Configuration space Faddeev calculations. II. Trinucleon Coulomb energy

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Coordinate space Faddeev techniques and a variety of potentials are used to calculate energies and wave functions for the trinucleon system, both with and without a static Coulomb interaction between the two protons. The wave functions are used to calculate first- and second-order perturbation theory contributions to the Coulomb energy of ^{3}He. Because too few partial-wave components of the potential are kept, the energy eigenvalues themselves are an inaccurate gauge of the Coulomb effect. The approximate hyperspherical formula was tested after calculating charge densities and found to be accurate to better than 2 percent. It is demonstrated that when using a phenomenological approach to the ^{3}He Coulomb energy, the second-order contribution *increases* the Coulomb energy by roughly 4 ± 1 keV. Finally, sum rules relating to the $T = 3/2$ state probability and the size of the second-order contribution are discussed.

[NUCLEAR STRUCTURE ^{3}He, Coulomb energy, Faddeev calculation.]

I. INTRODUCTION

An old problem[1] which has not yet been fully resolved is understanding the mass difference of ^{3}He and ^{3}H, the trinucleon system. Naively, one assumes that the charge-symmetry breaking in this isodoublet is due to the Coulomb repulsion between the two protons in ^{3}He, once the trivial n-p mass difference has been accounted for. Until recently, a serious problem in demonstrating this has been the lack of wave functions whose genesis was other than crude phenomenology. The advent of Faddeev techniques[2] and their implementation, as well as advanced variational calculations,[3] have largely alleviated this problem.

A more serious practical problem, however, is the fact that even the best "realistic" potentials do little more than incorporate commonly held prejudices into semiphenomenological two-nucleon forces; they contain a substantial number of free parameters which must be fit to data. In addition, there exist three-nucleon forces, necessitated by the constraints of relativity and quantum mechanics,[4] of which our understanding is even less than that of the more usual two-nucleon forces.

In view of these and other theoretical uncertainties, it is scarcely surprising that the gross properties of the trinucleon system are only moderately well reproduced by the best theory. The experimental binding energy of ^{3}H, 8.48 MeV, is larger than that calculated using realistic potentials by approximately 1 MeV, while the calculated charge radii of ^{3}He and ^{3}H are about 10 percent too large. Naively, the Coulomb energy should scale as α/R, where α is the fine structure constant and R is the "radius." Knowing that the calculated radius is incorrect, we should expect that the Coulomb energy is also incorrectly given.

In this work we will concern ourselves with just the Coulomb energy ΔE_c of ^{3}He. The complete 764 keV binding energy difference of ^{3}He and ^{3}H is certainly not entirely due to ΔE_c although this is by far the largest single contribution.[5] Other contributions are known to arise from the dynamical effect of the n-p mass difference,[6] magnetic and other relativistic interactions between nucleons,[7] isospin mixing in the mesons exchanged between nucleons,[8,9] and numerous other small effects.[7] Our approach will be to calculate wave functions by solving the Faddeev equations in coordinate space[10-12] and to use these wave functions in first-order perturbation theory to calculate first-order ($\Delta E_c^{(1)}$) and second-order ($\Delta E_c^{(2)}$) contributions to ΔE_c. The reason for our using this procedure is that only a few partial waves of the two-nucleon potential can be retained in order to keep the calculations tractable, and this is a serious limitation in the direct eigenvalue determination when dealing with the long-ranged Coulomb potential. The incorporation of the Coulomb potential into momentum space calculations is much more complicated and will not be discussed.

Our primary objective will be to test the "hyperspherical" formula, an approximation which allows one to estimate $\Delta E_c^{(1)}$ knowing only the trinucleon charge densities or, equivalently, the charge form factors. It will be shown in Sec. IV that this formula is accurate to considerably better

than 2 percent for five different potential models with very different properties. This lends confidence that the hyperspherical formula may be used with experimental data to estimate ΔE_c more reliably than using "good" wave functions with incorrect radii. Moreover, it will be seen in Sec. II that this formula has a simple semiclassical geometric origin, which allows us to use experimental data to scale model results to the correct α/R. In addition, the small second-order contribution will be calculated for these models and scaling arguments used to estimate its size for the physical ^{3}He nucleus. Our motivation for this is the very large (10–20 keV) $\Delta E_c^{(2)}$ found in some earlier calculations.[13,14] An interesting secondary result, demonstrated in Sec. III, is that when using phenomenological approaches to estimate $\Delta E_c^{(1)}$, such as the hyperspherical formula, the second-order contribution *increases* ΔE_c. A discussion of the exotic $T=\frac{3}{2}$ component of the ^{3}He wave function[15,16] and sum rules relating to the Coulomb energy are presented in Sec. IV. Results are discussed in Sec. V and a summary of the paper presented in Sec. VI. Details of the Faddeev calculation not found in Ref. 11 are relegated to an appendix.

II. THE HYPERSPHERICAL FORMULA

The hyperspherical formula[5] is most easily "derived" as a semiclassical approximation. We imagine the trinucleon as an equilateral triangle with the nucleons at the vertices. The distance between the two protons, x, is related to the distance between the center of gravity of the triangle and either of the two protons r [which is the coordinate that specifies the behavior of the charge density $\rho(r)$] by the relationship $x=\sqrt{3}r$. Thus the expectation value of α/x, which is $\Delta E_c^{(1)}$, becomes

$$\Delta E_c^{(1)}=\frac{\alpha}{\sqrt{3}}\langle 1/r\rangle=\frac{\alpha}{\sqrt{3}}\int d^3r\frac{\rho(r)}{r}. \tag{1}$$

