Few-nucleon systems studies with extended antisymmetrized molecular dynamics

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Abstract. Ground-state properties of three- and four-nucleon systems are studied with the angular momentum and parity projected antisymmetrized molecular dynamics. The Hamiltonian is constructed with realistic nucleon-nucleon interactions. The calculated ground-state energies, root-mean-square radii, and magnetic dipole moments are compared with the experimental results. In overall, the ground-state properties of the light nuclei considered are satisfactorily described.

1. Introduction

The structure of few-nucleon systems has been the subject of numerous theoretical and experimental investigations and reviews on a variety of their aspects can be found in the literature (see, for example, Refs. [1, 2]). The simplicity of these systems allows for an exact description and rigorous solutions of the corresponding dynamical equations can be obtained and thus accurate wave functions for bound states can now be constructed using realistic Hamiltonians. An illustration of the level of accuracy in describing ground state properties of the four-nucleon system by seven different state-of-the-art methods is given in Ref. [3]. However, the practical application of these methods become quite complicated as the number of particles involved increases and thus going beyond the $A = 4$ systems using exact methods still is a challenge.

In recent years, a very promising method, namely, the Antisymmetrized Molecular Dynamics (AMD), has been used to study the properties of A-particle systems. The AMD approach [4] is developed from the Time-Dependent Cluster Model [5] describing fermionic systems. This approach combines Fermi-Dirac statistics with quantum mechanics to treat the motion of the A particles [6]. Although the model is not fully quantum mechanical and does not assume a shell structure for the system, improved AMD wave functions are, nowadays, shown to give good predictions of the properties of few-body systems [7, 8]. In the present work the parity projected and angular momentum projected version of the AMD [9] is employed.

In Sect. 2 the general formalism of the AMD approach is summarized and the construction of the wave function, the equations of motion of the variable parameters, and the variational technique used are briefly outlined. Theoretical predictions of the ground state properties of three-nucleon and four-nucleon systems are presented in Sect. 3 while the conclusions drawn are given in Sect. 4.

2. The AMD formalism

The AMD wave function describing a system of A nucleons is constructed as a Slater determinant

$$\Psi_{AMD}(\vec{\mathrm{S}}) = \frac{1}{\sqrt{A!}} \det[\,\phi_j(\alpha, \vec{s}_i), \chi_j(\vec{\sigma}_i), \xi_j(\vec{\tau}_i)\,] \tag{1}$$

where ϕ, χ and ξ are, respectively, the spatial, spin and isospin components of the single-particle wave functions. The $\vec{s}_i$ are complex variational parameters, $\vec{\mathrm{S}} \equiv \{\vec{s}_1, \vec{s}_2, \vec{s}_3, \ldots, \vec{s}_A\}$, while α is a real constant width parameter. The single nucleon wave functions are given by [10]

$$\psi_i(\vec{r}_j) = \left(\frac{2\,\alpha}{\pi}\right)^{2/4} \exp\left[-\alpha\left(\vec{r}_j - \frac{\vec{s}_i(t)}{\sqrt{\alpha}}\right)^2 + \frac{1}{2}\,\vec{s}_i^{\,2}(t)\right] \otimes \chi_i \otimes \xi_i \tag{2}$$

where $\chi_i \otimes \xi_i \;\equiv \{\, N\otimes\uparrow \text{or} N\otimes\downarrow\}$ are the fixed spin-isospin states of the i-th nucleon, which represent nucleon with spin-up or spin-down. The width parameter is a free parameter and is common for all Gaussians terms.

A wave function with a definite parity π, a total angular momentum J, and angular momentum projection M, is constructed from the AMD wave function as

$$\Psi^{J\pi}_{MK}(\vec{\mathrm{S}}) = \frac{1}{2}\, P^J_{MK}(\Omega)\,[\,1 \pm P^\pi\,]\,\Psi_{AMD}(\vec{\mathrm{S}}) \tag{3}$$

where $P^J_{MK}(\Omega)$ is the angular momentum projection operator, P^π the parity projection operator. The angular momentum projection operator is defined by [11]

$$P^J_{MK}(\Omega) = \frac{2\,J+1}{8\,\pi^2} \int \mathrm{d}\Omega\, D^{J*}_{MK}(\Omega)\, \hat{R}(\Omega) \tag{4}$$

where $D^J_{MK}(\Omega)$ is the Wigner D-function, $\hat{R}(\Omega)$ the rotation operator and $\Omega \equiv \{\alpha, \beta, \gamma\}$ represents the Euler rotation angles.

