On a translationally invariant nuclear single particle picture

Walter Glöckle\textsuperscript{1,\textdagger} Hiroyuki Kamada\textsuperscript{2,*\textdoubleprime} and Jacek Golak\textsuperscript{3},

\textsuperscript{1}Institut für Theoretische Physik II, Ruhr-Universität Bochum, D-44780 Bochum, Germany
\textsuperscript{2}Department of Physics, Faculty of Engineering, Kyushu Institute of Technology, Kitakyushu 804-8550, Japan
\textsuperscript{3}M. Smoluchowski Institute of Physics, Jagiellonian University, PL-30059 Kraków, Poland

If one assumes a translationally invariant motion of the nucleons relative to the c. m. position in single particle mean fields a correlated single particle picture of the nuclear wave function emerges. A single particle product ansatz leads for that Hamiltonian to nonlinear equations for the single particle wave functions. In contrast to a standard not translationally invariant shell model picture those single particle s-, p- etc states are coupled. The strength of the resulting coupling is an open question. The Schrödinger equation for that Hamiltonian can be solved by few- and many-body techniques, which will allow to check the validity or non-validity of a single particle product ansatz.

Realistic nuclear wave functions exhibit repulsive 2-body short range correlations. Therefore a translationally invariant single particle picture – if useful at all – can only be expected beyond those ranges. Since exact \( A = 3 \) and 4 nucleon ground state wave functions and beyond based on modern nuclear forces are available, the translationally invariant shell model picture can be optimized by an adjustment to the exact wave function and its validity or non-validity decided.

§1. Introduction

The shell model for the nucleus has a long tradition. However, in its standard form expressed in single particle variables it is plagued by violating translational invariance. Various methods have been suggested to remedy this situation, like for instance the generator coordinate method\textsuperscript{1,\textendash}4). Clearly, if the shell model is realistic at all, the motion of the individual nucleons in a mean field happens in a translationally invariant manner, namely as a function of \( \vec{u}_i \equiv \vec{x}_i - \vec{X} \), where \( \vec{x}_i \) are the individual coordinates of particle \( i \) and \( \vec{X} \) is the c. m. coordinate. However, this set of coordinate vectors \( \vec{u}_i \) obeys the obvious condition \( \sum_{i=1}^{A} \vec{u}_i = 0 \), correlating the motion of all particles.

It is the aim of the present investigation to work out the consequences of choosing the coordinates \( \vec{u}_i \) for a shell model picture.

In Section II we provide some formal basis for this specific choice of coordinates. We restrict ourselves in this first investigation to systems of three and four nucleons. Furthermore, our most simplistic ansatz for the wave function shifts the antisymmetry requirement to the spin-isospin space, which leads to a symmetric space part

\textsuperscript{\textdagger} E-mail: Walter.Gloeckle@tp2.ruhr-uni-bochum.de
\textsuperscript{*\textdoubleprime} E-mail: kamada@mns.kyutech.ac.jp
under particle permutations. Then the very first ansatz for the space part is

\[ \Phi(\vec{u}_i) = \prod_{i=1}^{A} R(u_i), \]  

with \( A = 3 \) or 4. Here only s-wave states are assumed. We denote such a form a correlated single particle picture.

The nonlinear equations for 3 and 4 particles for the state \( R(u) \) assuming a sum of single particle potentials, \( V = \sum_{i=1}^{A} V(u_i) \), are presented in Section III.

In the case of the harmonic oscillator potential the nonlinear equations can be solved analytically and it is shown that the ansatz (1.1) is indeed the correct one.

Obviously the question arises whether the ansatz (1.1) for the wave function is at all valid for general single particle mean field potentials. To that effect the Hamiltonian, including the sum of single particle potentials, can be expressed in standard Jacobi variables. This is displayed in Section IV.

The resulting Schrödinger equations for 3 and 4 particles (in this case bosons for the space part) can be solved exactly in the form of the Faddeev-Yakubovsky equations, which will be formulated in that Section. Having the exact wave function at ones disposal, one can then investigate how well the above shell model ansatz (1.1) is realized, whether contributions beyond s-wave are needed, or whether that hope is not realistic at all. An optimization algorithm relating the shell model ansatz to the exact wave function is presented in Section V.

The numerical investigations for solving the nonlinear equations for \( R(u) \), for solving the Faddeev-Yakubovsky equations for the shell-model Hamiltonian and for the optimal extraction of \( R(u) \) from the exact wave functions is left to forthcoming investigations.

The main task however remains. The realistic nuclear wave function is determined by two- and three-nucleon forces. First estimates in the case of the \( \alpha \)-particle indicate that even small contributions from proper 4N forces\(^{5, 6}\) are needed. Based on these forces numerically exact wave functions are nowadays routinely generated for three and four nucleons.\(^{5, 6, 7, 8, 9, 10, 11, 12, 13}\) The question however arises, how well these wave functions for pair distances larger than a certain distance \( r_0 \) can be represented in the form of a correlated shell model ansatz like in (1.1), or whether higher partial waves and more complicated symmetries with respect to space-, spin- and isospin parts of the wave function are required. Clearly for pair distances smaller than \( r_0 \) short range repulsive features are present in the realistic wave functions which can not be represented in the shell model form. On the other hand it is known that the short pair distance behavior is essentially universal for light nuclei\(^{14, 15, 16}\) aside from proper normalization, which might allow an overall description: short range depletion and correlated shell model feature at larger distances. The value \( r_0 \) is expected to be somewhat smaller than 1 fm. Section VI provides some suggestion on how an optimal extraction of a correlated single particle picture can be obtained from realistic three- and four-nucleon wave functions. We summarize in Section VII.
The translationally invariant single particle coordinates for \( n \) particles are defined as

\[
\vec{u}_i \equiv \vec{x}_i - \frac{1}{n} \sum_{j=1}^{n} \vec{x}_j = \frac{n-1}{n} \vec{x}_i - \frac{1}{n} \sum_{j \neq i}^{n} \vec{x}_j
\]  