This argument does not specify the particular combination of wave function components which determines the various densities, or how the proton finite size enters. Neglecting the tiny neutron-neutron contribution to $\Delta E_c^{(1)}$, Eq. (2) of Ref. 5 may be Fourier transformed into the form given by Parseval's theorem

$$\Delta E_c^{(1)}=\frac{\alpha}{\sqrt{3}}\frac{4\pi}{(2\pi)^3}\int_0^\infty\frac{d^3q}{q^2}G_p^{\,2}(q^2/3)[F_s(q^2)+F_v(q^2)] \tag{2}$$

$$=\frac{\alpha}{\sqrt{3}}\int\frac{d^3r}{r}g(r)[\rho_s(r)+\rho_v(r)]\equiv\frac{\alpha}{\sqrt{3}}\langle 1/r\rangle_c, \tag{3}$$

where ρ_s and ρ_v are the point nucleon isoscalar and isovector densities, respectively, whose Fourier transforms are F_s and F_v. Our densities satisfy $\int d^3r\,\rho_s(r)=1$ and $\int d^3r\,\rho_v(r)=0$. The c subscript indicates the Coulomb combination of densities and the inclusion of the proton form factors G_p through g. In addition, we have defined g by

$$\frac{g(r)}{r}\equiv\frac{4\pi}{(2\pi)^3}\int\frac{d^3q}{q^2}G_p^{\,2}(q^2/3)e^{i\vec{q}\cdot\vec{r}}. \tag{4}$$

This generates

$$g_D(r)=1-e^{-x}(1+11x/16+3x^2/16+x^3/48) \tag{5a}$$

with $x=\sqrt{3}Ar$ if we assume a dipole form for G_p:

$$G_p(q^2)=(1+q^2/A^2)^{-2}. \tag{5b}$$

Naturally, $g_D(r)$ vanishes for $r\to 0$ and approaches 1 as $r\to\infty$ or as $A\to\infty$ (point protons). The scale of the Coulomb energies is given by $\hbar c\alpha/\sqrt{3}=831.37$ keV fm and that of the nucleons by $A=4.270$ fm^{-1}.

Equation (3), providing that it is accurate, allows us to extrapolate from charge distributions whose size is too large or small to the physical one. Although it has been known for a long time that the wrong radius would produce the wrong Coulomb energy, it had not been appreciated that one should scale this energy like $\langle 1/r\rangle$, rather than $1/\langle r^2\rangle^{1/2}$. Assuming that Eq. (3) is accurate, scaling ΔE_c for various distributions with $\langle r^2\rangle^{-1/2}$ would clearly not be as effective. It is fairly straightforward to use the Hölder inequality[17] to prove that for any non-negative $\rho(r)$, $\langle 1/r\rangle>\langle r^2\rangle^{-1/2}$, and for a selection of simple one-parameter densities (uniform, exponential, Gaussian) one finds that the product of $\langle r^2\rangle^{1/2}\langle 1/r\rangle$ is $[(\frac{27}{20})^{1/2},\ (6/\pi)^{1/2},\ \sqrt{3}]$ or (1.16, 1.38, 1.73). This shows a considerable variation of $\langle 1/r\rangle$ even when $\langle r^2\rangle^{1/2}$ is fixed. A similar relationship holds with the inclusion of the nucleon form factor. [A rough formula which works for either point nucleons, point nuclei, or Gaussian form factors for both nucleon and nucleus is $\langle 1/r\rangle_c=(\langle 1/r\rangle_N^{-2}+\langle 1/r\rangle_p^{-2})^{-1/2}$, where N refers to the point nuclear distribution $\rho_s+\rho_v$, while p refers to a moment with respect to the convolution of two identical proton distributions,[18] each scaled by $\sqrt{3}$:$\rho_p^{(2)}(\sqrt{3}r)$.]

III. PERTURBATION THEORY

Perturbation theory plays an important role in our calculation; because there appears to be no derivation of this in the literature for the coordinate space Faddeev problem and because we wish to make several points clear, we present a brief derivation. We define[10,11] permutation operators $P^{(+)}$ and $P^{(-)}$ for the *three-body problem* which are cyclic $[P^{(+)}(123)=(312)]$ and anticyclic $[P^{(-)}(123)=(231)]$; clearly these operators are inverses of each other and also $[P^{(\pm)}]^2=P^{(\mp)}$. In addition, it is

easy to prove that the P's are real operators and that $[P^{(\pm)}]^T = P^{(\mp)} = [P^{(\pm)}]^\dagger = [P^{(\pm)}]^{-1}$. Thus, $P^{(\pm)}$ are orthogonal operators. Defining $P = P^{(+)} + P^{(-)}$ with $P^\dagger = P$, the three Faddeev equations can be written in coordinate space in the form

$$(E - T - V_i)\psi_i = V_i P \psi_i , \tag{6}$$

where T is the kinetic energy and $V_i \equiv V_{jk}$ for a pair of nucleons $(j,k) \neq i$. The three Faddeev amplitudes ψ_i are permutations of each other and generate the total wave function according to

$$\Psi = \sum_i \psi_i = (1+P)\psi_i . \tag{7}$$

We choose to work with ψ_1, which we denote by ψ, and note that $\tilde{H} \equiv T + V_1 + V_1 P$ is not Hermitian in the usual sense because P and V_1 do not commute. However,

$$(1+P)\tilde{H} = \tilde{H}^\dagger (1+P) , \tag{8}$$

which is the Hermiticity relation allowing one to prove that energy eigenvalues are real, Faddeev wave functions corresponding to different energies (ψ_f and ψ_i) are orthogonal, etc. The latter condition becomes

$$\int \psi_f^\dagger (1+P)\psi_i = \delta_{fi}/3 . \tag{9}$$

If the potential V_1 is written as $\overline{V} + \Delta\overline{V}$, ($\Delta V = \Delta V_1 + \Delta V_2 + \Delta V_3$), perturbation theory may be derived by writing

$$(E - T - \overline{V} - \overline{V}P)\psi = \Delta\overline{V}(1+P)\psi \tag{10}$$

and postmultiplying by $\phi^\dagger(1+P)$. We have defined ϕ to be the solution ψ with $\Delta\overline{V} \equiv 0$, corresponding to $E = E_0$, and find using Eq. (7), $\Phi = (1+P)\phi$, and the antisymmetry of Φ and Ψ that

$$\Delta E \equiv E - E_0 = \frac{\langle \Phi \mid \Delta V \mid \Psi \rangle}{\langle \Phi \mid \Psi \rangle} = \frac{3\langle \phi \mid (1+P)\Delta\overline{V}(1+P) \mid \psi \rangle}{\langle \Phi \mid \Psi \rangle} . \tag{11}$$

This is the usual starting point for Schrödinger perturbation theory,[19] which exhibits the crucial importance of the permutation operator P.

