-momentum interaction. All these approaches are formulated either in a shell model basis or in momentum space. In contrast the Unitary Correlation Operator Method (UCOM) [2–4] is formulated in coordinate space and allows us to give explicit expressions for
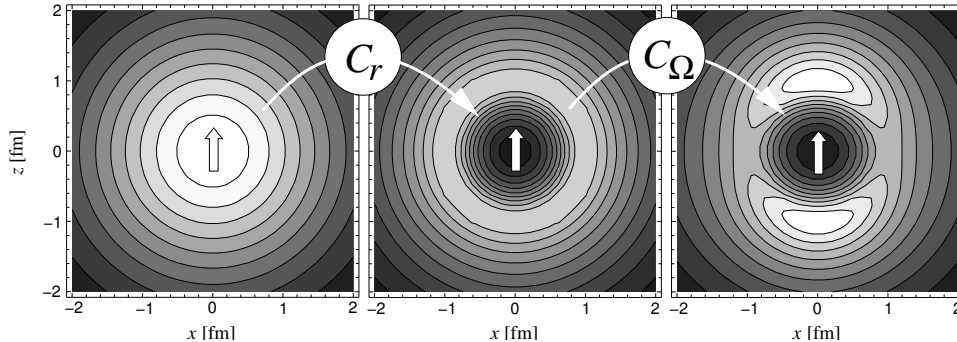
Fig. 1. Two-body density of ^{4}He $\rho^{(2)}(\mathbf{r})$ in the $S = 1, M_S = 1, T = 0$ channel as a function of the distance $\mathbf{r}$ of two nucleons. On the left the uncorrelated two-body density of the trial state is shown. In the middle the central correlator has shifted the nucleons out of the repulsive core into the attractive region of the potential. On the right the tensor correlator has achieved an alignment of the density with the spin of the two nucleons as energetically preferred by the tensor interaction.

the correlated (effective) interaction. The basic idea of the UCOM is to introduce the short-range correlations in the many-body explicitly by means of an unitary correlation operator $C = C_r \cdot C_\Omega$ that is the product of a central correlator C_r and a tensor correlator C_Ω. If the correlation operators are not applied onto the states but onto the operators we obtain correlated operators, e.g. the correlated Hamiltonian $C^\dagger H C$ that can be regarded as an effective interaction.

The central correlator $C_r = \sum_{i<j} \exp\left\{-s(r_{ij})p_{r_{ij}}\right\}$ moves nucleons ij pairwise apart from each other. This is achieved by using the radial part of the relative momentum p_r of the nucleons and a distance dependent shift function $s(r)$. The tensor correlator $C_\Omega = \sum_{i<j} \exp\left\{-\frac{1}{2}\theta(r_{ij})(\sigma_1 \cdot \mathbf{p}_{\Omega_{ij}})(\sigma_2 \cdot \mathbf{r}_{ij}) + 1 \leftrightarrow 2\right\}$ is constructed using the orbital part of the relative momentum of two nucleons $\mathbf{p}_\Omega = \mathbf{p} - \frac{\mathbf{r}}{r}p_r$ and performs shifts perpendicular to the distance vector of the nucleon pair as indicated in Fig. 1.

The parameters of the correlation operators are fixed in the two-body system by a variation with respect to the correlation functions $s(r)$ and $\theta(r)$ in each spin-isospin channel. The correlated interaction is a momentum-dependent soft interaction that can be used directly with simple many-body states. Its matrix elements in momentum space are almost identical to those of the V_{lowk}.

Unfortunately it is not enough to treat the nuclear interaction and the correlations on the two-body level. In our many-body calculations we will use the correlated interaction in a two-body approximation where contributions from three-body correlations are omitted. We also have not included genuine three-body forces in our approach yet. To simulate the effects of these missing parts of the interaction we introduce a two-body correction term (that contributes about 15% to the total

potential) to the interaction that consists of a central momentum-dependent and a spin-orbit part and is fitted to reproduce in the structure calculations the binding energies and charge radii of ^{4}He, ^{16}O and ^{40}Ca and binding energies of ^{24}O, ^{34}Si and ^{48}Ca. For ^{16}O and ^{40}Ca tetrahedral α-cluster configurations are used, all other nuclei are treated as spherical closed-shell configurations.