(2.1)

Since \( \sum_{i=1}^{n} \vec{u}_i = 0 \), the mapping from the \( n \vec{x}_i \) to the \( n \vec{u}_i \) can not be inverted and we choose the new variables as the first \((n-1)\) \( \vec{u}_j \) together with the c.m. coordinate \( \vec{X} \)

\[
\vec{X} = \frac{1}{n} \sum_{j=1}^{n} \vec{x}_j.
\]  

(2.2)

It is a straightforward exercise to express the kinetic energy in terms of the new variables

\[
T = -\frac{1}{2m} \sum_{k=1}^{n} \nabla^2 x_k = -\frac{1}{2m} \left( \frac{n-1}{n} \sum_{i=1}^{n-1} \nabla^2 u_i - \frac{1}{n} \sum_{i \neq j}^{n} \vec{\nabla} u_i \cdot \vec{\nabla} u_j \right) - \frac{1}{2mn} \nabla^2 \vec{X}
\]  

(2.3)

Clearly, the first part refers to the relative motion, the second part to the c.m. motion. While the choice of Jacobi coordinates avoids mixed terms in the kinetic energy, here they are unavoidable.

Let us now restrict ourselves to three and four particles. If one chooses a Slater determinant with equal space-dependent single particle wave functions, the symmetric part of the form (1.1) factors out and one is left with a totally antisymmetric spin-isospin part. For a proton-proton-neutron (ppn) system this has the form

\[
\chi_3 = |(t = 0 \frac{1}{2})T = \frac{1}{2} > |(s = \frac{1}{2})S = \frac{1}{2} > \\
- |(t = 1 \frac{1}{2})T = \frac{1}{2} > |(s = 0 \frac{1}{2})S = \frac{1}{2} >,
\]  

(2.4)

where the two-body spin or isospin state is coupled with the spin or isospin \( \frac{1}{2} \) of the third particle to total spin \( S = \frac{1}{2} \) or total isospin \( T = \frac{1}{2} \). This state together with a symmetric space part is known as the principal \( S \)-state for realistic \( ^3 \)He wave functions and contributes with about 90% to the norm. This result by itself clearly indicates that this choice of the one Slater determinant can not exhaust the full wave function but at least a very large portion of it.

For the \( ppnn \) system the totally antisymmetric spin-isospin part of the wave function has the form

\[
\chi_4 = (1 - P_{23} - P_{24}) |(\frac{1}{2} \frac{1}{2} 0)(\frac{1}{2} \frac{1}{2} 0)S = 0 > \\
(1 + P_{13}P_{24}) |(\frac{1}{2} \frac{1}{2} 11 >12 |(\frac{1}{2} \frac{1}{2} 1 - 1 >_{34},
\]  

(2.5)
where $P_{ij}$ is a transposition of particles $i$ and $j$. That state has total spin $S = 0$ and total isospin $T = 0$. Again in relation to the norm of a realistic $\alpha$-particle wave function it accounts for about 90\%.\[11\]

Now we provide some formal properties, whose verification is left to the reader. The Heisenberg commutation relations

$$[w_{k\alpha}, u_{j\beta}] = \delta_{kj} \frac{1}{i} \delta_{\alpha\beta}$$

are obeyed, where $w_{k\alpha} \equiv \frac{\partial T}{\partial \dot{u}_{k\alpha}}$ are components of the conjugate momenta.

The relative orbital angular momentum has the form

$$\vec{L}_{rel} = \vec{u}_1 \times \vec{\nabla} u_1 + \vec{u}_2 \times \vec{\nabla} u_2,$$  \hspace{1cm} (2.7)

which justifies that standard Clebsch-Gordon coupling in the variables $\vec{u}_1$ and $\vec{u}_2$ can be used.

Using (2.3) for $n = 3$, the translationally invariant shell model Hamiltonian is given by

$$H_3 = -\frac{1}{3m} (\nabla^2 u_1 + \nabla^2 u_2 - \vec{\nabla} u_1 \cdot \vec{\nabla} u_2) + V(u_1) + V(u_2) + V(u_3),$$  \hspace{1cm} (2.8)

where $u_3 = |\vec{u}_1 + \vec{u}_2|$.Obviously, a separation of variables is not possible. However, the symmetry of the kinetic energy under particle exchanges is valid:

$$\nabla^2 u_1 + \nabla^2 u_2 - \vec{\nabla} u_1 \cdot \vec{\nabla} u_2 = \nabla^2 u_2 + \nabla^2 u_3 - \vec{\nabla} u_2 \cdot \vec{\nabla} u_3$$

$$= \nabla^2 u_3 + \vec{\nabla} u_1 \cdot \vec{\nabla} u_1.$$  \hspace{1cm} (2.9)

In the case of four particles the translationally invariant shell model Hamiltonian is given as

$$H_4 = -\frac{3}{8m} (\nabla^2 u_1 + \nabla^2 u_2 + \nabla^2 u_3 - 2 \left( \vec{\nabla} u_1 \cdot \vec{\nabla} u_2 + \vec{\nabla} u_1 \cdot \vec{\nabla} u_3 + \vec{\nabla} u_2 \cdot \vec{\nabla} u_3 \right)$$

$$+ V(u_1) + V(u_2) + V(u_3) + V(u_4),$$  \hspace{1cm} (2.10)

with $u_4 = |\vec{u}_1 + \vec{u}_2 + \vec{u}_3|$. All the formal relations corresponding to (2.6), (2.7), and (2.9) are valid for four particles as is expected.