The first two orders of perturbation theory may be derived by writing $\Psi \cong \Phi + \Delta\Psi$, with $\Delta\Psi$ of order ΔV. We use normalized wave functions Φ and Ψ, which means that $\langle \Phi \mid \Delta\Psi \rangle = 0$; normalization corrections arise in second order in ΔV. This leads immediately to

$$\Delta E \cong \langle \Phi \mid \Delta V \mid \Phi \rangle + \langle \Phi \mid \Delta V \mid \Delta\Psi \rangle \equiv \Delta E^{(1)} + \Delta E^{(2)} . \tag{12}$$

If we choose a method for estimating ΔE which uses Ψ instead of Φ, and if $\Delta E^{(3)}$, the third-order contribution, is negligible, we find

$$\Delta\tilde{E}^{(1)} \equiv \langle \Psi \mid \Delta V \mid \Psi \rangle \cong \langle \Phi \mid \Delta V \mid \Phi \rangle + \langle \Phi \mid \Delta V \mid \Delta\Psi \rangle + \langle \Delta\Psi \mid \Delta V \mid \Phi \rangle = \Delta E^{(1)} + 2\Delta E^{(2)} . \tag{13}$$

This interesting result demonstrates that using wave functions which include the effect of ΔV (in our case, wave functions which include the effect of Coulomb distortion) requires us to *subtract* $\Delta E^{(2)}$ from $\Delta\tilde{E}^{(1)}$ in order to obtain ΔE:

$$\Delta E \cong \Delta\tilde{E}^{(1)} - \Delta E^{(2)} . \tag{14}$$

Since $\Delta E^{(2)}$ is always negative, ΔE is greater than $\Delta\tilde{E}^{(1)}$. Furthermore, forming sums and differences we obtain two useful expressions:

$$\Delta E \cong \frac{\Delta\tilde{E}^{(1)} + \Delta E^{(1)}}{2} , \tag{15a}$$

$$\Delta E^{(2)} = \frac{\Delta\tilde{E}^{(1)} - \Delta E^{(1)}}{2} . \tag{15b}$$

Finally, we note that these results hold even if a nonlocal potential is used, which is the usual case with Faddeev calculations. That is, two-body forces are partial-wave projected and only a limited number of such waves are kept:

$$V_{ij} = \mid ij\rangle V(x) \langle ij \mid + \cdots , \tag{16}$$

where $\mid ij\rangle$ is a channel projector for the interacting pair (ij) in some partial wave. As first noted by Gignoux and Laverne,[12] the long-range nature of the Coulomb force can lead to serious inaccuracies if we truncate it to a single partial wave ($^1S_0$). The missing ^3P and higher partial waves can make an important Coulomb energy contribution in the Faddeev eigenvalues. But even in the absence of ^3P forces our perturbation theory wave functions include induced (relative coordinate, two-body) ^3P components because the permutation operators $P^{(+)}$ and $P^{(-)}$ generate such wave function elements in rearranging the various nuclear coordinates [see Eq. (11)]. If one truncates the Coulomb potential in the manner of Eq. (16), these components do not contribute to ΔE_c in perturbation theory because they are eliminated by the projection operators. However, used with the complete (all partial waves) Coulomb interaction, the permutation induced components can generate significant contributions. We note that the induced components are always used when the density ρ is calculated [see Eq. (9)]. Thus, because we wish to correlate ΔE_c and ρ, it is important for us to calculate the Coulomb energy using the perturbation theory approach, a method which includes the effect of all wave function components.

IV. SUM RULES AND SCALING

Exact wave functions for the Coulomb problem contain several ingredients which are not present in the absence of this force. In particular, the Coulomb force averaged over all nucleons (i.e., $\frac{1}{3}\sum_{i<j}\alpha/r_{ij}$) simply *expands* the wave function, without changing its symmetry character.[15] The remainder of the force is of mixed-symmetry character and *distorts* the wave function by changing the amounts of S' (mixed-symmetry) states, for example, as well as creating a $T=\frac{3}{2}$ isospin component of the wave function.[15] This classification of the Coulomb effect into distortion and expansion categories is due to Ohmura.[15] The $T=\frac{3}{2}$ component is quite small, as we will see, and neglecting it does no serious damage to Coulomb calculations. As noted by Gignoux and Laverne,[12] if the $T=\frac{3}{2}$ component of the Faddeev wave function is dropped, the resulting Faddeev equations for the usual set of S- and D-wave potentials is made smaller by one component and differs from the charge-symmetric case by the addition of $2/3V_c$ to the $^1S_0$ potential, presuming of course that only S waves are kept for the isospin triplet channel. This may be verified using Eq. (A4). This approximation is therefore extremely easy to implement in standard two-, three-, four-, and five-channel Faddeev calculations.

The first-order wave function change $\Delta\Psi$ due to the Coulomb interaction can be written in the form[19]

$$|\Delta\Psi\rangle=\sum_{N\neq 0}\frac{|N\rangle\langle N|V_c|\Phi\rangle}{E_0-E_N}. \tag{17}$$

Introducing a projection operator $\hat{P}_{3/2}$, which is nonvanishing only when acting on $T=\frac{3}{2}$ states, we can write

$$|\Delta\Psi\rangle_{3/2}\equiv\frac{-\hat{P}_{3/2}V_c|\Phi\rangle}{\delta\overline{E}}, \tag{18a}$$

which defines $\delta\overline{E}$, and the $T=\frac{3}{2}$ probability becomes

$$P_{3/2}=\frac{\langle\Phi|V_c\hat{P}_{3/2}V_c|\Phi\rangle}{(\delta\overline{E})^2} \tag{18b}$$

expressed in terms of $\delta\overline{E}$, the effective excitation energy. As noted by Werntz and Valk,[20] $\delta\overline{E}>E_B$, the total binding energy, and this allows an inequality to be written for $P_{3/2}$:

$$P_{3/2}\leq\langle\Phi|V_c\hat{P}_{3/2}V_c|\Phi\rangle/{E_B}^2. \tag{19}$$

Their estimate was $P_{3/2}\leq 1.7\cdot 10^{-3}$ for the Coulomb potential. We will see later that (19) overestimates $P_{3/2}$ by a factor of 50–200 for the cases we have examined, because $\delta\overline{E}>50$ MeV, while $E_B=8.5$ MeV.

