Nuclear structure and reactions in the Fermionic Molecular Dynamics approach

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Abstract. The Fermionic Molecular Dynamics (FMD) model uses Gaussian wave packets as single-particle states. Intrinsic many-body basis states are constructed as Slater determinants which have to be projected on parity, angular momentum and total linear momentum to restore the symmetries of the Hamiltonian. The flexibility of the Gaussian basis allows to economically describe states with shell structures as well as states featuring clustering or halos. We use an effective interaction that is derived from the realistic Argonne V18 interaction by means of the Unitary Correlation Operator Method (UCOM). A phenomenological momentum-dependent two-body correction simulates contributions from missing three-body forces and three-body correlations. We discuss $^{12}$C with a special emphasis on the structure of the excited $0^+$ and $2^+$ states. We analyze the degree of $\alpha$-clustering and confirm, taking inelastic electron scattering data into account, the conjecture that the Hoyle state has to be understood as a loosely bound system of alpha particles. We will also present first results on the application of FMD for the calculation of scattering phase shifts in $^3$He – $^4$He.

1. Introduction

In recent years ab initio calculations for light nuclei have become possible. The Green’s Function Monte Carlo Method (GFMC) [1] or the No-Core Shell Model (NCSM) [2] allow to calculate the properties of light nuclei with realistic two- and three-body forces. However because of the huge numerical effort these approaches are currently only viable for very light nuclei. Furthermore the harmonic oscillator basis used in the NCSM is not very well suited for the description of loosely bound systems with halos or clustering. The famous first excited $0^+$ state in $^{12}$C is completely missing in NCSM calculations. Such cluster states have been described quite successfully in cluster models where the $\alpha$-particles are the constituents. On the other hand cluster models are not able to describe the single-particle structure of shell model like configurations. In the ground state band of $^{12}$C the $\alpha$-cluster structure is broken by the spin-orbit force and the $p_{3/2}$ orbits are preferred over the $p_{1/2}$ orbits.

In the Antisymmetrized Molecular Dynamics (AMD) [3] and Fermionic Molecular Dynamics (FMD) [4] approaches one uses Gaussian wave packets as single-particle states. The Gaussian wave-packets have the great advantage that shell model states and Brink-type cluster wave functions are just special limiting cases in this basis.

2. Unitary Correlation Operator Method

In the FMD approach we use an effective interaction that is derived from the realistic Argonne V18 interaction by means of the Unitary Correlation Operator Method (UCOM) [5]. Short-range
central and tensor correlations, which are essential for a successful description of the nuclear many-body state, are treated explicitly by a unitary correlation operator. In Fig. 1 the two-body uncorrelated and correlated two-body densities are shown for \(^4\)He. One can see how the central correlation operator shifts nucleons apart, out of the repulsive core of the interaction into the region of most attraction at about 1fm distance. The tensor correlation operator then aligns the probability with the orientation of the spins of the nucleons. The correlated Hamiltonian is evaluated in a two-body approximation and has been tested in exact calculations for the 3- and 4-body systems [6]. We are missing genuine three-body forces and three-body correlations and also suffer from some restrictions of the FMD model space regarding the treatment of medium range tensor correlations. To obtain good agreement with experimental observations we simulate these missing components for now by a two-body correction term with momentum dependence and an additional spin-orbit force. The correction term is fitted to reproduce binding energies and radii of doubly-magic nuclei [7] and contributes about 15% to the potential energy.

3. Fermionic Molecular Dynamics
3.1. Basis
The FMD basis states are Slater determinants

\[
|\psi\rangle = \mathcal{A}\{|q_1\rangle \otimes \ldots \otimes |q_A\rangle\}.
\]

The single-particle states are given by a single or a superposition of Gaussian wave packets

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

The complex parameter \(\vec{b}\) encodes the mean position and the mean momentum of each wave packet. The parameter \(a\) describes the spread of the wave packet in coordinate and momentum space. The spin of each wave packet is given by a spinor that allows orientation in all directions. The isospin can assume values of \(\pm 1\) describing protons and neutrons respectively.

The wave packets provide a very flexible basis. Localized wave packets can be used to create cluster wave functions in the Bloch-Brink sense. Harmonic oscillator single-particle wave functions are obtained by linear combinations (provided by antisymmetrization) of slightly shifted Gaussians. Loosely bound nucleons require width parameters \(a\) that are much larger than those of nucleons in the core. Different widths are also helpful if one has a competition
between shell model states, which prefer larger widths, and cluster states, which prefer smaller widths to describe the clusters.