§3. Nonlinear Equations for the Translationally Invariant Shell Model States

For three particles the simplest ansatz for a symmetrical space part wave function is

$$\Phi(u_1, u_2, u_3) = R(u_1) R(u_2) R(u_3),$$  \hspace{1cm} (3.1)

with $u_3 = |\vec{u}_1 + \vec{u}_2|$.

It is straightforward, though tedious, to evaluate the action of the kinetic energy in (2.8) onto (3.1). If we put $R(u) = \frac{r(u)}{u}$, the Schrödinger equation based on $H_3$
and the ansatz (3.1) results in

\[- \frac{1}{3m^2}r''(u_1)r(u_2)r(u_3) - r(u_1)r''(u_2)r(u_3) - r(u_1)r''(u_3)\]

\[- \frac{(u_1)}{u_2}(r''(u_2) - r''(u_3))u_1 \cdot u_3\]

\[- r(u_1)(r''(u_2) - r''(u_3))u_2 \cdot u_3\]

\[- r(u_1)(r''(u_2) - r''(u_3))r(u_3)u_1 \cdot u_2\]

\[+ (V(u_1) + V(u_2) + V(u_3) - E)r(u_1)r(u_2)r(u_3) = 0, \quad (3.2)\]

where

\[\hat{u}_1 \cdot \hat{u}_3 = - \frac{u_1 + \hat{u}_1 \cdot \hat{u}_2}{u_3}\]

\[\hat{u}_2 \cdot \hat{u}_3 = - \frac{u_2 + \hat{u}_2 \cdot \hat{u}_1}{u_3} \quad (3.3)\]

Here the independent variables are \(u_1, u_2\) and \(x = \hat{u}_1 \cdot \hat{u}_2\).

We can not exclude that higher partial waves should be included. The simplest ansatz for a p-wave admixture is given by

\[\Phi_1(\hat{u}_1, \hat{u}_2, \hat{u}_3) = R_1(u_1)R_1(u_2)R(u_3)\hat{u}_1 \cdot \hat{u}_2 + R(u_1)R_1(u_2)R_1(u_3)\hat{u}_2 \cdot \hat{u}_3\]

\[+ R_1(u_1)R(u_2)R_1(u_3)\hat{u}_1 \cdot \hat{u}_3, \quad (3.4)\]

where for the sake of simplicity we assumed that the ‘third’ state, which is not involved in the p-wave admixture, remains unchanged. We leave it to the reader to derive the resulting equation.

For four particles the most simple ansatz is

\[\Phi(u_1, u_2, u_3, u_4) = R(u_1)R(u_2)R(u_3)R(u_4), \quad (3.5)\]

with \(|u_4| = |\vec{u}_1 + \vec{u}_2 + \vec{u}_3|\). The resulting equation based on \(H_4\) is

\[- \frac{3}{8m^2}r''(u_1)r(u_2)r(u_3)r(u_4)\]

\[+ r(u_1)r(u_2)r(u_3)r''(u_4) + r(u_1)r''(u_2)r(u_3)r(u_4)\]

\[+ r(u_1)r(u_2)r''(u_3)r(u_4) + r(u_1)r(u_2)r''(u_3)r(u_4)\]

\[+ r(u_1)r(u_2)r''(u_3)r(u_4)\]

\[\frac{3}{3m^2}r(u_1)r(u_2)r''(u_3)r(u_4)\]

\[\quad (3.3)\]
we consider four particles and introduce standard Jacobian coordinates
state may be poor.
Choosing the mean field potential
Again, extensions to the ansatz (3.5) are obvious. Already the presence of the
Choosing the mean field potential
Then the potential energy
allow for a separation of the variables with the result

\[ T_{rel} = -\frac{1}{2m} (2\nabla_x^2 + 3\nabla_y^2 + 4\nabla_z^2) \]

(3.8)

allow for a separation of the variables with the result

\[ \Phi(x, y, z) = e^{-\frac{m\omega}{2} x^2} \]

(3.9)

where

\[ R(u) = e^{-\frac{m\omega}{2} u^2}. \]

(3.10)
This goes with the lowest energy \( E = \frac{9}{2} \omega \). The corresponding result for three particles, now for \( E = 3 \omega \), is

\[
\Phi(x, y) = \prod_{i=1}^{3} R(u_i),
\]

(3.11)

with the same function \( R(u) \). It is straightforward to verify that (3.9) and (3.11) fulfill the nonlinear equations (3.6) and (3.2).