Equation (17) may also be used to write the second-order perturbation theory result in the form

$$\Delta E_c^{(2)}=\sum_{N\neq 0}\frac{|\langle N|V_c|\Phi\rangle|^2}{E-E_N}$$
$$\equiv\frac{-1}{\delta\overline{E}_2}[\langle\Phi|V_c^2|\Phi\rangle-|\langle\Phi|V_c|\Phi\rangle|^2], \tag{20}$$

where $\delta\overline{E}_2$ in this equation is not the same as $\delta\overline{E}$ in Eq. (18). Furthermore, because there are only two protons, the Coulomb potential between the protons, $V_c=\alpha/r_{pp}$, when squared becomes $V_c^2=\alpha^2/r_{pp}^2$. This is easy to generalize to include finite size; the important point is that the isospin structure is identical to that of the Coulomb interaction. An interesting phenomenon in deuteron photodisintegration[21] is that the dipole strength function peaks at $E_\gamma\cong 2E_B$, where E_γ is the incident photon energy. Roughly the same behavior occurs in trinucleon photodisintegration.[22] It is therefore reasonable to assume that $\delta\overline{E}_2\cong\lambda E_B$; furthermore, it is also plausible from dimensional considerations that $\langle\Phi|V_c^2|\Phi\rangle\cong\mu|\langle\Phi|V_c|\Phi\rangle|^2$. These assumptions lead to

$$\Delta E_c^{(2)}=\frac{-(\mu-1)|\Delta E_c^{(1)}|^2}{\lambda E_B}. \tag{21a}$$

We will demonstrate numerically that the assumptions are very reasonable. In a manner similar to that used in deriving Eq. (3), a hyperspherical formula for $\langle V_c^2\rangle$ may be written in the form $\alpha^2\langle g(r)/r^2\rangle_c/3$. Note also that the $T=\frac{3}{2}$ contribution to $\Delta E_c^{(2)}$ can be written in the form

$$\Delta E_c^{(3/2)}=-\langle\Phi|V_c\hat{P}_{3/2}V_c|\Phi\rangle/\delta\overline{E}=-\delta\overline{E}P_{3/2}. \tag{21b}$$

Clearly this contribution is second order in V_c, because only $\Delta\Psi$, as opposed to Φ, contains $T=\frac{3}{2}$ components. (The coupled $T=\frac{1}{2}$, $T=\frac{3}{2}$ set of equations for the isospin triplet channel is a 2×2 problem in which the off-diagonal matrix element contribution to the energy comes in second order, as is well-known.) Obviously, $\Delta E_c^{(3/2)}$ is small, although the large value of $\delta\overline{E}$ makes the energy shift larger than simple estimates might produce.

V. RESULTS AND DISCUSSION

Specific numerical calculations of Coulomb energies were performed for several models: (1) a one-channel (three-boson) model using a local potential[23] with repulsion (*MT V*); (2) a two-channel calculation using the local S-wave Malfliet-Tjon *I–III* potential[23] (*MT I–III*); (3) a two-channel calculation using the local S-wave Malfliet-Tjon *II–IV* potential[23] (*MT II–IV*); (4) a truncated three-channel calculation using the $^1S_0$, $^3S_1-{}^3D_1$ components of the Reid soft-core potential[24]

(RSC3); (5) a complete five-channel calculation using the same components of the RSC potential (RSC5). In cases (2) and (3) two distinct approaches were used: (a) add $2/3V_c$ to the $^1S_0$ potential; (b) introduce an extra channel (for a total of 3) by adding the $T=\frac{3}{2}$ wave function component. The RSC cases were computed using the spectator approximation ($2/3V_c$) in the $^1S_0$ channel. The one-channel case was used only to test the hyperspherical formula.

Our results indicate that differencing the eigenvalues of the Faddeev equations with and without the Coulomb interaction is less stable than using perturbation theory, Eqs. (15), particularly for the RSC cases. In addition, the use of perturbation theory allows us to include the complete Coulomb potential, rather than just the S-wave projection. We feel that this is important, since the density is calculated using all of the wave function rather than selected projections. Our procedure will allow us to correlate size and Coulomb energy in a far more effective manner. A summary of these results is presented in Table I. Not all the numbers are well converged in the last significant figure, but they have been listed so that differences may be taken. Our results for the Coulomb energy calculation in perturbation theory correspond to a model with the *complete* Coulomb potential (i.e., all partial waves) and the usual set of partial-wave strong interaction potentials. Quantities labeled with an overscore indicate that the dipole form of the nucleon finite size was used in constructing the Coulomb potential. We emphasize that wave functions calculated using $\overline{V}_c$ must be used when taking the expectation values of $\overline{V}_c$ in order for the perturbation approach to be consistent. A superscript H indicates the hyperspherical formula was used to calculate $\Delta E_c^{(1)}$ and the prime indicates that Coulomb distorted densities were used. *The rms radii were calculated for point nucleons only*. The quantities ΔE_F and ΔE_P are the eigenvalue differences from the Faddeev equations and the perturbation theory estimates of ΔE_c using the S-wave projected Coulomb potential, respectively. The latter quantities should be equal, and in fact are quite close except for the RSC5 case which is the least well converged of all our calculations. We expect that the perturbation theory estimate is more accurate than ΔE_F. Note the substantial difference between

TABLE I. Properties of ^{3}He and ^{3}H for various potential models. Entries are discussed in the text.

	MT II–IV	*MT I–III*	RSC3	RSC5
E_B (MeV)	11.88	8.54	6.38	7.01
ΔE_c (keV)	1028	666	608	631
$\Delta E_c^{(2)}$ (keV)	−14	−5	−6	−5
$\Delta\overline{E}_c$ (keV)	847	634	585	605
$\Delta\overline{E}_c^{(2)}$ (keV)	−5	−4	−5	−4
$\Delta E_c^{(1)}$ (keV)	1042	671	614	636
ΔE_c^H (keV)	1026	700	640	660
$\Delta\overline{E}_c^{(1)}$ (keV)	853	638	590	609
$\Delta\overline{E}_c^H$ (keV)	851	647	598	617
$\Delta\overline{E}_c^{H'}$ (keV)	841	639	589	609
$P_{S'}$ (%)	0.68/0.79	1.95/2.17	1.88/2.21	1.66/1.93
P_D (%)	0	0	8.01/8.06	9.10/9.17
$\langle r^2\rangle^{1/2}_{^3\mathrm{He}}$ (fm)	1.367/1.394	1.772/1.805	1.987/2.036	1.894/1.933
$\langle r^2\rangle^{1/2}_{^3\mathrm{H}}$ (fm)	1.287	1.616	1.770	1.698
ΔE_F (keV)	1020	656	546	558
ΔE_P (keV)	1020	656	547	554
$\Delta\overline{E}_F$ (keV)	839	624	525	535
$\Delta\overline{E}_P$ (keV)	840	623	525	530
$P_{3/2}$ ($\cdot 10^6$)	12/5	6/4		

ΔE_c and ΔE_F or ΔE_P. This reflects the difference between using the complete V_c and its S-wave projection, and is particularly large for the RSC cases. The error due to using projected Coulomb wave functions in matrix elements of the complete Coulomb potential should be quite small.

