Variational calculation of the ground state properties of the trinucleon system

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A practical and flexible variational method is employed to calculate the trinucleon ground state energy, wave function, and charge form factor, using the s-wave Malfliet-Tjon potentials V and VI. The results are compared with existing accurate solutions of the same potentials. The charge form factor is found to be rather insensitive to the addition of different three-body forces.

Due to their simple structure, the Malfliet-Tjon (MT) potentials[1] have become the testing ground for approximation methods.[2–4] It is in this spirit that we report the following calculation. Our variational method is rather unconventional although it has been used a number of times.[5,6] We briefly outline it as follows.

Starting from a known function $(x|0)$ not orthogonal to the ground state wave function of a quantum mechanical system, one can construct the ground state wave function $\langle x|0\rangle$ by the following process:

$$|0\rangle = \lim_{N\to\infty} |XN) = [1/(H-a)]^N|0) \quad . \tag{1}$$

H is the Hamiltonian and a a numerical energy parameter that lies closer to the ground state energy than any other.

The Green's function–Monte Carlo method used in Ref. 2 evaluates Eq. (1) using the Monte Carlo method. We evaluate the operator $1/(H-a)$ in a truncated space of a complete set of basis functions. In other words, the variational functions $(x|XN)$ are expanded in terms of the basis functions. For our three-body systems, we have the expansion,

$$\psi = \sum_{(n_1n_2n_3)} C_{1(n_1n_2n_3)} T(r_{12}^{n_1} r_{13}^{n_2} r_{23}^{n_3}) \exp[-a_1(r_{12}+r_{13}+r_{23})] + \sum_{(n_1n_2n_3)} C_{2(n_1n_2n_3)} T(r_{12}^{n_1} r_{13}^{n_2} r_{23}^{n_3}) \exp[-a_2(r_{12}+r_{13}+r_{23})] . \tag{2}$$

The r's are the internucleon distances, T the completely symmetric Young operator, and a_1, a_2 two nonlinear variational parameters. These simple basis functions are chosen so that no numerical integration is necessary for our wave function calculations.

From our experience in applying this method to various systems, we found that for a reasonably chosen a and $(x|0)$, $N=2$ in Eq. (1) is quite sufficient.

Our calculation has adopted the same values for the potential parameters as in Ref. 2. Namely, we have,

$$\frac{\hbar^2}{M} = 41.47 \text{ MeV fm}^2 ,$$

$$V(r) = [1458.05\exp(-3.11r)/r - 578.09\exp(-1.55r)/r] \text{ MeV} ,$$

for the MT V potential, and

$$V(r) = -58.795\exp(-0.723r)/r \text{ MeV} ,$$

for the MT VI potential. The various parameters in the variational wave functions and the corresponding energies, evaluated using MT VI and MT V are listed in Tables I and II, respectively. The number of digits retained in the energies is determined by the last digit where the variational energy and the variational lower bound from the method of moments[5] both are equal. Note that the variational upper and lower bounds are not the absolute upper and lower bounds of the exact energy. They only measure how close Eq. (1) has converged with respect to a particular expansion in Eq. (2). It is a reflection of the numerical accuracy however.

It is seen from Table I that the ground state wave function of MT VI is very smooth, so that even the five-term expansion is sufficiently accurate. The energy of this potential was reported in Ref. 1 to be -10.6 MeV.

Table II shows that a good MT V wave function needs considerably more terms in the expansion. Our calculation is consistent with the exact energy -8.26 ± 0.01 MeV reported in Ref. 2. Our 40-term expansion is comparable with theirs.

The Malfliet-Tjon potential VI is a purely attractive potential. Its wave function in configuration space is fairly smooth. That was demonstrated by a graphical study in Ref. 7. The Malfliet-Tjon potential V consists of a short range repulsive term as well as an attractive term. The wave function in configuration space consists of peaks and valleys.[7] Despite such seemingly difficult situations, our simple variational function converges quite well at about 40 terms.

Our charge form factors $F(q^2)$ are obtained with a limited amount of numerical integration. Since $F(0)=\int \Psi^*\Psi d\tau$, the integrals in $F(0)$ can be checked with those obtained in the wave function calculation where no numerical integration was used. This gives us a very useful means of finding

TABLE I. Parameters of wave functions and energies calculated using the Malfliet-Tjon potential VI.

Total number of terms	a_1	Number of terms in a_1	a_2	Number of terms in a_2	Energy (MeV)
5	0.4	1	0.75	4	−10.6819
14	0.5	4	0.7	10	−10.7018

TABLE II. Parameters of wave functions and energies calculated using the Malfliet-Tjon potential V.