In the simplest FMD approach the many-body wave function is obtained by minimizing the expectation value of the intrinsic energy

$$E[|Q\rangle] = \frac{\langle Q|H - T_{\text{cm}}|Q\rangle}{\langle Q|Q\rangle}$$

with respect to all the single-particle parameters. This corresponds to a Hartree-Fock calculation in the restricted FMD model space.

3.2. Projection after Variation, Variation after Projection

The many-body states obtained in the minimization in general no longer possess the symmetries of the Hamiltonian with respect to parity, rotational and translational invariance. To restore the symmetries the intrinsic wave function is projected on parity and angular momentum with the projection operators

$$P^\pi = \frac{1}{2}(1 + \pi \Pi)$$

and

$$P^{\vec{J}\vec{M}K\vec{P}}_\sim = \frac{2J + 1}{8\pi^2} \int d\Omega \, D^{\vec{J}\vec{M}K\vec{P}}_\sim^* (\Omega) R(\Omega) \cdot .$$

For the special case of identical width parameters $a$ for all the single-particle states the total wave function separates in the intrinsic and the center-of-mass wave function. In the general case the FMD wave function has to be projected on total momentum $\vec{P} = 0$ to restore the translational invariance of the wave function.

$$P^\vec{P} = \frac{1}{(2\pi)^3} \int d^3X \exp\{-i(\vec{P} - \vec{P}) \cdot \vec{X}\}$$

The effects of projection can be quite large especially for nuclei in the $p$-shell. Therefore the results of a variation after projection (VAP) can be quite different from the simple projection after variation (PAV) approach. A full VAP calculation is quite costly and can only be performed for light nuclei. For heavier nuclei a variation after parity projection (VAP$^\pi$) is combined with a VAP in the sense of the generator coordinate approach. The energy is minimized under constraints on certain generator coordinates like radius or quadrupole deformation. The states obtained in this manner are later projected on angular momentum and the state of minimum energy is found in the energy surface as a function of the generator coordinates.

3.3. Multiconfiguration

In general we will obtain for each nucleus a set of intrinsic states $|Q^{(a)}\rangle$. To calculate the eigenstates of the Hamiltonian the generalized eigenvalue problem

$$\sum_{K'K} \langle Q^{(a)}| (H - T_{\text{cm}}) P_{KK'}^{J \vec{P}} P^{\vec{P}=0} |Q^{(b)}\rangle \cdot c_{K'b}^{(i)} = E^{J \vec{P}}(i) \sum_{K'K} \langle Q^{(a)}| P_{KK'}^{J \vec{P}} P^{\vec{P}=0} |Q^{(b)}\rangle \cdot c_{K'b}^{(i)}$$

has to be solved. Technically we first perform a $K$-mixing calculation for each intrinsic state and then diagonalize the Hamiltonian in the set of $K$-mixed eigenstates. In both calculations a singular value decomposition is performed to take care of linear dependent states within our set of non-orthogonal basis states.
4. Cluster States in $^{12}$C

As indicated the FMD wave functions are flexible enough to describe both shell model and cluster configurations. It is therefore an ideal tool to study the spectrum of $^{12}$C. The ground state band of $^{12}$C is well described in a shell model picture. The shell model on the other hand completely fails to describe the first excited $0^+$ state $[8, 9]$, the famous Hoyle state. Our aim is to get a consistent picture within the FMD approach including the shell model like ground state band and the cluster states in $^{12}$C $[10]$. We will also compare to a pure microscopic cluster model to get a better understanding with regard to features and problems of the different approaches. For the cluster model we use the same modified Volkov interaction as Kamimura $[11, 12]$ used in his RGM calculations. It has been adjusted to reproduce the $^{12}$C ground state energy with respect to the three-alpha threshold. This interaction has also been used in $[13]$ where the cluster model results were reproduced with an ansatz of condensate wave functions.

Our cluster model calculation makes use of Bloch-Brink type wave functions $[14]$ where we define a complete $\alpha$-cluster model basis using 165 configurations. A converged result for the three lowest $0^+$ states is obtained by selecting 55 of these basis states in an iterative procedure. In the FMD calculation we build our many-body basis with 16 states obtained in full VAP calculations for $0^+$ and $2^+$ states with different radii. In addition we selected additional 57 configurations out of FMD states obtained in variation after parity projection with constraints on radius and quadrupole deformation and the $\alpha$ cluster configurations.