The first important observation is that the first- and second-order results vary over a wide range for the point Coulomb interaction and over a substantial range for the finite-size Coulomb results. The next thing to note is the correlation between ΔE_c and $1/\langle r^2\rangle_{\mathrm{He}}^{1/2}$. This correlation is only partially present in $\Delta E_c^{(2)}$ indicating that the latter quantity depends on other variables (such as E_B). The two separate radii for ^{3}He quoted in each entry were calculated without (Φ) and with (Ψ) Coulomb modified wave functions, respectively. The effect of the nucleon finite size in V_c was relatively unimportant, except for the tiny $T=\frac{3}{2}$ state probabilities quoted in the last line (quoted without and with finite size) and the large change in ΔE_c in the *MT II–IV* case. The latter effect is due to the lack of repulsion in the potential, which produces wave functions that are sensitive to the short-range behavior of the Coulomb interaction. Repulsion in the other potential models makes them relatively insensitive to this unphysical effect. The entire $T=\frac{3}{2}$ state and the indicated increases in S'- and D-state probabilities when the Coulomb potential is introduced, are examples of the distortion effect of the Coulomb interaction.

Of primary interest is the comparison of $\Delta E_c^{(1)}$ and the corresponding quantity calculated using the hyperspherical formula, ΔE_c^H. The ΔE_c^H for the *MT II–IV* case is too small, but the inclusion of finite size (overscored quantities) dramatically decreases the discrepancy. The remaining cases have values for ΔE_c^H which are too large by approximately 4 percent, in agreement with Ref. 7, while the inclusion of the proton finite size reduces the discrepancy to less than 1.5 percent. In addition, the *MT-V* potential generates a ^{3}H energy of 7.54 MeV, rms radius of 1.727, $\Delta E_c^{(1)}/\Delta\bar{E}_c^{(1)}$ equal to 718/674 keV and $\Delta E_c^H/\Delta\bar{E}_c^H$ equal to 736/674 keV. These results are summarized in Fig. 1, which illustrates $\Delta E_c^{(1)}$ plotted against $\langle 1/r\rangle_c$, the hyperspherical quantity. The circles and triangles refer to point Coulomb and dipole form factor cases. The solid line indicates the hyperspherical prediction, while the "error bar" of ±2 percent is only meant to give the eye a scale. The arrows point to the values of $\langle 1/r\rangle_c$ calculated using the experimental form factors for ^{3}He and ^{3}H, which allows us to deduce 682 and 639 keV for the point and finite-size Coulomb energies.[25] If the deviations we have observed are representative of the actual physical situation (which is by no means guaranteed), assuming a 2 percent error for the hyperspherical formula is reasonable. Table I also contains a calculation ($\Delta\bar{E}_c^{H'}$) using the finite-size version of the hyperspherical formula and the Coulomb modified densities. These results should differ from $\Delta\bar{E}_c^H$ by $2\Delta\bar{E}_c^{(2)}$ approximately, as suggested by Eq. (13), and they do.

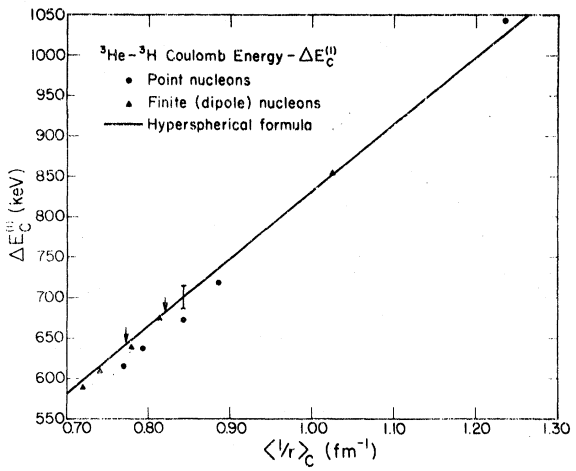

FIG. 1. Test of the hyperspherical formula $\Delta E_c^{(1)}$ vs $\langle 1/r\rangle_c$ for point Coulomb (circles) and finite-size triangles) Coulomb potentials. The error bar (±2%) is to guide the eye only. The arrows indicate point and finite-size values of $\langle 1/r\rangle_c$, calculated using the physical values of the trinucleon charge distributions.

One notable effect is the non-negligible change in the ^{3}He rms radius due to Coulomb expansion, which further increases the discrepancy between theory and experiment. In many previous calculations, it was remarked that the experimentally known radii[26,27] of 1.70 ± 0.05 fm for ^{3}H and 1.89 ± 0.05 fm for ^{3}He were in good agreement with the RSC5 calculations. These remarks are incorrect because they fail to take into account the finite size[28] of protons and neutrons which are necessarily included in experimental data, but are often left out of calculations. Using[29] $\langle r^2\rangle_p^{1/2}=0.836$ fm and $\langle r^2\rangle_n^{1/2}=-0.34$ fm, one finds the "experimental" point nucleon values of the ^{3}H and ^{3}He rms radii, 1.56 and 1.69 fm. Alternatively, our point values of 1.698 and 1.933 fm correspond to finite nucleon radii of 1.831 and 2.092 fm. We note that the Coulomb interaction changes the isoscalar and isovector components of the ^{3}He density by roughly equal amounts, 0.033 and 0.039 fm.

We indicated earlier that the $T=\frac{3}{2}$ component of the wave function makes a very small contribution to observables. We have isolated this contribution to ΔE_c and $\langle r^2\rangle_{\mathrm{He}}^{1/2}$ for the two cases we examined. Defining

TABLE II. Second-order Coulomb properties of ^{3}He for various potentials. An overscore indicates the use of $\overline{V}_c$. Entries are discussed in the text.