2. Many-body Approach

The nuclear many-body states in Fermionic Molecular Dynamics (FMD) [4,5] are given by Slater determinants

$$\left| Q \right\rangle = \mathcal{A} \left\{ \left| q_1 \right\rangle \otimes \cdots \otimes \left| q_A \right\rangle \right\} \tag{1}$$

with Gaussian wave packets for the spatial part of the single-particle states

$$\left\langle \mathbf{x} \,\middle|\, q \right\rangle = \sum_i c_i \exp \left\{ -\frac{(\mathbf{x} - \mathbf{b}_i)^2}{2a_i} \right\} \otimes \left| \chi_i^\uparrow, \chi_i^\downarrow \right\rangle \otimes \left| \xi \right\rangle . \tag{2}$$

The spin is given by the spinor $\left| \chi_i^\uparrow, \chi_i^\downarrow \right\rangle$, the isospin $\left| \xi \right\rangle$ can be either proton or neutron. Minimizing the intrinsic energy expectation value of the Slater determinant

$$\min_{\{q_k\}} \frac{\left\langle Q \,\middle|\, H_{eff} - T_{cm} \,\middle|\, Q \right\rangle}{\left\langle Q \,\middle|\, Q \right\rangle} \tag{3}$$

with respect to all the single-particle parameters provides the intrinsic state of the nucleus.

2.1. Restoration of Symmetries

This minimization corresponds to a mean-field calculation in our basis and may yield intrinsic states that violate the symmetries of the Hamiltonian. We perform projections on total momentum, parity and angular momentum to restore the translational and rotational symmetry and the symmetry under parity transformation. We therefore obtain from a single intrinsic state $\left| Q \right\rangle$ projected states

$$\left| Q; J^\pi M K \right\rangle = P_{MK}^J P^\pi P_{\mathbf{P}=0} \left| Q \right\rangle . \tag{4}$$

If the intrinsic state has no axial symmetry we need to consider K-mixing and have to diagonalize the Hamiltonian matrix. The projections are implemented in a straightforward manner as the FMD Slater determinants can be moved and rotated without difficulty.

2.2. Variation after Projection and Multiconfiguration Calculations

For the often strongly deformed and clustered nuclei of the p- and sd-shell the effects of the projection can be large. In principle a Variation after Projection should

be performed. As this is quite costly we do this explicitly only with respect to the parity projection. Beyond that we generate sets of intrinsic states that are obtained by minimizing the energy under constraints on collective variables like dipole moment (Helium isotopes), quadrupole moments (Lithium, Beryllium, Carbon isotopes) or octupole moments (Carbon isotopes). We can then study the projected energy surface as a function of the external constraints. The different intrinsic states can also be used to perform multiconfiguration calculations by diagonalizing the Hamiltonian in this many-body basis

$$
\sum_{bK'} \left\langle Q^{(a)} \left| H P_{KK'}^{J} P^{\pi} P_{\mathbf{P}=0} \right| Q^{(b)} \right\rangle c_{bK'}^{J^{\pi}(i)} =
$$
$$
E^{J^{\pi}(i)} \sum_{bK'} \left\langle Q^{(a)} \left| P_{KK'}^{J} P^{\pi} P_{\mathbf{P}=0} \right| Q^{(b)} \right\rangle c_{bK'}^{J^{\pi}(i)} . \quad (5)
$$

The eigenstates

$$
\left| \Psi; J^{\pi} M(i) \right\rangle = \sum_{bK'} \left| Q^{(b)}; J^{\pi} M K' \right\rangle c_{bK'}^{J^{\pi}(i)} \quad (6)
$$

of the Hamiltonian are then linear combinations of projected Slater determinants. This improves the description of the ground state and is in general necessary to describe states that do not belong to a ground state (rotational) band.

We also observe that the structure of a nucleus is related to the strength of the spin-orbit force. A weak spin-orbit forces favors cluster structures while a strong spin-orbit force usually leads to shell model like structures. As the effects of the angular momentum projection are usually more pronounced for clustered nuclei the
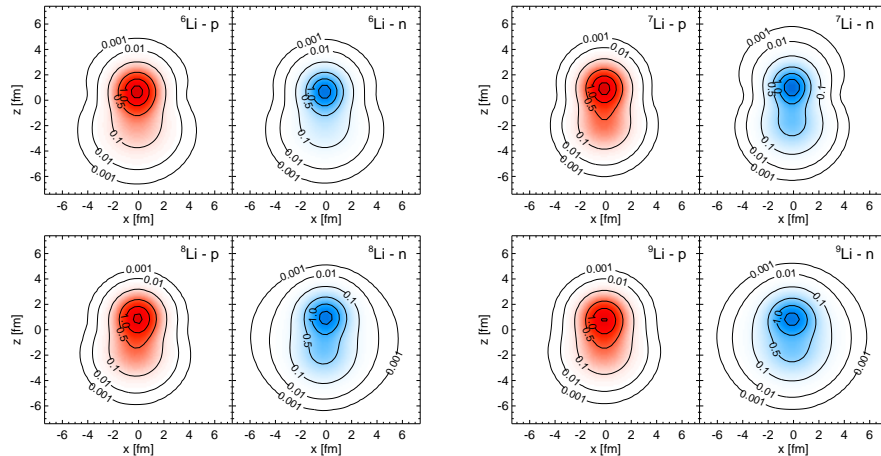
Fig. 2. Cuts through the proton- and neutron densities of intrinsic states with minimum energy obtained in the FMD calculations.

strength of the spin-orbit force can be used as a generator coordinate. The final projected energies are of course always calculated with the same interaction.