§4. The Faddeev-Yakubovsky Equations for Three and Four Particles

The shell model Hamiltonians \( H_3 \) and \( H_4 \), Eqs. (2.8) and (2.10), can be rewritten in terms of standard Jacobi coordinates. This allows one to solve the two Schrödinger equations exactly in the form of the Faddeev-Yakubovsky equations and therefore to test the quality of shell model ansatz. For three particles one defines the Jacobi coordinates as

\[
\begin{align*}
\bar{x} &= \bar{u}_2 - \bar{u}_3 = 2\bar{u}_2 + \bar{u}_1 \\
\bar{y} &= \bar{u}_1 - \frac{1}{2}(\bar{u}_2 + \bar{u}_3) = \frac{3}{2} \bar{u}_1,
\end{align*}
\]

(4.1)

or

\[
\begin{align*}
\bar{u}_1 &= \frac{2}{3} \bar{y} \\
\bar{u}_2 &= \frac{1}{2} \bar{x} - \frac{1}{3} \bar{y}.
\end{align*}
\]

(4.2)

This gives for the Hamiltonian

\[
H_3 = -\frac{1}{m} \nabla_x^2 - \frac{3}{4m} \nabla_y^2 + V(\frac{2}{3} \bar{y}) + V(\frac{1}{2} \bar{x} - \frac{1}{3} \bar{y}) + V(\frac{1}{2} \bar{x} + \frac{1}{3} \bar{y})
\]

(4.3)

The above expression has a formal similarity to a three-body Hamiltonian composed of two-body forces:

\[
H_{3,2b} = -\frac{1}{m} \nabla_x^2 - \frac{3}{4m} \nabla_y^2 + V_{2b}(x) + V\left(\frac{1}{2} \bar{x} + \bar{y}\right) + V\left(\frac{1}{2} \bar{x} - \bar{y}\right).
\]

(4.4)

However, Eqs. (4.2) and (4.4) are different. Nevertheless the formal structure of the Faddeev equation[19] can be used. The three-body bound state obeys

\[
\Psi = G_0 \sum_{i=1}^{3} V_i \Psi \equiv \sum_{i=1}^{3} \psi_i,
\]

(4.5)

where \( G_0 \) represents the free three-body propagator, and \( V_i \equiv V(u_i) \). Then one arrives in a standard manner[20] at

\[
\psi_i = G_0 T_i \sum_{j \neq i} \psi_j,
\]

(4.6)
where $T_i$ obeys the Lippmann Schwinger equation

$$T_i = V_i + V_i G_0 T_i \tag{4.7}$$

Because of the identity of the particles one arrives at the well known form for the total state

$$\Psi = (1 + P) \psi_1, \tag{4.8}$$

with $P \equiv P_{12} P_{23} + P_{13} P_{23}$, which is a sum of a cyclical and an anticyclical permutation of three particles. One Faddeev equation is sufficient, namely

$$\psi_1 = G_0 T_1 P \psi_1 \tag{4.9}$$

The Faddeev equation can be solved in configuration space as an integro-differential equation or, what we prefer, in momentum space as an integral equation. In the latter case one needs the momentum space representation of the shell model potential as well as of the Lippmann Schwinger equation in terms of the conjugate momenta $\vec{p}_x$ and $\vec{p}_y$ of the Jacobi momenta $\vec{x}$ and $\vec{y}$.

With standard (unit) normalizations it results in

$$\langle \vec{x} \vec{y} | \vec{u}_1 \vec{u}_2 \rangle = \left( \frac{1}{3} \right)^3 \delta(\vec{u}_1 - \frac{2}{3} \vec{y}) \delta(\vec{u}_2 - \frac{1}{2} \vec{x} + \frac{1}{3} \vec{y}) \tag{4.10}$$

Furthermore, as consequence of the locality assumption

$$\langle \vec{u}_1 \vec{u}_2 | V(u_1) | \vec{u}_1 \vec{u}_2 \rangle = \delta(\vec{u}_2 - \vec{u}_1') \delta(\vec{u}_1 - \vec{u}_1') V(u_1) \tag{4.11}$$

and using (4.10) one obtains

$$\langle \vec{p}_x \vec{p}_y | V(u_1) | \vec{p}_x \vec{p}_y \rangle = \delta(\vec{p}_x - \vec{p}_x') t_1(\vec{p}_y, \vec{p}_y, z = E - \frac{p_x'^2}{m}) \tag{4.12}$$

Due to that structure the T-matrix element in (4.7) must have the form

$$\langle \vec{p}_x \vec{p}_y | T_1 | \vec{p}_x \vec{p}_y \rangle = \delta(\vec{p}_x - \vec{p}_x') t_1(\vec{p}_y, \vec{p}_y, z = E - \frac{p_x'^2}{m}), \tag{4.13}$$

where $t_1$ obeys

$$t_1(\vec{p}_y, \vec{p}_y, z) = V_1(\vec{p}_y', \vec{p}_y') + \int d^3 \vec{p}_y'' V(\vec{p}_y', \vec{p}_y'') \frac{1}{E - \frac{p_x'^2}{m} - \frac{3}{4 m} p_y'^2} t_1(\vec{p}_y'', \vec{p}_y', z). \tag{4.14}$$

For two-body forces the $\delta$-function in (4.13) would have been for the spectator momentum $\vec{p}_y$. We assume that the mean field forces are spin-independent and require symmetry in the spatial part.