	$-\Delta E_c^{(2)}$	$-\Delta\tilde{E}_c^{(2)}$	$(\mu-1)$	$\delta\overline{E}_2$	$\delta\overline{E}_2/E_B$	$\delta\overline{E}(\frac{3}{2})$
MT II–IV	13.6	7.2	0.970	78±3	6.5±0.3	171
$\overline{MT\ II–IV}$	5.4	4.4	0.219	29±3	2.4±0.2	96
MT I–III	5.1	4.7	0.358	32±3	3.7±0.4	83
$\overline{MT\ I–III}$	3.9	4.0	0.226	23±3	2.7±0.4	63
RSC3	5.6	4.6	0.352	24±2	3.7±0.3	
$\overline{\text{RSC3}}$	4.6	4.1	0.255	19±2	3.0±0.3	
RSC5	4.9	4.1	0.334	28±3	3.9±0.4	
$\overline{\text{RSC5}}$	4.0	3.6	0.239	22±3	3.2±0.4	
MT V			0.374			
$\overline{MT\ V}$			0.221			

$\Delta E_c = \Delta E_c^0 + \Delta E_c^{3/2}$ and $\langle r^2\rangle_{\rm He}^{1/2} = (\langle r^2\rangle_0 + \Delta\langle r^2\rangle_{\rm He}^{3/2})^{1/2}$, we find that the isovector part of the matrix elements involving the $T=\frac{3}{2}$ components generates (essentially) the entire contribution. For the *MT II–IV* case, the $T=\frac{3}{2}$ contributions are $\Delta E_c^{3/2} = -0.99/-0.31$ keV and $[\Delta\langle r^2\rangle_{\rm He}^{3/2}]^{1/2} = 0.052/0.043$ fm for the point and finite-size problems, while the *MT I–III* case generates $-0.32/-0.22$ keV and 0.053/0.049 fm for the corresponding cases. Both changes are negligible. Table II lists the effective energy for the $T=\frac{3}{2}$ state $[\delta\overline{E}(\frac{3}{2})]$ calculated using our value of $P_{3/2}$ and Eq. (18b). These numbers are only significant in that they are large; using Eq. (21b) leads to different (but large) values for $\delta\overline{E}$, for example. This is a reflection of the mixed symmetry of the $T=\frac{3}{2}$ components, whose spatial structure is typical of states of high energy and leads directly to a tiny $P_{3/2}$. Alternatively, the matrix element of the Coulomb potential between $T=\frac{1}{2}$ and $T=\frac{3}{2}$ states is small because the Coulomb potential is smooth and does not easily connect primarily space-symmetric and mixed-symmetry wave functions. These two statements are not really different in content.

Table II also contains the second-order Coulomb energies $\Delta E_c^{(2)}$. The second column contains the scaled values of $\Delta E_c^{(2)}(\Delta\tilde{E}_c^{(2)})$; that is, we assume that $\Delta E_c^{(2)} \sim |\Delta E_c^{(1)}|^2/E_B$ and have scaled the numbers to the "physical" values of $\Delta E_c^{(1)} = 640$ keV and $E_B = 8.5$ MeV. Except for the *MT II–IV* point Coulomb result, these numbers are approximately the same, with the point Coulomb results roughly $\frac{1}{2}$ keV higher. The scaled sum rule $(\mu-1)$ from Eq. (20) is listed in the next column. The finite-size results are all approximately the same, indicating that the scaling assumption is reasonably good. The effective excitation energy $\delta\overline{E}_2$ is listed in the next column, with an error estimated by *assuming* that the error on $\Delta E_c^{(2)}$ is ±0.5 keV. Scaling these numbers by the appropriate E_B results in the next column. Note that the inclusion of the $T=\frac{3}{2}$ state increases $\Delta\tilde{E}_c^{(1)}$, which increases $\Delta E_c^{(2)}$, thereby lowering $\delta\overline{E}_2$. This would bring the RSC results closer to the *MT* results, particularly for the (physical) finite-size case. We thus expect $\mu - 1 \cong 0.24 \pm 0.03$ and $\lambda \cong 2.75 - 3$ for this case, which results in a *scaled* value of $\Delta\overline{E}_c^{(2)} \cong -4 \pm 1$ keV. A plot of unscaled and scaled values of $\Delta E_c^{(2)}$ is shown in Fig. 2. Our value for λ is somewhat higher than that found for dipole excita-

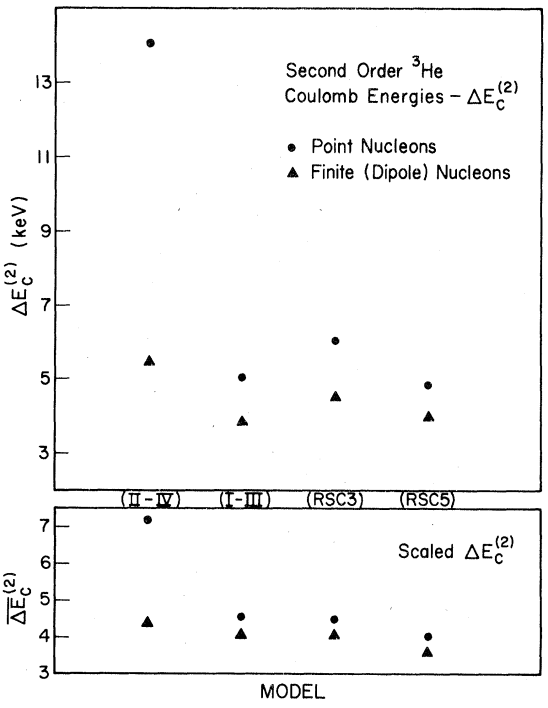

FIG. 2. Magnitude of the second-order Coulomb energies $\Delta E_c^{(2)}$ before (above) and after (below) scaling for the four potential models discussed in the text. Circles and triangles indicate the point and finite-size cases.

tions.[21] If one uses the hyperspherical formula for the sum rule, one finds values of $\langle V_c^2 \rangle$ somewhat too large by 5–10 percent; it therefore works less well than for $\langle V_c \rangle$. This is quite a reasonable result, since V_c is a smoother operator than V_c^2, and the hyperspherical approach is better for smoother operators.