Total number of terms	a_1	Number of terms in a_1	a_2	Number of terms in a_2	Energy (MeV)
5	0.27	1	1.0	4	−7.191 46
14	0.45	4	0.85	10	−7.955 73
20	0.75	10	1.0	10	−8.068 83
30	0.75	10	1.1	20	−8.200 35
40	0.77	20	1.15	20	−8.237 83

out how many Gaussian points are needed for sufficient accuracy. In fact, without sufficient accuracy in the numerical integration, the form factor gives large oscillations in $F(q^2)$ for $q^2 > 14\ \text{fm}^{-2}$, even though $F(q^2)$ was correctly obtained for smaller q^2.

For comparison, we plotted the charge form factor obtained from the 14-term MTVI wave function in Fig. 1. The monotonic appearance of the form factor is a reflection of the smoothness of its wave function. That, of course, is due to the purely attractive nature of its underlying potential.

In Fig. 2, we plotted $|F(q^2)|$ obtained with the 40-term MTV wave function together with the $|F(q^2)|$ obtained with the 14-term MTV wave function. The energies calculated from these two functions differ by 0.28 MeV.

The MTV charge form factors have the familiar appearance of those calculated from the realistic potentials. It has the usual shortcomings in that the zero of the form factor is too far out (at $q^2 = 18.5\ \text{fm}^{-2}$), and the secondary maximum in $|F(q^2)|$ is about 2.2 times too small compared to experiment data. All these potentials have the short range repulsion.

Comparing the charge form factors in Figs. 1 and 2, one cannot help but take notice of the drastic affect that the short range repulsion has on $F(q^2)$, and one expects the likelihood that the charge form factor is strongly two-body potential model dependent!

To test the sensitivity of the charge form factor due to the addition of three-body forces in the Hamiltonian, we used two drastically different forms of three-body forces. These potentials were chosen for their computational expediency, lack of numerical integration, and the need for only minor

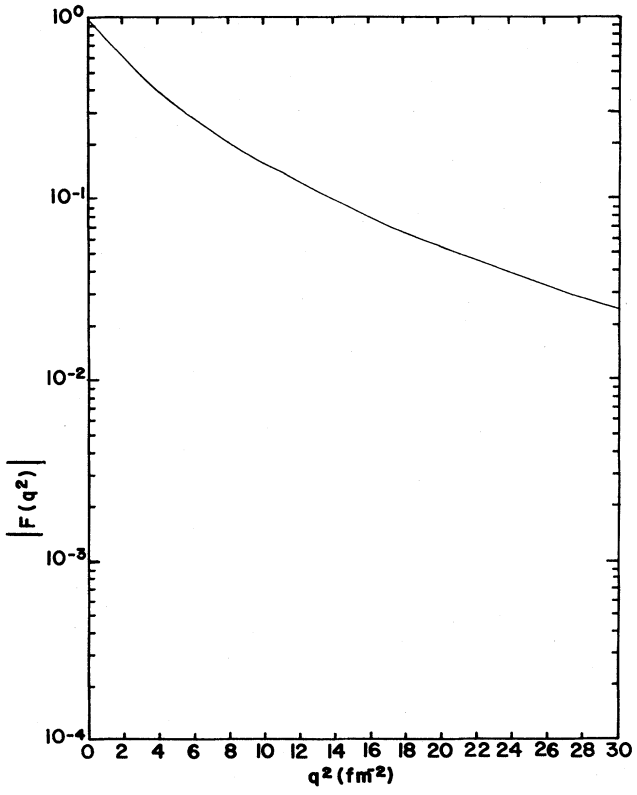

FIG. 1. Charge form factor $|F(q^2)|$ calculated using the 14-term wave function and the Malfliet-Tjon potential VI.

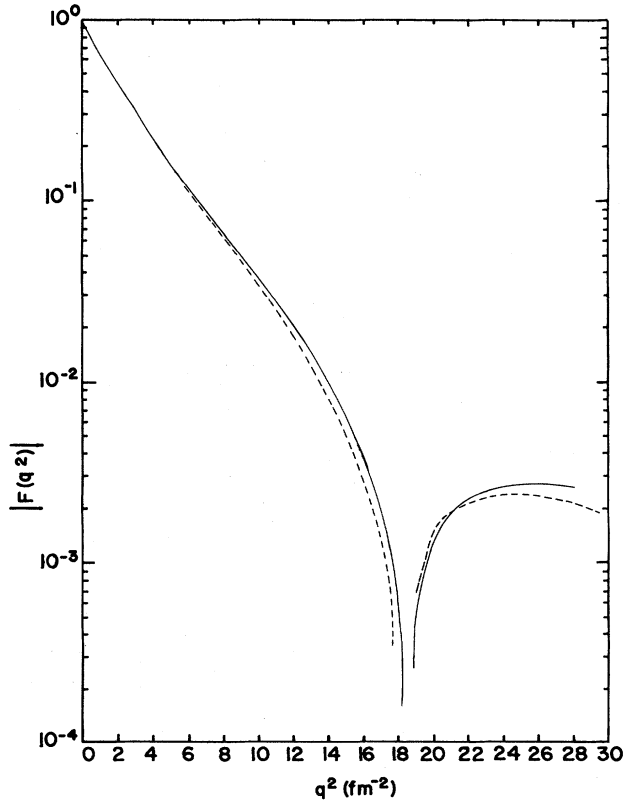

FIG. 2. Charge form factors $|F(q^2)|$ calculated using the 40-term wave function and the Malfliet-Tjon potential V—solid line, and using the 14-term wave function and the Malfliet-Tjon potential V—dashed line.