In such a system has been shown to be easily solvable using directly momentum vectors and thus avoiding any partial wave decomposition. We follow the same approach. Then (4.9), using (4.13) has the form

$$\langle \vec{p}_x \vec{p}_y | \psi_1 \rangle = \frac{1}{E - \frac{p_x'^2}{m} - \frac{3}{4 m} p_y'^2} \int d^3 \vec{p}_y' t_1(\vec{p}_y, \vec{p}_y', z = E - \frac{p_x'}{m})$$
\[ \int d^3 p_{x''} d^3 p_{y''} < \vec{p}_x \vec{p}_y | P | \vec{p}_{x''} \vec{p}_{y''} > < \vec{p}_{x''} \vec{p}_{y''} | \psi_1 > . \] (4.15)

The permutation matrix element is well known and is given as
\[ < \vec{p}_x \vec{p}_y | P | \vec{p}_{x''} \vec{p}_{y''} > = \left( \frac{8}{3} \right)^3 (\delta(\vec{p}_y' + \frac{2}{3} \vec{p}_x - \frac{4}{3} \vec{p}_{x''}) \delta(\vec{p}_{y''} - \frac{4}{3} \vec{p}_x - \frac{2}{3} \vec{p}_{x''}) \\
+ \delta(\vec{p}_y' - \frac{2}{3} \vec{p}_x - \frac{4}{3} \vec{p}_{x''}) \delta(\vec{p}_{y''} + \frac{4}{3} \vec{p}_x + \frac{2}{3} \vec{p}_{x''})). \] (4.16)

Therefore, Eq. (4.15) turns into
\[ < \vec{p}_x \vec{p}_y | \psi_1 > = \frac{1}{E - \frac{p_x^2}{m} - \frac{3}{4m} \vec{p}_y^2} \left( \frac{8}{3} \right)^3 \int d^3 p_{x''} \\
(t_1(\vec{p}_y, \frac{3}{2} \vec{p}_x - \frac{4}{3} \vec{p}_{x''}, z = E - \frac{p_y^2}{m}) < \vec{p}_{x''}, \frac{4}{3} \vec{p}_x + \frac{2}{3} \vec{p}_{x''} | \psi_1 > \\
+ t_1(\vec{p}_y, \frac{3}{2} \vec{p}_x + \frac{4}{3} \vec{p}_{x''}, z = E - \frac{p_y^2}{m}) < \vec{p}_{x''}, -\frac{4}{3} \vec{p}_x - \frac{2}{3} \vec{p}_{x''} | \psi_1 > . \] (4.17)

Because of the uniqueness of the solution, any solution of (4.17) has the property
\[ - \vec{p}_x, \vec{p}_y | \psi_1 > = \vec{p}_x, \vec{p}_y | \psi_1 > . \] This equation is then be solved by iteration using a Lanczos type algorithm.

As follows from (4.16) the total state given by (4.18) has the form
\[ < \vec{p}_x, \vec{p}_y | \psi > = < \vec{p}_x, \vec{p}_y | \psi_1 > + \left( \frac{3}{4} \right)^3 < -\frac{1}{2} \vec{p}_x - \frac{3}{4} \vec{p}_y, \vec{p}_x + \frac{1}{2} \vec{p}_y | \psi_1 > \\
+ \left( \frac{3}{4} \right)^3 < -\frac{1}{2} \vec{p}_x + \frac{3}{4} \vec{p}_y, -\vec{p}_x + \frac{1}{2} \vec{p}_y | \psi_1 > . \] (4.18)

In the case of four particles we use the Yakubovsky equations. For four bosons and two-body forces this has been solved rigorously the first time in. Now we have different potentials depending on the relative coordinates \( \vec{u}_i \), which require a renewed derivation. Starting from
\[ \Psi = G_0 \sum_{i=1}^{4} V(u_i) \Psi \equiv \sum_{i=1}^{4} \psi_i \] (4.19)

one arrives in a standard first step at
\[ \psi_1 = G_0 T_1 (\psi_2 + \psi_3 + \psi_4), \] (4.20)

where \( T_1 \) obeys the Lippmann Schwinger equation (4.14). (Note however, the modified free four-body propagator.)

In the spirit of the Yakubovsky scheme one regards a three-body subsystem by defining
\[ \psi_{1;123} \equiv G_0 T_1 (\psi_2 + \psi_3) \] (4.21)

and a remaining component
\[ \psi_{1;14} \equiv G_0 T_1 \psi_4. \] (4.22)
Then
\[ \psi_1 = \psi_{1;123} + \psi_{1;1,4}. \] (4.23)

Correspondingly one defines
\[
\begin{align*}
\psi_{2;231} &= G_0 T_2 (\psi_3 + \psi_1) \\
\psi_{3;312} &= G_0 T_3 (\psi_1 + \psi_2) \\
\psi_{2;2,4} &= G_0 T_2 \psi_4 \\
\psi_{3;3,4} &= G_0 T_3 \psi_4
\end{align*}
\] (4.24)

where
\[
\begin{align*}
\psi_2 &= \psi_{2;231} + \psi_{2;2,4} \\
\psi_3 &= \psi_{3;312} + \psi_{3;3,4}.
\end{align*}
\] (4.25)

Then (4.21) and (4.25) yield
\[
\psi_{1;123} = G_0 T_1 (\psi_{2;231} + \psi_{3;312} + \psi_{2,2,4} + \psi_{3,3,4}).
\] (4.26)

Due to the identity of the particles one has
\[
\begin{align*}
\psi_{2;231} + \psi_{3;312} &= P \psi_{1;123} \\
\psi_{3;3,4} &= P_{23} \psi_{2,2,4},
\end{align*}
\] (4.27)

and (4.26) can be rewritten as
\[
(1 - G_0 T_1 P) \psi_{1;123} = G_0 T_1 (1 + P_{23}) \psi_{2,2,4}.
\] (4.28)