There exist few previous calculations which can be used to compare with our results. Kiang and Ng[13] calculated variational wave functions using two different central potentials with a point Coulomb interaction and found −20 keV and −9 keV, respectively, for $\Delta E_c^{(2)}$. Their results, scaled as we conjectured, give −4.6 and −5.4 keV, consistent with ours. Delves and Hennell's[30] variational results for the Hamada-Johnston potential yield −4.5 keV for a point Coulomb interaction, which scales to −4.4 keV. Erens[14] found −12 and −5 keV for the *MT II–IV* and *MT I–III* potentials, which agree with our results fairly well. His results for the Coulomb energies for the former potential are approximately 3–5 keV larger than ours and 10 keV larger for the latter potential. Correspondingly, his radii are slightly smaller, more so for the latter potential. Overall agreement on the second-order scaling hypothesis must be considered good, and the physical value of $\Delta E_c^{(2)}$ correspondingly small.

Few calculations exist for the $T = \frac{3}{2}$ state. Using a variety of models without tensor forces, Ohmura[16] found $T = \frac{3}{2}$ state probabilities generated by a dipole modified Coulomb force ranging from 3 to 7×10^{-6}. He also found changes in P_S, of roughly 0.1 percent. Both numbers are consistent with ours. Gignoux and Laverne[12] found $20 \cdot 10^{-6}$ for the RSC3 model, which also included other charge-symmetry-breaking potentials. Their change in the ^{3}He radius, 0.08 fm, was somewhat larger than ours, as was the change in P_S. A similar calculation for the *dTS* potential gave $10 \cdot 10^{-6}$. Bell and Delves,[31] on the other hand, found 50×10^{-6} for a simple Yukawa potential in a variational calculation. Gignoux and Laverne[12] found ~610 keV for $\Delta E_c^{(1)}$ in the RSC3 model, while Haftel[32] found 608 keV. Hennell and Delves[33] found smaller values of ΔE_c but their radii are also somewhat different for the RSC case. Malfliet and Tjon[34] found 630 keV for the RSC potential, in general agreement with our result. The Gignoux and Laverne[10] result for RSC5 appears to use the projected Coulomb potential and thus is considerably smaller.

VI. SUMMARY

We have calculated first- and second-order Coulomb energies using perturbation theory and Faddeev wave functions for several different *NN* potential models. The first-order results have been compared with those of the hyperspherical formula in each case, and the agreement was found to be good (better than 2%) for nucleons with finite size. This permits us to scale model results for $\Delta E_c^{(1)}$ to the correct physical size. The validity of scaling for the second-order results has also been tested and found to be more than adequate for our purposes. The difference between "first-order" Coulomb energy estimates using wave functions with and without Coulomb distortion is essentially $2\Delta E_c^{(2)}$. Thus, the use of phenomenological methods which fit the ^{3}He charge density double counts the second-order contribution, and it must be *subtracted* in those cases, which *increases* the ^{3}He Coulomb energy.

The hyperspherical formula, *when applied to experimental data*,[8] uses $(4\rho_{\mathrm{He}} - \rho_{\mathrm{H}})/3$ (if we ignore the neutron's form factor). This is equivalent to $\rho_s + \rho_v$ if these latter quantities are identical for ^{3}He and ^{3}H, which was assumed in the derivation of the formula. Since ρ_{He} contains Coulomb effects, the assumption is untrue, and the numerical output of the formula contains a multiple of the hyperspherical approximation to $\Delta E_c^{(2)}$. We find

$$\Delta E_H^{\mathrm{exp}} \cong \Delta E_H^{(1)} + \tfrac{8}{3}\Delta E_H^{(2)} - \tfrac{4}{3}\Delta E_H^{(2)}(v), \tag{22}$$

where $\Delta E_H^{(1)}$ and $\Delta E_H^{(2)}$ are the hyperspherical estimates of $\Delta E_c^{(1)}$ and $\Delta E_c^{(2)}$, respectively, while $\Delta E_H^{(2)}(v)$ is the isovector part of $\Delta E_H^{(2)}$. The latter quantity is roughly $\frac{1}{4}$ of $\Delta E_H^{(2)}$ in the cases we have examined, and $\Delta E_H^{(2)}$ itself is a reasonably good approximation to $\Delta E_c^{(2)}$. Thus, $\Delta E_H^{\mathrm{exp}} \cong \Delta E_H^{(1)} + 7\Delta E_H^{(2)}/3$, and in order to correct this overestimate of $\Delta E_c^{(2)}$ we must subtract $4\Delta E_H^{(2)}/3$ from $\Delta E_H^{\mathrm{exp}}$, which *increases* the hyperspherical estimate of ΔE_c from experimental data: $\Delta E_H^{\mathrm{exp}}$.

Using the previously calculated value[8] of $\Delta E_H^{\mathrm{exp}}$ (639 keV), we estimate the pure Coulomb trinucleon energy difference to be $\Delta E_c = 644 \pm 12$ keV, where we have utilized our estimate of $\Delta E_c^{(2)} = -4 \pm 1$ keV. We find a substantial change of approximately 0.04 fm in $\langle r^2 \rangle_{\mathrm{He}}^{1/2}$, when Coulomb distorted wave functions are used; this results from the Coulomb expansion of the wave function. We confirm the small probability for the $T = \frac{3}{2}$ wave function component ($P_{3/2} \leq 10^{-5}$), which is attributed to its mixed-symmetry nature.

