Variational Monte Carlo Calculations of ^{3}H and ^{4}He with a Relativistic Hamiltonian - II

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(Sept. 22, 1994)

Abstract

In relativistic Hamiltonians the two-nucleon interaction is expressed as a sum of $\tilde{v}_{ij}$, the interaction in the $\mathbf{P}_{ij} = 0$ rest frame, and the "boost interaction" $\delta v(\mathbf{P}_{ij})$ which depends upon the total momentum $\mathbf{P}_{ij}$ and vanishes in the rest frame. The δv can be regarded as a sum of four terms: δv_{RE}, δv_{LC}, δv_{TP} and δv_{QM}; the first three originate from the relativistic energy-momentum relation, Lorentz contraction and Thomas precession, while the last is purely quantum. The contributions of δv_{RE} and δv_{LC} have been previously calculated with the variational Monte Carlo method for ^{3}H and ^{4}He. In this brief note we report the results of similar calculations for the contributions of δv_{TP}

and δv_{QM}. These are found to be rather small.

PACS numbers: 21.30.+y, 21.45.+v

Recently we reported [1] results of variational Monte Carlo calculations of ^{3}H and ^{4}He with a relativistic Hamiltonian based on the work of Foldy [2], Krajcik and Foldy [3] and Friar [4]. This Hamiltonian has the form:

$$H = \sum_i \left[\left(m^2 + p_i^2 \right)^{1/2} - m \right] + \sum_{i<j} \left[\tilde{v}_{ij} + \delta v(\mathbf{P}_{ij}) \right] + \sum_{i<j<k} V_{ijk}, \tag{1}$$

where $\mathbf{p}_i$ label momenta of particles, and $\mathbf{P}_{ij} = \mathbf{p}_i + \mathbf{p}_j$ is the total momentum of the pair ij. The two-nucleon interaction $\tilde{v}_{ij}$ is obtained by fitting the scattering data in the $\mathbf{P}_{ij} = 0$ frame. The boost interaction $\delta v(\mathbf{P}_{ij})$ is zero when $\mathbf{P}_{ij} = 0$, and is generally given by:

$$\delta v(\mathbf{P}_{ij}) = -\frac{P_{ij}^2}{8m^2}\tilde{v}_{ij} + \frac{1}{8m^2}\left[\mathbf{P}_{ij} \cdot \mathbf{r}_{ij} \mathbf{P}_{ij} \cdot \boldsymbol{\nabla}_{ij}, \tilde{v}_{ij} \right] + \frac{1}{8m^2}\left[(\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j) \times \mathbf{P}_{ij} \cdot \boldsymbol{\nabla}_{ij}, \tilde{v}_{ij} \right] \tag{2}$$

up to order P_{ij}^2/m^2. Only the first two terms of this $\delta v(\mathbf{P}_{ij})$ were considered in ref. [1]. The last term, having $(\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j)$, does not have diagonal matrix elements in eigenstates of $S^2 = (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j)^2$. Hence it was neglected in [1]. The Urbana model VII of V_{ijk} is used, and its boost correction $\delta V_{ijk}(\mathbf{P}_{ijk})$ is neglected. This correction is zero for ^{3}H in its rest frame, and in ^{4}He it is expected to contribute much less than the $\delta v(\mathbf{P}_{ij})$.

In the present work we calculate the expectation value of the $(\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j)$ term in $\delta v(\mathbf{P}_{ij})$. This term can couple the dominant two-nucleon $T, S = 1, 0$ and $0, 1$ waves in the wave function of ^{3}H and ^{4}He to the small P-waves having $T, S = 1, 1$ and $0, 0$ respectively. The $\tilde{v}_{ij}$ has fourteen terms like those of the Urbana v_{14} interaction [5]. The first six of these have operators $(1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}) \otimes (1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j)$, and are denoted by $\tilde{v}_{6,ij}$:

$$\begin{aligned} \tilde{v}_{6,ij} = {} & v_c(r_{ij}) + v_\sigma(r_{ij}) \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + v_t(r_{ij}) S_{ij} \\ & + \left[v_\tau(r_{ij}) + v_{\sigma\tau}(r_{ij}) \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j + v_{t\tau}(r_{ij}) S_{ij} \right] \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j. \end{aligned} \tag{3}$$

The $\tilde{v}_{6,ij}$ gives $> 98\%$ of the $\langle \tilde{v}_{ij} \rangle$ in ^{3}H and ^{4}He, therefore we approximate the $\tilde{v}_{ij}$ in the $(\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j)$ term of $\delta v(\mathbf{P}_{ij})$ by $\tilde{v}_{6,ij}$.