The left hand side by itself defines a three-body problem. After inversion one obtains
\[
\psi_{1;123} = G_0 \tilde{T} (1 + P_{23}) \psi_{2,2,4},
\] (4.29)

where \( \tilde{T} \) obeys
\[
\tilde{T} = T_1 + T_1 P G_0 \tilde{T}.
\] (4.30)

It remains to consider (4.22), which in analogy to (4.25) has the form
\[
\psi_{2,2,4} = G_0 T_2 (\psi_{4;413} + \psi_{4,4,2}).
\] (4.31)

Using now
\[
\psi_{4,4,2} = P_{24} \psi_{2,2,4}
\] (4.32)

we rewrite (4.31) as
\[
(1 - G_0 T_2 P_{24}) \psi_{2,2,4} = G_0 T_2 \psi_{4,413}.
\] (4.33)

Inversion yields
\[
\psi_{2,2,4} = G_0 \tilde{T} \psi_{4,413},
\] (4.34)
where $\tilde{T}$ obeys

$$\tilde{T} = T_2 + T_2P_{24}G_0\tilde{T}$$

Finally permutation symmetry yields

$$\psi_{4;423} = P_{23}P_{14}\psi_{1;123}$$

and one ends up with two coupled equations

$$\psi_{1;123} = G_0\hat{\tilde{T}}(1 + P_{23})\psi_{2;2,4}$$
$$\psi_{2;2,4} = G_0\tilde{T}P_{23}P_{14}\psi_{1;123}.$$ (4.37)

The total wave function is now given as

$$\Psi = \psi_1 + \psi_2 + \psi_3 + \psi_4 = (1 + P)\psi_{1;123} + P_{14}P_{23}(\psi_{1;123} + \psi_{2;2,4}) + (1 + P_{24} + P_{12})\psi_{2;2,4}.$$ (4.38)

While a corresponding coupled set based on two-body forces has been rigorously solved in a partial wave representation, it is also possible to directly use momentum vectors as has been demonstrated in §2.6.

We would propose to follow that second option. We leave it to the reader to work out the explicit momentum space representation of (4.37) and (4.38) in terms of appropriate Jacobi momentum vectors.

§5. Shell Model Ansatz versus Exact Wave Function

The solution of the Faddeev equation (4.17) yields the full three-dimensional three-boson Faddeev component in momentum space. This is the input for the full wave function given in (4.18). Since we search for the lowest energy state, $\Psi$ is a scalar and therefore depends only on 3 variables

$$\langle \vec{p}_x, \vec{p}_y | \Psi \rangle \rightarrow \Psi(p_x, p_y, \hat{p}_x \cdot \hat{p}_y)$$

As a consequence, the dependence of the configuration space wave function $\langle \vec{x}, \vec{y} | \Psi \rangle$ will also reduce to a three-variable dependence $\Psi(x, y, \hat{x} \cdot \hat{y})$:

$$\langle \vec{x}, \vec{y} | \Psi \rangle = \frac{1}{(2\pi)^3} \int d^3p_x d^3p_y e^{i(\vec{p}_x \cdot \vec{x} + \vec{p}_y \cdot \vec{y})}\Psi(p_x, p_y, \hat{p}_x \cdot \hat{p}_y)$$
$$= \frac{1}{(2\pi)^3} \int d^3p_x d^3p_y \cos(\vec{p}_x \cdot \vec{x} + \vec{p}_y \cdot \vec{y})\Psi(p_x, p_y, \hat{p}_x \cdot \hat{p}_y)$$
$$\equiv \Psi(x, y, \hat{x} \cdot \hat{y}).$$ (5.2)

We used the reality property of $\Psi$ to replace the exponential by the cosine.

The expectation is now that

$$\Psi_{SM}(\vec{x}, \vec{y}) \equiv R(u_1)R(u_2)R(u_3),$$

with $u_3 = |\vec{u}_1 + \vec{u}_2|$ being a good approximation to $\Psi(x, y, \hat{x} \cdot \hat{y})$. In the case of the harmonic oscillator this is exactly fulfilled.
In general one faces the task to minimize $|\Psi(x, y, \hat{x} \cdot \hat{y}) - R(u_1)R(u_2)R(u_3)|$ for all $x, y, \hat{x} \cdot \hat{y}$ or $u_1, u_2, \hat{u}_1 \cdot \hat{u}_2$. Explicitly this requirement is $|\Psi(x, y, \hat{x} \cdot \hat{y}) - R(\hat{x} \cdot \hat{y})R((\hat{x}^2 - \frac{1}{2} \hat{y}^2))R((\hat{x}^2 + \frac{1}{2} \hat{y}^2))| \text{ or } |\Psi(|\hat{u}_1 + 2\hat{u}_2|, \frac{3}{2}u_1, \frac{u_1 + 2\hat{u}_2 \cdot \hat{u}_1}{|\hat{u}_1 + 2\hat{u}_2|} - R(u_1)R(u_2)R(|\hat{u}_1 + 2\hat{u}_2|) \text{ to be minimal.}

Instead of an optimized pointwise adjustment one can try an average adjustment minimizing

$$\int du_1 du_2 d\hat{u}_1 \cdot \hat{u}_2 (\Psi(|\hat{u}_1 + 2\hat{u}_2|, \frac{3}{2}u_1, \frac{u_1 + 2\hat{u}_2 \cdot \hat{u}_1}{|\hat{u}_1 + 2\hat{u}_2|} - R(u_1)R(u_2)R(|\hat{u}_1 + 2\hat{u}_2|))^2$$

in relation to the choice of $R(u)$. For instance, one can expand $R(u)$ into harmonic oscillator wave functions $\Phi_m(u)$, where $\frac{d\Phi}{du}$ is optimally adjusted to the given mean field potential $V(u)$.