changes in our programming. We have

$$V_{31} = -5 \sum_{\text{cyclic}} (r_{12}+r_{13}-r_{23})(r_{13}+r_{23}-r_{12})(r_{12}+r_{23}-r_{13}) \times \exp[-0.5(r_{12}+r_{13})]/(r_{12}r_{13}r_{23}) \text{ MeV} .$$

The corresponding energy obtained with the addition of V_{31} to the MTV potential is -9.0362 MeV. This is an increase in binding energy of 1.48 MeV. V_{31} is attractive only when the three nucleons form triangles. It becomes zero when they take a collinear formation.

For the second three-body force, we used $V_{32} = -90|\Psi|^2$ MeV. The energy obtained with V_{32} and MTV is $-8.523\,80$ MeV. This is an increase in binding of 0.57 MeV. Again the 14-term wave function is used. With the nonlinear V_{32}, the algebraic equations in our method were solved iteratively. It takes seven iterations for the six digits convergent result quoted above. Since there is no integration needed for subsequent iterations, the computer time required is minimum.

The charge form factors calculated with the 14-term MTV wave function without three-body force, with V_{31} and with V_{32}, are plotted, respectively, in Fig. 3 for comparison. One notices that in both cases, their effect on the form factor is rather small. In the case of V_{31}, it increases the secondary maximum by 16% even when the strength of the three-body forces are adjusted to increase the binding energy by 1.48 MeV, which is about a 20% increase in binding energy. Their effect on the position of the zero in $F(q^2)$ is even weaker and it is not always in the right direction. In the case of V_{32}, it increases the secondary maximum by 9% with an energy increase of 0.57 MeV or a 7% increase in binding energy. The zero in $F(q^2)$ always moves in the wrong direction.

For all practical purposes, such as binding energy and charge form factor calculations, our 40-term wave function seems to be quite adequate. This calculation is carried out on our small on-campus Cyber 750. The computer core space available for our use is very limited. In a calculation using more realistic potentials, comparable wave function involves 180 terms.[8] Such calculation is easily manageable on computers with large core memory.

Our three-body force calculation indicates that the charge form factor is very insensitive to the addition of purely attractive three-body forces, such as V_{31} and V_{32}. Perhaps a short range repulsive part in the three-body force is essential. The three-body force used in Ref. 2 is repulsive when the nucleons are on or near collinear configuration and becomes attractive in triangle formation. Yet unrealistically large strength is needed to get the desirable effect.[2] Such three-body force when properly regularized at $r_{ij}=0$ for our use, will be investigated in our subsequent calculation using more realistic potentials.

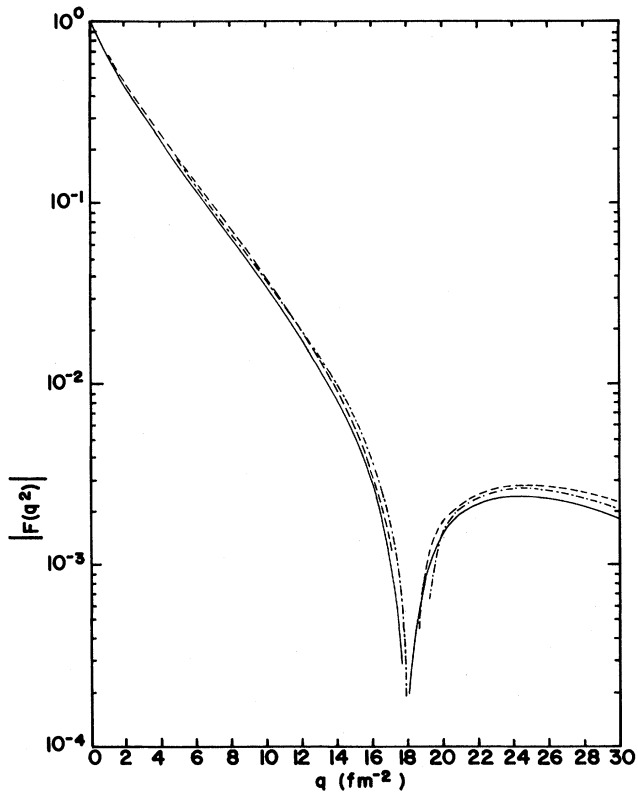

FIG. 3. Charge form factors $|F(q^2)|$ calculated using the 14-term wave function and Malfliet-Tjon potential V without three-body force—solid line, with the three-body force V_{31}—dashed line, with the three-body force V_{32}—dot dashed line.

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