Structure of Few-Nucleon Systems Studied with the Extended Antisymmetrized Molecular Dynamics

G J Rampho and S A Sofianos

Department of Physics, University of South Africa, Pretoria 0003, South Africa

E-mail: `rampho@science.unisa.ac.za`

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

1. Introduction

The structure of few-nucleon systems is widely and continuously investigated, both theoretically and experimentally, mainly because of the simplicity of the systems. Reviews on a variety of aspects of nuclear structure can be easily found in the literature [1, 2]. Over the years a variety of theoretical methods have been developed and refined in the study of few-body systems. Very accurate wave functions for bound states in few-nucleon systems can now be constructed using realistic Hamiltonian for the systems. A demonstration of the level of accuracy in describing ground state properties of the four-nucleon system by seven different state-of-the-art methods is shown in reference [3]. The practical application of these methods become quite involved as the systems become slightly increased. This work focuses on the use of one of the microscopic simulation methods, the antisymmetrized molecular dynamics (AMD) in the study of ground state properties of three-nucleon and four-nucleon systems. These type of methods are continuously developing.

The AMD approach was developed [4] from the Time-Dependent Cluster Model [5] for the study of fermionic systems. This approach combines Fermi-Dirac statistics with elementary quantum mechanics to treat the motion of particles in a system [6]. However, the model is not fully quantum mechanical and does not assume a shell structure for the system. Improved AMD wave functions are shown to give good predictions of few-body systems [7, 8]. In this work the parity projected and angular momentum projected AMD approach [9] is employed.

In the next Section 2 the general formalism of the AMD approach is summarised. In this section 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 ground state properties of three-nucleon and four-nucleon systems are presented in Section 3. Conclusions drawn are given in Section 4.

2. The AMD Formalism

The antisymmetrised molecular dynamics (AMD) wave function describing a nuclear 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-nucleon wave functions. The spatial components are non-orthogonal Gaussian with complex variational parameters $\vec{s}_i$. The width parameter α is taken as real and free. A wave function with definite parity(π) and total angular momentum (J) with the angular momentum projection (M) is constructed from the AMD wave function as

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

where $P_{MK}^{J}(\Omega)$ is the angular momentum projection operator, P^{π} the parity projection operator and $\vec{\mathrm{S}} \equiv \{\vec{s}_1, \vec{s}_2, \vec{s}_3, \ldots, \vec{s}_A\}$. The angular momentum projection operator is defined by [10]

$$P_{MK}^{J}(\Omega) \; = \; \frac{2\,J+1}{8\,\pi^2} \int \mathrm{d}\Omega\, D_{MK}^{J*}(\Omega)\, \hat{R}(\Omega) \tag{3}$$

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

The single particle wave functions are given by

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

where $\chi_i \otimes \xi_i$ are the fixed spin-isospin states of the i-th nucleon. These states are compactly expressed in the form $\kappa_i = \{\, N\uparrow$ or $N\downarrow\,\}$ for nucleon with spin-up or spin-down. The Gaussian width parameter α is a real constant and the variational parameter $\vec{s}(t)$ is complex. The time-dependent variational principle [11]

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

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]

$$\frac{\mathrm{d}\vec{s}_i}{\mathrm{d}t} = -\mu\,\frac{\partial E_0^{J\pm}(\vec{S}, \vec{S}^*)}{\partial \vec{s}_i^*} \qquad , \qquad \frac{\mathrm{d}\vec{s}_i^*}{\mathrm{d}t} = -\mu\,\frac{\partial E_0^{J\pm}(\vec{S}, \vec{S}^*)}{\partial \vec{s}_i} \tag{7}$$

where μ is an arbitrary positive real constant and

$$E_0^{J\pm}(\vec{S}, \vec{S}^*) \; = \; \frac{\langle\, \Psi_{MK}^{J\pm}(\vec{\mathrm{S}})|\,H\,|\Psi_{MK}^{J\pm}(\vec{\mathrm{S}})\,\rangle}{\langle\, \Psi_{MK}^{J\pm}(\vec{\mathrm{S}})|\Psi_{MK}^{J\pm}(\vec{\mathrm{S}})\,\rangle} \;\;. \tag{8}$$

the variational energy of the nucleus. Solving these equations minimizes E_0 and determines the variational parameters. The Hamiltonian of the system is given by

$$H \; = \; -\sum_i \frac{\hbar^2}{2\,M_i}\,\nabla_i^2 + \frac{1}{2}\sum_{i \neq j}\left[\,V_{NN}(\vec{r}_{ij}) + V_C(\vec{r}_{ij})\,\right] \tag{9}$$

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

3. Ground State Properties

The variational energy for the three-nucleon and four-nucleon systems were calculated from equation (8). The results are compared with experimental data in Table 1. The theoretical energy for the ^{3}H system overestimates the experimental energy by 5 % and for the ^{3}He system the experimental energy is overestimated by 12 %. Since the nuclear systems are described with spherical wave functions, spatial rotations are not expected to introduce significant modifications to the results obtained with the unprojected wave functions.