Thus

$$R(u) = \sum_m \phi_m(u)C_m,$$

and the set $C_m$ is to be varied minimizing the above integral. Differentiating with respect to $C_k$ and putting the result to zero yields a nonlinear relation for the coefficients $C_m$. This might be solved by an iterative procedure allowing first $C_0 \neq 0$. Then keeping also $C_1 \neq 0$ in addition one might start with $C_0$ from the previous step and determine $C_1$. Finally one can iterate the nonlinear equation for $C_0$ and $C_1$ starting with the values found before; etc. Very likely, however, one has to allow in addition for p-wave admixtures as given in (5.4) and possibly even higher orbital angular momentum values.

The direct solution of the nonlinear equation (3.2) poses a severe problem. Moreover, very likely p-wave and possibly higher order admixtures have to be taken into account, which requires an extension of the nonlinear equation (3.2) as mentioned above. Discretization in the $u_1, u_2, \hat{x} \cdot \hat{y}$ - values is necessary and iterative procedures appear unavoidable. Thereby each run is of course an eigenvalue problem for the energy $E$.

In the case of four nucleons the symmetric state of lowest energy is again a scalar and thus depends on 5 variables:

$$\Psi = \Psi(x, y, z, \hat{x} \cdot \hat{y}, \hat{x} \cdot \hat{z}, \hat{y} \cdot \hat{z}),$$

where $\hat{x}, \hat{y}, \hat{z}$ are one choice of standard Jacobi coordinates. The optimal extraction of $R(u)$ in

$$\Psi_{SM}(\hat{x}, \hat{y}, \hat{z}) \equiv R(u_1)R(u_2)R(u_3)R(u_4)$$

and possibly higher angular momentum admixture follows analogous strategies as for three nucleons.

§6. Realistic Three- and Four-Nucleon Wave Functions

Based on modern nuclear forces like27, 28, 29 combined with three-nucleon (3N) forces of the Tucson-Melbourne type30 or based on the most recent consistent two-
and three-nucleon forces generated from chiral effective field theory\cite{30} numerically exact solutions of the Faddeev - Yakubovsky equations are available. If a correlated single particle picture applies at all it can only be valid beyond a certain value $r_0$ of the pair distances. The two-body correlation function to find two nucleons at a distance $r$ has its maximum around $r = 1$ fm universally for all light nuclei\cite{13,14,15}. Thus $r_0$ has to be smaller than 1 fm. For the most simple correlated shell model ansatz of Eq. (3.1) or symmetric extensions beyond s-wave and (3.5) the exact wave function for $^3$He and $^4$He is to be projected onto the totally antisymmetric spin-isospin states $\chi_3$ and $\chi_4$, Eqs. (2.4) and (2.5), respectively:

$$\Psi_{3,4}^{\text{exact}} \equiv <\chi_{3,4}|\Psi_{3,4}^{\text{exact}} >. \quad (6.1)$$

For a global adjustment one has to minimize

$$\int dV (\Psi_{3,4}^{\text{exact}} - \prod_{i=1}^{3,4} R(u_i))^2 \prod_{i<j}^{3,4} \Theta(r_{ij} - r_0) \quad (6.2)$$

or an extension including higher partial waves but still keep the symmetry in the space part.

The resulting $R(u)$ and $R'$s related to higher partial waves should be independent of $r_0$. This requirement should determine the smallest possible value for $r_0$.

Knowing $R(u)$ one can compare the norms

$$N_{\text{exact}}^{\text{short}} \equiv \int dV |\Psi_{3,4}^{\text{exact}}| \prod_{i<j}^{3,4} \Theta(r_{ij} - r_0)$$

$$N_{\text{SM}} \equiv \int dV \prod_{i=1}^{3,4} R(u_i)^2 \prod_{i<j}^{3,4} \Theta(r_{ij} - r_0) \quad (6.3)$$

In addition the short range behavior is not accessible to the single particle picture and provides the norm contribution

$$N_{\text{short}}^{\text{exact}} \equiv \int dV |\Psi_{3,4}^{\text{exact}}|^2 \prod_{i<j}^{3,4} \Theta(r_0 - r_{ij}) \quad (6.4)$$

Finally, one has to keep in mind that only about 90% of the total norm is related to the spin-isospin states $\chi_{3,4}$. The rest is of more complicated structure\cite{13}.

\section{Summary}

In nature a nuclear wave function is translationally invariant. Therefore, if a shell model picture is a good representation of a nuclear wave function, the single particle states have to depend on translationally invariant coordinates. Our choice of coordinates $\vec{u}_i \equiv \vec{x}_i - \vec{X}$ relating the individual position vectors $\vec{x}_i$ to the c. m. coordinate $\vec{X}$ fulfills this condition with the additional constraint that they have to sum up to zero: $\sum_{i=1}^{n} \vec{u}_i = 0$. Choosing the first $n - 1$ of them together with the
c. m. coordinate one can formulate a shell model Hamiltonian composed of kinetic energy containing now also mixed terms $\vec{\nabla} u_i \cdot \vec{\nabla} u_j$ and single particle potentials depending on the coordinates $|u_i|$. Assuming the energetically lowest energy state to that Hamiltonian to be a Slater determinant with equal space dependent single particle wave functions, $R(u_i)$, which is the most simple choice, one obtains nonlinear equations for $R(u_i)$. They have been worked out for nucleon numbers $A = 3$ and $4$. For the special choice of harmonic oscillator potentials the nonlinear equations can be analytically solved and that most simple ansatz for the wave function turns out to be correct. In the case of general mean field potentials partial wave contributions beyond s-states might be necessary.