The time-dependent variational principle [10]

$$\delta \int_{t_1}^{t_2} \frac{\langle\, \Psi(\vec{S})\,|\, \mathrm{i}\hbar\,\frac{\partial}{\partial t} - H \,|\, \Psi(\vec{S})\,\rangle}{\langle\, \Psi(\vec{S})\,|\,\Psi(\vec{S})\,\rangle}\, \mathrm{d}t = 0 \tag{5}$$

with the constraints

$$\delta\Psi(t_1) = \delta\Psi(t_2) = \delta\Psi^*(t_1) = \delta\Psi^*(t_2) = 0. \tag{6}$$

is used to determine the dynamical equations for the variational parameters. The resulting equations can be transformed into the form [12]

$$\frac{\mathrm{d}\vec{s}_i}{\mathrm{d}t} = -b\,\frac{\partial E^{J\pm}_0(\vec{S}, \vec{S}^*)}{\partial \vec{s}^{\,*}_i} \quad , \quad \frac{\mathrm{d}\vec{s}^{\,*}_i}{\mathrm{d}t} = -b\,\frac{\partial E^{J\pm}_0(\vec{S}, \vec{S}^*)}{\partial \vec{s}_i} \tag{7}$$

where b is an arbitrary positive real constant and $E^{J\pm}_0(\vec{S}, \vec{S}^*)$,

$$E^{J\pm}_0(\vec{S}, \vec{S}^*) = \frac{\langle\, \Psi^{J\pm}_{MK}(\vec{\mathrm{S}})|\, H\,|\Psi^{J\pm}_{MK}(\vec{\mathrm{S}})\,\rangle}{\langle\, \Psi^{J\pm}_{MK}(\vec{\mathrm{S}})|\Psi^{J\pm}_{MK}(\vec{\mathrm{S}})\,\rangle}. \tag{8}$$

is the variational energy determined from the Hamiltonian H of the nucleus given by

$$H = -\sum_i \frac{\hbar^2}{2\,m_i}\,\nabla^2_i + \frac{1}{2}\sum_{i\neq j}\Big[\,V_{NN}(\vec{r}_{ij}) + V_C(\vec{r}_{ij})\,\Big] \tag{9}$$

where m_i is the mass of nucleon i, $V_{NN}(\vec{r})$ the two-body nuclear potential, $V_C(\vec{r})$ the Coulomb potential and $\vec{r}$ the relative position vector of the interacting nucleons. In this work the AV4′ NN potential with the $V_{C1}(\vec{r})$ Coulomb component is used [13]. The evaluation of the energy expectation values is explained in Ref. [14].

Table 1. AMD results for the ground-state energies E_0, rms radii $\langle r^2 \rangle^{1/2}$, and magnetic moments μ of the three- and four-nucleon systems. The experimental values are taken from reference [15].

	E_0 (MeV)		$\langle r^2 \rangle^{1/2}$ (fm)		μ (μ_N)	
	AMD	EXP	AMD	EXP	AMD	EXP
^{3}H $\left(\frac{1}{2}^+\right)$	-8.95	-8.48	1.33	1.60	2.769	2.979
^{3}He $\left(\frac{1}{2}^+\right)$	-8.61	-7.72	1.33	1.77	-1.847	-2.128
^{4}He $\left(0^+\right)$	-23.04	-28.30	1.16	1.47	0.000	

3. Ground state properties

The "frictional cooling" equations (7) were solved with the values $b \approx 30/\hbar$ and $\alpha = 0.12$. The α is chosen to reproduce, to reasonable accuracy, the ground state energies of light nuclei using only the parity-projected wave functions. The variational energy for the three- and four-nucleon systems was calculated using Eq. (8) and the results obtained are compared with experimental data in Table 1. The root-mean-square (rms) radii of the nuclei were calculate using the expression

$$\left\langle r^2 \right\rangle_{MK} = \frac{1}{A} \frac{\langle \Psi^{J\pm}_{MK} \,|\, \sum_{i=1}^{A} [\vec{r}_i - \vec{R}]^2 \,|\, \Psi^{J\pm}_{MK} \rangle}{\langle \Psi^{J\pm}_{MK} \,|\, \Psi^{J\pm}_{MK} \rangle} \tag{10}$$

where A is the number of nucleons in the nucleus and $\vec{R}$ the center-of-mass of the nucleus. The results obtained are also presented in Table 1.