The root-mean-square radii of the nuclei were calculate using the expression

$$\left\langle r^2 \right\rangle_{MK} = \frac{1}{A} \frac{\langle \Psi_{MK}^{J\pm} | \sum_{i=1}^{A} \left(\vec{r}_i - \vec{R} \right)^2 | \Psi_{MK}^{J\pm} \rangle}{\langle \Psi_{MK}^{J\pm} | \Psi_{MK}^{J\pm} \rangle} \tag{10}$$

where A is the number of nucleons in the nucleus and $\vec{R}$ the center-of-mass of the nucleus. The results obtained are presented in Table 1. As can be observed from the table the AMD approach generates poor predictions of the experimental values for the root-mean-square radii of the nuclei. The experimental values of the radii are underestimated by the theoretical model for all the nuclei. The predicted radius for the ^{3}H system is about 16 % less and for the ^{3}He system is about 22 % less than the experimental values. The theoretical radius for the ^{4}He system also underestimated the experimental value by about 21 %.

The magnetic moment $\vec{\mu}$ of a nucleon in nuclear magnetons (μ_N) is given by [16]

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

where $\left\langle \vec{\ell} \right\rangle$ ($\langle \vec{s} \rangle$) 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]

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

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

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

Table 1. The ground-state energies (E_0), root-mean-square radii ($\sqrt{\langle r^2 \rangle}$) and magnetic moments ($\mu$) of the three-nucleon and four-nucleon systems. The values are for the parity and angular momentum projected wave function. The experimental values are taken from reference [15].

	E_0 (MeV)		$\sqrt{\langle r^2 \rangle}$ (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	

The values of the magnitude $\mu_{MK}^{\pm} = |\vec{\mu}_{MK}^{\pm}|$ for the three-nucleon 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. The discrepancy can be rectified by including other components of the ground-state wave function, like the mixed-symmetry S-state and the D-state. Also, the implementation of the full version of the Argonne V18 potential including three-nucleon forces, and the addition of relativistic corrections to the magnetic moment operator, are expected to reduce the discrepancy between the theoretical results and experimental data.

4. Conclusions

To demonstrate the competency of the AMD model wave function in nuclear structure studies, the angular momentum and parity projected AMD wave function was used to construct ground state wave functions of selected few-nucleon systems. In the past the construction of AMD wave functions was restricted to the use of phenomenological nucleon-nucleon potentials of Gaussian radial form. In this work the nuclear Hamiltonian was described with the semi-realistic Argonne V4' nucleon-nucleon potential. Ground-state energies, root-mean-square radii, magnetic moments and clustering in the nuclei were calculated using the constructed wave functions and results were compared with experimental data. The AMD wave functions reproduce the experimental values of these ground-state properties of light nuclei satisfactorily, given the crude form of the model. The AMD wave function has limited flexibility which limits the accuracy with which it can predict the nuclear properties. As was demonstrated in this work, it is possible to construct the AMD wave function with realistic nuclear Hamiltonian. The use of a more realistic nuclear Hamiltonian is important for a realistic description of nuclear systems. However, because of the rigidity of the wave function, such a Hamiltonian may introduce very little improvements in the accuracy of the theoretical results of the nuclear properties. A more flexible variational wave function constructed with a more realistic nucleon-nucleon potentials, including three-nucleon potentials may reduce the overall discrepancy between the experimental observation and theoretical AMD predictions of the nuclear properties.

References

[1] Golak J, Skibiński R, Witala H, Glöckle W, Nogga A and Kamada H 2005 *Phys. Rep.* **C 415** 89
[2] Carlson J, Schiavilla R 1998 *Rev. Mod. Phys.* **70** 743
[3] Kamada H *et al* 2001 *Phys. Rev.* **C 64** 044001
[4] Horiuchi H 1991 *Nucl. Phys.* **A 522** 257c
[5] Caurier E, Grammaticos B and Sami T 1982 *Phys. Lett.* **B 109** 150
[6] Feldmeier H 1990 *Nucl. Phys.* **A 515** 147
[7] Togashi T, Katō K 2007 *Prog. Theor. Phys.* **117** 189
[8] Watanabe T and Oryu S 2006 *Prog. Theor. Phys.* **116** 429
[9] Kanada-En'yo Y, Horiuchi H and Ono A 1995 *Phys. Rev.* **C 52** 628
[10] Peierls R E and Yoccoz J 1957 *Proc. Phys. Soc.* **A 70** 381
[11] Ono A, Horiuchi H, Maruyama T and Ohnishi A 1992 *Prog. Theor. Phys.* **87** 1185
[12] Ono A and Horiuchi H 2004 *Prog. Part. Nucl. Phys.* **53** 501
[13] Wiringa R B and Pieper S C 2002 *Phys. Rev. Lett.* **89** 182501-1
[14] Rampho G J 2010 *PhD Thesis*, University of South Africa, unpublished.
[15] Suzuki Y, Horiuchi W, Orabi M and Arai K 2008 *Few-Body Systems.* **42** 33
[16] Wong S S M 1998 *Introductory Nuclear Physics*, 2nd Edition
        (John Wiley and Sons, Inc. New York)