In order to shed light on the question how well such a shell model ansatz is justified we regarded in some detail three and four nucleons. The corresponding shell model Hamiltonian can be written in terms of standard Jacobi coordinates and numerically exact solutions can be generated based on the Faddeev-Yakubovsky equations. Knowing the exact wave functions one can check the validity of the Slater determinant ansatz. Optimization algorithms are provided to perform the comparison of exact wave function with the Slater determinant ansatz.

The main task however, is to confront such a shell model ansatz to realistic three- and four-nucleon wave functions (and beyond), which are based on modern two- and three-nucleon forces. Clearly at short pair distances the well established repulsive nature of the nuclear forces invalidates the shell model ansatz and therefore only for pair distances beyond a certain value $r_0$ the shell model picture can make sense, if at all. To that aim numerical investigations are planned for both, the shell-model Hamiltonians and realistic Hamiltonians composed of two- and three-nucleon forces.

References

1) B. Giraud, J. C. Hocquenghem, and A. Lumbroso, Proc. Colloque de la Toussuire, lecture 61 (Fevrier 1971).
2) D. L. Hill and J. A. Wheeler, Phys. Rev. 80 (1953), 1102.
3) J. J. Griffin and J. A. Wheeler, Phys. Rev. 108 (1957), 328.
4) C. W. Wong, Phys. Rep. 15C (1975), 283.
5) D. Rozpedzik et al., Acta Phys. Polon. B 37 (2006) 2889.
6) A. Nogga, E. Epelbaum, J. Golak, H. Kamada, H. Witała, D. Rozpedzik, R. Skibiński, and W. Glöckle, Four-nucleon force contribution to the binding energy of $^4\text{He}$, in 19th International IUPAP Conference on Few-Body Problems in Physics, Vol. 3 of EPJ Web of Conferences, (2010) 05006.
7) H. Kamada, W. Glöckle, Phys. Lett. B 292 (1992), 1.
8) A. Nogga, H. Kamada, W. Glöckle, Nucl. Phys. A 689 (2001), 357c.
9) A. Nogga, D. Hueber, H. Kamada, W. Glöckle, Phys. Lett. B 409 (1997), 19.
10) W. Glöckle, H. Kamada, Phys. Rev. Lett. 71 (1993), 971.
11) A. Nogga, H. Kamada, W. Glöckle, Phys. Rev. Lett. 85 (2000), 944.
12) H. Kamada et al., Phys. Rev. C 64 (2001), 044001.
13) A. Nogga, H. Kamada, W. Glöckle, B. R. Barrett, Phys. Rev. C 65 (2002), 054003.
14) W. Glöckle, H. Kamada, J. Golak, A. Nogga, H. Witała, R. Skibiński, J. Kuroś-Zołnierczuk, Acta Phys. Polon. B 32 (2001) 3053.
15) W. Glöckle, H. Kamada, H. Witała, D. Hüber, J. Golak, K. Miyagawa, S. Ishikawa, Few Body Syst Suppl 8 (1995) 9.
16) W. Glöckle, H. Witała, H. Kamada, D. Hüber, J. Golak, Few Body Syst Suppl 9 (1995) 384.
17) B. Blankleider and R. M. Woloshyn, Phys. Rev. C 29 (1984), 538.
On a translationally invariant nuclear single particle picture

18) J. L. Friar et al., Phys. Rev. C 42 (1990), 2310.
19) L. D. Faddeev, Sov. Phys. JETP 12 (1961) 1014.
20) W. Glöckle, The quantum mechanical few-body problem, Springer Verlag 1983.
21) H. Liu, Ch. Elster, W. Glöckle, Computer Physics Communications 147 (2002) 170.
22) H. Liu, Ch. Elster, W. Glöckle, Few-Body Syst. 33 (2003) 241.
23) A. Stadler, W. Glöckle, P. U. Sauer, Phys. Rev. C 44 (1991), 2319.
24) O. A. Yakubovsky, Sov. J. Nucl. Phys. 5 (1967) 937.
25) H. Kamada, W. Glöckle, Nucl. Phys. A 548 (1992), 205.
26) M. R. Hadizadeh, S. Bayegan, Few-Body Syst. 40 (2007) 171.
27) R. B. Wiringa, V. G. J. Stoks, R. Schiavilla, Phys. Rev. C 51 (1995), 38.
28) R. Machleidt, Phys. Rev. C 63 (2001), 024001.
29) V. G. J. Stoks et al., Phys. Rev. C 49 (1994), 2950.
30) E. Epelbaum, Prog. Part. Nucl. Phys 57 (2006) 654.
31) S. A. Coon, M. T. Peña, Phys. Rev. C 48 (1993), 2559; J. L. Friar, D. Hüber, U. van Kolck, Phys. Rev. C 59 (1999), 53; S. A. Coon, H. K. Han, Few-Body Syst 30 (2001) 131.