In Fig. 2 the spectra obtained in both approaches are compared with experimental data. In both approaches the Hoyle state is found like in experiment slightly above the 3-$\alpha$ threshold. In the cluster model a typical shortcoming is the too small excitation energy of the first $2^+$ state, which is a result of the missing spin-orbit force. This problem is not found in the FMD calculation. In the FMD calculations we also find an improved description of the negative parity states. Another interesting point concerns the second $2^+$ and the third $0^+$ state. The experimental situation for these states is not settled yet. The $2^+_2$ has been seen in $\alpha$-scattering $[15]$ at 2.7(3)MeV which agrees with the FMD calculations but could not be found in $\beta$-decay studies $[16, 17]$. The third $0^+$ state has a very large width which makes it difficult to determine precisely its energy. The present calculations also use a bound state approximation which might influence the results, especially for broad states.

A characteristic feature of the excited $0^+$ and $2^+$ states is their very large radius. The rms point radii in the FMD approach are 2.39 fm for the ground state, 3.38 fm for the Hoyle state and 4.62 fm for the $0^+_3$ state. The $2^+_1$ state has a radius of 2.50 fm while the $2^+_2$ again has a
very large radius of 4.43 fm. To further analyze our results we calculate the overlap of the FMD eigenstates with the $\alpha$-cluster space. For that we define a projection operator $P_{\alpha}$ with our 165 $\alpha$-cluster configurations. We find $\langle 0_1^+ | P_{\alpha} | 0_1^+ \rangle = 0.52$, $\langle 0_2^+ | P_{\alpha} | 0_2^+ \rangle = 0.85$, $\langle 0_3^+ | P_{\alpha} | 0_3^+ \rangle = 0.92$, $\langle 2_1^+ | P_{\alpha} | 2_1^+ \rangle = 0.67$ and $\langle 2_2^+ | P_{\alpha} | 2_2^+ \rangle = 0.99$. The ground state therefore has a large admixture of non-cluster shell model configurations whereas the Hoyle state is dominated by spatially extended cluster configurations but still has a sizeable admixture of shell model configurations. The $2_2^+$ state on the other hand is almost purely of cluster nature which might explain why it is not seen in the $\beta$-decay experiments. The GT transition strength to this state is proportional to the very small admixture of shell model configurations. We can furthermore analyze the FMD and cluster model wave functions in terms of harmonic oscillator basis used by the no-core shell model. The occupation numbers displayed in Fig. 3 show that the FMD ground state is essentially a $p$-shell configuration in contrast to the Hoyle state where about half of the nucleons are distributed in a coherent fashion over many harmonic oscillator orbits. This explains why the Hoyle state is not accessible even in the largest no-core shell model calculations.

A further test of the wave functions is a comparison with electron scattering cross sections. This is a direct way to measure the spatial extension of the wave function. In Fig. 4 we compare the cross sections calculated with DWBA for the FMD and cluster model wave functions with experimental data. For the elastic scattering on the ground state the FMD wave function

**Figure 3.** Occupation numbers of harmonic oscillator single-particle orbits for the ground (left) and the Hoyle state (right) calculated with the FMD wave functions.

**Figure 4.** Electron scattering cross-sections for elastic scattering on the ground state (left) for inelastic scattering into the Hoyle state (right).
provides an almost perfect description of the cross section, the cluster model is only slightly off. The cross section for the transition into the Hoyle state on the other hand is better described by the cluster model wave function but also the FMD results are not that far off. The good agreement with experiment confirms the picture of a spatially extended Hoyle state.

5. Resonances, Scattering States and Reactions

The FMD basis is also very well suited for the description of nuclear reactions. In the asymptotic channels the wave function is constructed using Brink-type cluster wave functions where the clusters are given by the corresponding FMD states. In this sense the FMD approach is very similar to microscopic cluster models. In the interaction region, where the clusters overlap, additional FMD configurations are added. The difficult part is to include the proper boundary conditions for resonances and scattering states. Asymptotically we have to match the FMD many-body wave functions with the known Coulomb solutions for two point-like nuclei. To perform this matching we developed the so-called “Collective Coordinate Method” [18]. In Fig. 5 we show first results for the calculation of $^3\text{He} - ^4\text{He}$ phase shifts.

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