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APPENDIX A: FADDEEV EQUATIONS

For ^{3}He we consider three identical particles with spin equal to one-half and isospin equal to

one-half. For the independent center-of-mass coordinates we use

$$\vec{x}_i = \vec{r}_j - \vec{r}_k ,$$

the distance between the interacting pair j and k, and

$$\vec{y}_i = \tfrac{1}{2}(\vec{r}_j + \vec{r}_k) - \vec{r}_i ,$$

the distance between the third particle and the center of mass of the interacting pair. The three-particle totally antisymmetric wave function is written as

$$\Psi = (1 + P^{(-)} + P^{(+)})\psi(\vec{x}_1, \vec{y}_1)$$
$$= \psi(\vec{x}_1, \vec{y}_1) + \Psi(\vec{x}_2, \vec{y}_2) + \psi(\vec{x}_3, \vec{y}_3) , \qquad \text{(A1)}$$

where $\Psi(\vec{x}_1, \vec{y}_1)$ is antisymmetric under the interchange of the interacting particles 2 and 3. The operators $P^{(+)}$ and $P^{(-)}$ are the cyclic permutation operators for the three particles. The Hamiltonian for the three-particle system is

$$H = T + V(x_1) + V(x_2) + V(x_3) ,$$

where $V(x_1) = V_N(x_1) + \frac{1}{4}[1 + \tau_z(2)][1 + \tau_z(3)]V^c(x_1)$ is the nuclear interaction plus the Coulomb interaction. Since Ψ is totally antisymmetric, the three Faddeev equations are identical, and it is only necessary to solve one of the three equations. Consequently, we consider only the equation for $\psi(x_1, y_1)$, i.e.,

$$[T + V(x_1) - E]\psi(\vec{x}_1, \vec{y}_1)$$
$$= -V(x_1)[\psi(\vec{x}_2, \vec{y}_2) + \psi(\vec{x}_3, \vec{y}_3)] . \qquad \text{(A2)}$$

For $\psi(\vec{x}_1, \vec{y}_1)$ we use a partial-wave expansion in the L-S basis:

TABLE III. The quantum numbers of the three $J = \frac{1}{2}$ states formed from three particles interacting in relative S states by means of strong plus Coulomb potentials.

α	$(\frac{1}{2}, s_\alpha)S_\alpha$	$(\frac{1}{2}, t_\alpha)T_\alpha$
1	$(\frac{1}{2}, 0)\frac{1}{2}$	$(\frac{1}{2}, 1)\frac{1}{2}$
2	$(\frac{1}{2}, 1)\frac{1}{2}$	$(\frac{1}{2}, 0)\frac{1}{2}$
3	$(\frac{1}{2}, 0)\frac{1}{2}$	$(\frac{1}{2}, 1)\frac{3}{2}$

$$\psi(\vec{x}_1, \vec{y}_1) = \sum_\alpha \frac{\phi_\alpha(x_1, y_1)}{x_1 y_1} |[(l_\alpha \lambda_\alpha)L_\alpha, (\tfrac{1}{2}, s_\alpha)S_\alpha] \times JM, (\tfrac{1}{2}, t_\alpha)T_\alpha\rangle , \qquad \text{(A3)}$$

where

l_α = orbital angular momentum of particles 2 and 3,
λ_α = orbital angular momentum of particle 1,
s_α = spin angular momentum of particles 2 and 3,
t_α = isospin of particles 2 and 3,
L_α = total orbital angular momentum,
S_α = total spin,
T_α = total isospin, and
J = total angular momentum.

For the calculations of $T = \frac{3}{2}$ wave function components presented in this paper we consider only particles in relative s states, i.e., $l_\alpha = \lambda_\alpha = L_\alpha = 0$. For a system with a total angular momentum of one-half, only the three states listed in Table III are needed.

The coupled equations for the three channels listed in Table III are obtained by substituting Eq. (A3) into Eq. (A2) and projecting out the various channels. The resulting equations are

$$\left(\frac{\partial^2}{\partial x_1^2} + \frac{3}{4}\frac{\partial^2}{\partial y_1^2} - K^2\right)\phi_1(x_1, y_1) = U_{1S_0}(x_1)\left\{\phi_1(x_1, y_1) + \int_{-1}^{1} d\mu \frac{x_1 y_1}{x_2 y_2}[\tfrac{1}{4}\phi_1(x_2, y_2) - 3/4\phi_2(x_2, y_2)]\right\}$$
$$+ U_c(x_1)\left\{2/3\phi_1(x_1, y_1) - \frac{\sqrt{2}}{3}\phi_3(x_1, y_1)\right.$$
$$\left. + \int_{-1}^{1} d\mu \frac{x_1 y_1}{x_2 y_2}[1/6\phi_1(x_2, y_2) - \tfrac{1}{2}\phi_2(x_2, y_2) + \sqrt{2}/6\phi_3(x_2, y_2)]\right\}, \qquad \text{(A4a)}$$

$$\left(\frac{\partial^2}{\partial x_1^2} + \frac{3}{4}\frac{\partial^2}{\partial y_1^2} - K^2\right)\phi_2(x_1, y_1) = U_{3S_1}(x_1)\left\{\phi_2(x_1, y_1) + \int_{-1}^{1} d\mu \frac{x_1 y_1}{x_2 y_2}[-3/4\phi_1(x_2, y_2) + \tfrac{1}{4}\phi_2(x_2, y_2)]\right\}, \qquad \text{(A4b)}$$

$$\left(\frac{\partial^2}{\partial x_1^2} + \frac{3}{4}\frac{\partial^2}{\partial y_1^2} - K^2\right)\phi_3(x_1, y_1) = U_{1S_0}(x_1)\left\{\phi_3(x_1, y_1) + \int_{-1}^{1} d\mu \frac{x_1 y_1}{x_2 y_2}[-\tfrac{1}{2}\phi_3(x_2, y_2)]\right\}$$
$$+ U_c(x_1)\left\{-\frac{\sqrt{2}}{3}\phi_1(x_1, y_1) + \tfrac{1}{3}\phi_3(x_1, y_1)\right.$$
$$\left. + \int_{-1}^{1} d\mu \frac{x_1 y_1}{x_2 y_2}\left[-\frac{\sqrt{2}}{12}\phi_1(x_2, y_2) + \frac{\sqrt{2}}{4}\phi_2(x_2, y_2) - \tfrac{1}{6}\phi_3(x_2, y_2)\right]\right\}, \qquad \text{(A4c)}$$

where

$$K^2 = -\frac{M}{\hbar^2}E\,,$$

$$U(x_1) = \frac{M}{\hbar^2}V(x_1)$$

and the nuclear force has a $^1S_0$ part and a $^3S_1$ part. The quantity μ is the cosine of the angle between $\vec{x}_1$ and $\vec{y}_1$. For the numerical solution of these equations, they are rewritten in terms of the variables ρ and θ_1, where

$$x_1 = \rho\cos\theta_1$$

and

$$y_1 = \tfrac{1}{2}\sqrt{3}\,\rho\sin\theta_1\,,$$

and the resulting equations are solved using the techniques in Ref. 11.

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