As can be seen, the binding energy found for the ^{3}H system overestimates the experimental energy by 5 % and for the ^{3}He system by 12 % while . In contrast, the ^{4}He results are lower than the experimental value by $\sim$ 19 %, a result which is in line with other calculations in the field using the same rank in the potential and without the use of three-body forces. The rms radii obtained for the ^{3}H and ^{3}He systems are lower than the experimental values by $\sim$ 16 % and $\sim$ 22 % less, respectively. Similar results are obtained for the ^{4}He system where the calculated rms radius is underestimated by $\sim$ 21 %.

We turn now our attention to the magnetic moment of a nucleon which is given (in nuclear magnetons) by [16]

$$\mu = g_\ell \langle \vec{\ell} \rangle + g_s \,\langle \vec{s} \rangle \tag{11}$$

where $\langle \vec{\ell} \rangle$ ($\langle \vec{s} \rangle$) is the expectation value of the orbital (spin) angular momentum and g_ℓ (g_s) the orbital (spin) g-factor of the nucleon. The nucleon g-factors are constants, the values of which are [16]

$$g_\ell = \begin{cases} 1 & \text{for proton} \\ 0 & \text{for neutron} \end{cases} \quad : \quad g_s = \begin{cases} 5.585695 & \text{for proton} \\ -3.826085 & \text{for neutron} \end{cases} \tag{12}$$

The magnetic moment of the nuclei $\vec{\mu}_A$ is calculated from

$$\vec{\mu}^{\pm}_{MK} = \frac{\langle \Psi^{J\pm}_{MK} \,|\, \sum_{i=1}^{A} [\, g_\ell \,\vec{\ell}_i + g_s \,\vec{s}_i \,] | \, \Psi^{J\pm}_{MK} \rangle}{\langle \Psi^{J\pm}_{MK} \,|\, \Psi^{J\pm}_{MK} \rangle} \,. \tag{13}$$

The values of the magnitude $\mu^{\pm}_{MK} = |\,\vec{\mu}^{\pm}_{MK}|$ for the three- and four-nucleon systems are given in Table 1. In general, the AMD approach reproduces the experimental values for the magnetic moment of the nuclei quite satisfactorily.

4. Conclusions

To test the suitability of the AMD model in nuclear structure studies, the angular momentum and parity projected AMD wave function was used to calculate the binding energies, rms radii, and the magnetic moments for ^{3}H, ^{3}He, and ^{4}He few-nucleon systems. The nuclear Hamiltonian is constructed from the Argonne AV4$'$ nucleon-nucleon potential that includes also the Coulomb interaction.

Comparison with the experimental data revealed that the reproduction of the ground-state properties of light nuclei is quite satisfactory. The discrepancies observed can be attributed to reasons not related to the AMD. These include i) the omission of mixed-symmetric states (for three-body) ii) the use of a limited rank for the Argonne AV18 potential, and iii) the omission of three-nucleon forces. As far as the magnetic moment is concerned, the inclusion of relativistic corrections to the magnetic moment operator, are also expected to contribute to the reduction of the discrepancy between theory and experiment.

It short, we demonstrated that it is possible to construct a variational AMD wave function using realistic nucleon-nucleon potentials. The inclusion of three-nucleon forces in the Hamiltonian is also possible and this is expected to reduce the overall discrepancy between the experimental observation and theoretical AMD predictions of the nuclear properties. It should be noted that in nuclear systems described with spherical wave functions, like the ^{4}He nucleus, spatial rotations are not expected to introduce modifications to the results obtained with the parity-projected wave functions and therefore the use of the AMD method should be accurate.

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