The commutator can be written as:

$$\frac{1}{8m^2}\left[(\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j) \times \mathbf{P}_{ij} \cdot \boldsymbol{\nabla}_{ij}, \tilde{v}_{6,ij} \right] = \delta v_{TP}(\mathbf{P}_{ij}) + \delta v_{QM}(\mathbf{P}_{ij}), \tag{4}$$

where

$$\delta v_{TP}(\mathbf{P}_{ij}) = \frac{1}{8m^2} (\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j) \times \mathbf{P}_{ij} \cdot (\boldsymbol{\nabla}_{ij} \tilde{v}_{6,ij}) \,, \tag{5}$$

and $\delta v_{QM}(\mathbf{P}_{ij})$ contains terms that come from the commutator of $(\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j)$ with the spin operators in $\tilde{v}_{6,ij}$. The $\delta v_{TP}(\mathbf{P}_{ij})$ originates from the classical Thomas precession [6,7]. The precession of the spin $\mathbf{s}_i$ in the frame moving with velocity $\mathbf{P}_{ij}/2m$ is given by $-\boldsymbol{\nabla}_{ij}\tilde{v}_{ij} \times \mathbf{P}_{ij}/4m^2$ up to order $1/m^2$. Thus the Thomas precession potential for particle i is:

$$-\frac{1}{2}\boldsymbol{\sigma}_i \cdot \frac{\boldsymbol{\nabla}\tilde{v}_{ij} \times \mathbf{P}_{ij}}{4m^2} = \frac{1}{8m^2}\boldsymbol{\sigma}_i \times \mathbf{P}_{ij} \cdot (\boldsymbol{\nabla}_{ij}\tilde{v}_{ij}) \,. \tag{6}$$

Both particles have same velocity due to their center of mass motion, but their accelerations due to $\tilde{v}_{ij}$ are equal and opposite. Therefore the Thomas precession potential for the particle j is $-\boldsymbol{\sigma}_j \times \mathbf{P}_{ij} \cdot (\boldsymbol{\nabla}_{ij}\tilde{v}_{ij})/8m^2$, and together with (6) it makes up the $\delta v_{TP}(\mathbf{P}_{ij})$. After some algebra we obtain:

$$\begin{aligned}\delta v_{TP}(\mathbf{P}_{ij}) = \frac{1}{8m^2 r} \Big[& \left(v_c' - v_\sigma' + v_t' + 3\frac{v_t}{r}\right) \mathbf{P}\cdot\mathbf{r} \times (\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j) \\ & -i\left(2v_\sigma' + v_t' + 3\frac{v_t}{r}\right) (\mathbf{P}\cdot\boldsymbol{\sigma}_i\ \mathbf{r}\cdot\boldsymbol{\sigma}_j - \mathbf{P}\cdot\boldsymbol{\sigma}_j\ \mathbf{r}\cdot\boldsymbol{\sigma}_i)\Big] + \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j \text{ term,}\end{aligned} \tag{7}$$

where v_x' denotes $\partial v_x/\partial r$, the ij subscripts of $\mathbf{r}$, $\mathbf{P}$ and v_x are omitted for brevity, and the $\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$ term has v_τ, $v_{\sigma\tau}$ and $v_{t\tau}$ in place of v_c, v_σ and v_t.

The $\delta v_{QM}(\mathbf{P}_{ij})$ does not have a classical analogue; it is found to be:

$$\begin{aligned}\delta v_{QM}(\mathbf{P}_{ij}) = & \frac{i}{2m^2}(v_t - v_\sigma)\,(\mathbf{P}\cdot\boldsymbol{\sigma}_i\ \boldsymbol{\sigma}_j\cdot\boldsymbol{\nabla} - \mathbf{P}\cdot\boldsymbol{\sigma}_j\ \boldsymbol{\sigma}_i\cdot\boldsymbol{\nabla}) \\ & -\frac{3i}{4m^2}\ \frac{v_t}{r^2}\ \mathbf{P}\cdot\mathbf{r}\,(\boldsymbol{\sigma}_i\cdot\mathbf{r}\ \boldsymbol{\sigma}_j\cdot\boldsymbol{\nabla} - \boldsymbol{\sigma}_j\cdot\mathbf{r}\ \boldsymbol{\sigma}_i\cdot\boldsymbol{\nabla}) \\ & -\frac{3i}{4m^2}\ \frac{v_t}{r^2}\,(\mathbf{P}\cdot\boldsymbol{\sigma}_i\ \mathbf{r}\cdot\boldsymbol{\sigma}_j - \mathbf{P}\cdot\boldsymbol{\sigma}_j\ \mathbf{r}\cdot\boldsymbol{\sigma}_i)\,\mathbf{r}\cdot\boldsymbol{\nabla} \\ & +\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j \text{ terms}\end{aligned} \tag{8}$$

from eq. (4).

It is convenient [7] to express $\delta v(\mathbf{P}_{ij})$ given by eq. (2) as:

$$\delta v(\mathbf{P}_{ij}) = \delta v_{RE}(\mathbf{P}_{ij}) + \delta v_{LC}(\mathbf{P}_{ij}) + \delta v_{TP}(\mathbf{P}_{ij}) + \delta v_{QM}(\mathbf{P}_{ij}). \tag{9}$$

Its first term:

$$\delta v_{RE}(\mathbf{P}_{ij}) = -\frac{P_{ij}^2 \ \tilde{v}_{ij}}{8m^2} \tag{10}$$

comes from the relativistic energy, and the second:

$$\delta v_{LC}(\mathbf{P}_{ij}) = \frac{1}{8m^2}\mathbf{P}_{ij} \cdot \mathbf{r}_{ij} \ \mathbf{P}_{ij} \cdot (\boldsymbol{\nabla}_{ij} \, \tilde{v}_{ij}) \tag{11}$$

from Lorentz contraction. The $[\mathbf{P}_{ij} \cdot \mathbf{r}_{ij}\mathbf{P}_{ij} \cdot \boldsymbol{\nabla}_{ij}, \tilde{v}_{ij}]$ can have terms in addition to those in δv_{LC} when $\tilde{v}_{ij}$ depends upon the relative momentum $\mathbf{p}_{ij}$. These terms are to be regarded as a part of δv_{QM}. However, they vanish when $\tilde{v}_{ij}$ is approximated with $\tilde{v}_{6,ij}$.

The expectation values of $\delta v_{TP}(\mathbf{P}_{ij})$ and $\delta v_{QM}(\mathbf{P}_{ij})$ are calculated with the variational wave function of ref. [1] using the Monte Carlo methods described in [1]. The results are tabulated in table I along with others of interest from [1]. The contributions of δv_{TP} and δv_{QM} are much smaller than those of δv_{RE} and δv_{LC} as expected. These contributions would be exactly zero if there were no two-nucleon P-waves in these nuclei.

Stadler and Gross [8] have also estimated these contributions in ^{3}H with a different method and obtained similar results.

The authors would like to thank Dr. J. L. Friar for illuminating discussions. The work of JLF and VRP is partly supported by the U.S. National Science Foundation via grant PHY–89–21025, that of JC and RS was performed under the auspices of the U.S. Department of Energy.

TABLES

TABLE I. Expectation values in MeV

	^{3}H	^{4}He
$\langle \sum_i (m^2 + p_i^2)^{1/2} - m \rangle$	48.7(2)	105.0(6)
$\langle \sum_{i<j} \tilde{v}_{ij} \rangle$	-55.9(2)	-127.4(5)
$\langle \sum_{i<j<k} \tilde{v}_{ijk} \rangle$	-1.21(2)	-5.43(15)
$\langle \sum_{i<j} \delta v_{RE}(\mathbf{P}_{ij}) \rangle$	0.23(2)	1.17(3)
$\langle \sum_{i<j} \delta v_{LC}(\mathbf{P}_{ij}) \rangle$	0.10(1)	0.53(1)
$\langle \sum_{i<j} \delta v_{TP}(\mathbf{P}_{ij}) \rangle$	0.016(2)	0.074(4)
$\langle \sum_{i<j} \delta v_{QM}(\mathbf{P}_{ij}) \rangle$	-0.004(2)	-0.014(4)
$\langle H \rangle$	-8.07(3)	-25.90(8)

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