3. Nuclear Structure

In this section we illustrate the use of the FMD for the structure of Lithium isotopes. Calculations for Helium, Beryllium and Carbon isotopes have been presented in [6]. We use the quadrupole deformation and the strength of the spin-orbit force as generator coordinates and create sets of six intrinsic states for each isotope. In Fig. 2 the intrinsic states with the lowest projected energies are shown. Obviously the intrinsic states are not parity or angular momentum eigenstates. ^{6}Li and ^{7}Li are to a large extend of α - d and α - t structure. This can be verified by calculating the overlap with Brink type cluster wave functions. For the heavier isotopes ^{8}Li and ^{9}Li the filling of the $p_{3/2}$ neutron orbitals leads to more shell model like structures. This effect can also be observed in the calculated quadrupole moments and charge radii as shown in Tab. 1.

4. Reactions

The FMD basis is also very well suited for doing reaction theory. The possibility to localize wave packets allows us to construct Brink type cluster model wave functions as FMD many-body states. These cluster model wave functions are used in the asymptotic region to define proper asymptotics for the formulation of the boundary conditions. In the internal region we can use for example adiabatic configurations in addition to the cluster wave functions. We can directly use our effective interaction which provides a good description of nuclear structure properties in the reaction theory.

As a first example we have calculated molecular resonances in the ^{16}O-^{16}O

Table 1. Experimental and calculated properties of Lithium isotopes.

| J^π		E_B [MeV]	μ [μ_N]	Q [e^2fm^4]	r_{matter} [fm]	r_{charge} [fm]
^{6}Li	FMD	31.42	+0.85	+0.08	2.44	2.58
1^+	Experiment	31.995	+0.822	-0.083(8)	2.32(3)	2.55(3)
^{7}Li	FMD	39.26	+3.25	-3.61	2.40	2.42
$3/2^-$	Experiment	39.245	+3.256	-4.06	2.33(2)	2.40(5)
^{8}Li	FMD	40.16	+1.73	+2.76	2.42	2.37
2^+	Experiment	41.277	+1.654	3.17(4)	2.37(2)	
^{9}Li	FMD	44.36	+3.48	-3.22	2.43	2.30
$3/2^-$	Experiment	45.341	3.439	2.78(8)	2.32(2)	

reaction where we used angular momentum projected GCM many-body states

$$\big| \Psi^{JM}(R) \big\rangle = P_{M0}^J \big| \Psi(\mathbf{R}) \big\rangle \tag{7}$$

with

$$\big| \Psi(\mathbf{R}) \big\rangle = \mathcal{A}\{ \big| {}^{16}\text{O}; \tfrac{1}{2}\mathbf{R} \big\rangle \big| {}^{16}\text{O}; -\tfrac{1}{2}\mathbf{R} \big\rangle \} \tag{8}$$

In the asymptotic region a transformation in the corresponding RGM wave function is performed and Gamov boundary conditions (purely outgoing Coulomb wave) are assumed for the relative motion of the nuclei. With this boundary conditions we solve the Schrödinger equation in the interaction region. The complex eigenvalues of this eigenvalue problem directly give resonance energies and widths. In Fig. 3 the first two calculated molecular bands are shown.
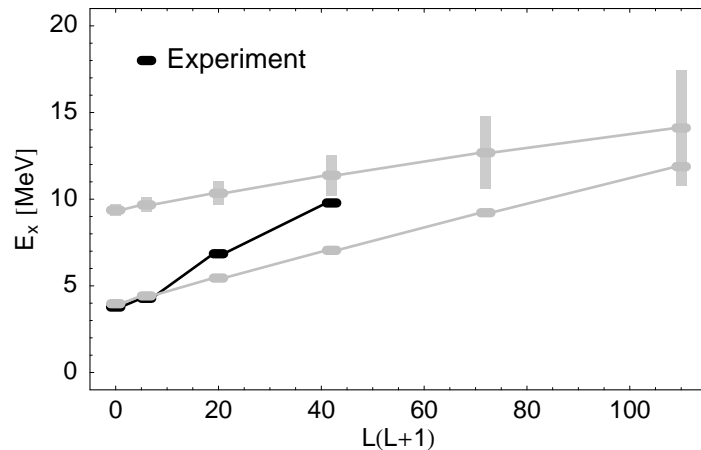
Fig. 3. Molecular resonances in the ^{16}O-^{16}O system calculated in the FMD framework. Gray bars indicate the calculated widths. The experimental data show a good agreement for low angular momentum with the calculated resonances. For higher angular momentum a stronger mixing with the ground state band of ^{32}S is expected but not yet included in the FMD calculation.

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