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The binding energy of the deuteron in the exponentially damped Breit-Pauli-Schrödinger (XBPS) Model

Robert J Buenker

Abstract
The XBPS method that is successful in obtaining a low-energy state of positronium which is equivalent to the photon is employed to study the effects of nuclear binding. The theoretical treatment of interactions that are capable of holding an electron within the small volume of a neutron, with the requisite 500 MeV kinetic energy expected for it on the basis of the de Broglie $p=h/\lambda$ relation, is applied to the description of the structure of the deuteron (^{2}H). In agreement with the nuclear-shell model of Goeppert-Mayer and Jensen, it is found that spin-dependent nuclear forces must be added to the Breit-Pauli electromagnetic Hamiltonian in order to obtain agreement with the experimental finding of a triplet ground state. In particular, a spin-spin δ operator with a proton coupling constant of 1.0 bohr magneton succeeds in producing the desired multiplicity and approximate total energy of the ^{2}H ground state. Two s-type orbitals φ_a and φ_b are needed to describe the ground state wavefunction, one of which characterizes the neutron and the other, the proton. Double occupation of one of these orbitals produces a satisfactory description of ^{3}He. As for the neutron, it is found that an electron-antineutrino $e^-\overline{\nu}$ complex is essential for obtaining a proper description of the binding process in all cases.

Keywords: Exponentially-damped Breit-Pauli-Schrödinger (XBPS) equation, deuteron binding energy, spin-dependent nuclear forces, spin-spin-δ Interaction, ^{3}He and light nuclides

Introduction
In preceding work [1-3] it has been argued that a theoretical model based on the exponentially damped Breit-Pauli-Schrödinger (XBPS) equation is capable of explaining how electrons can be confined to the small radius of a nucleus. This supposition is supported in large part by the fact that calculations [4, 5] employing the same model have demonstrated that an electron and positron can be bound to one another so strongly that they form a mass-less system which can reasonably be identified with the photon. To accomplish this objective, it has been argued that neutrinos must have charge-to mass ratios that allow them to participate significantly in the Breit-Pauli short-range interactions such as spin-orbit coupling and the Darwin term [2]. How this can be possible given the capacity of neutrinos to pass nearly undetected through matter for very long distances is an important question that has been dealt with in a convincing manner [3].
The simplest nucleus consists of a single neutron and proton. They are assumed to be bound together by a force generally referred to as the strong or hadronic interaction. By analogy to the quantum electrodynamics description of the Coulomb force as involving the exchange of a virtual photon, Yukawa [6] suggested in 1935 that the exchange of a heavier particle was responsible for the force joining any two nucleons together. By contrast, according to the XBPS model, the reaction of a proton and a neutron to form the deuteron product ^{2}H involves four separate particles, three of which are found in the neutron itself. The question that will be taken up next is whether the forces which have been proposed above to explain how three separate particles can be bound together to form a neutron might not also be involved in the nuclear binding process as well. Having computed a value for the charge-to-mass ratio of the antineutrino on the basis of the results of the $p^+e^-\overline{\nu}$ XBPS treatment in a given one-particle basis, the next step will be to examine the effects of adding a second

proton to this system, while otherwise proceeding in an equivalent manner as in the calculations already discussed.

II. Initial overview of the deuteron binding process

On the basis of the treatment of the helium atom in the standard quantum mechanical theory, one might expect the ground state of this two-proton system to correspond to double occupation of the same s orbital found to be optimal for the $p^+e^-\bar{\nu}$ system. Experiment tells us that the resulting singlet state is not favored by the deuteron, however, but rather one of triplet multiplicity [7]. Moreover, no other bound state is known to exist for the deuteron [8]. The fact that the triplet multiplicity is so favored by the deuteron has given rise to the well-known characterization of the nuclear force as being spin-dependent [9]. The XBPS calculations for the $p^+e^-\bar{\nu}$ system [2, 3] have indicated quite strongly that the $e^-\bar{\nu}$ complex itself retains the 0^- character preferred in its isolated state, and thus it is reasonable to expect that such relatively light particles themselves do not make a significant contribution to the total angular momentum of this system. Especially since the traditional description of this nucleus is in terms of a proton $s_{1/2}$ and a neutron $s_{1/2}$ orbital [10, 11], it seems clear that the only way to obtain a satisfactory explanation for the deuteron ground state's triplet multiplicity in the present model is therefore to assume that *there is a second* $s_{1/2}$ *proton orbital with nearly the same energy as the first, but orthogonal to it.* For simplicity, let us refer to these two orbitals as φ_a and φ_b, whereby it can be anticipated that one of them will be quite similar to that found to be most strongly occupied in the $p^+e^-\bar{\nu}$ ca1culations [2, 3].

In view of the above experimental findings one is led to expect that neither of the closed shell φ_a^2 or φ_b^2 configurations leads to a bound deuteron state, i.e. the energies of the related singlet states must lie above that of the separated proton and neutron, or some 29000 hartree higher than that of the constituent protons, electron and antineutrino separated to infinity. According to the convention employed in earlier work [2, 3], the deuteron ground state itself has a total energy of -52972.813 hartree, corresponding to the measured binding energy of 2.22452 MeV relative to the separated proton and neutron. To see how this general picture is reflected in actual calculations, we will begin by employing the simplest one-particle basis considered previously, with 2s and 2p functions for each particle type. The same values for the exponential damping constant A and the $\bar{\nu}$ charge-to-mass ratio are assumed as in the analogous $p^+e^-\bar{\nu}$ calculations which employ the same AO basis. After optimization of the scaling factor η for this basis, it is found that the lowest-energy state of the $p^{+2}e^-\bar{\nu}$ system has 0^- symmetry, with both protons occupying the φ_a $s_{1/2}$ orbital with opposite spins. As expected, the electron and antineutrino form a singlet unit similar to that favored by the e^+e^- system [5] and this part of the wavefunction is responsible for the negative parity of the four-particle state as a whole. The total energy obtained for the 0^- state is -254512.252 hartree. The lowest-lying 1^- state with a $s_{1/2}$ $s_{1/2}$ $\varphi_a\varphi_b$ proton configuration has a much higher energy of +21955.705 hartree, but is still bound relative to the $p^+e^-\bar{\nu}$ system plus an isolated proton by 6941.856 hartree, or 0.189 MeV (see Table 1).

In Ref. [3] it was found that the proton of the $p^+e^-\bar{\nu}$ system preferred a considerably more contracted charge distribution than either the electron or antineutrino. In the next series of $p^{+2}e^-\bar{\nu}$ calculations the same 4s, 2p basis is employed which demonstrated this effect in the first case. The additional two s functions (α_1 = 2.56 x 10^8 and α_2 = 0.80 x 10^8 a_0^{-2}) are found to have a much greater effect on the total energies of the $p^{2+}e^-\bar{\nu}$ states than before for the corresponding one-proton system. For A=1.0567 a.u. and q/m_o ($\bar{\nu}$)=0.5375 a.u., the values of these parameters which lead to the desired binding energies of the e^+e^- and $p^+e^-\bar{\nu}$ systems in this basis, results of -401335.635 and -86856.876 hartree are obtained for the 0^- and 1^- $p^{+2}e^-\bar{\nu}$ states, respectively. The corresponding computed binding energies are thus 430897.744 hartree (11.72 MeV) and 116418.985 hartree (3.17 MeV), respectively, considerably larger in each case than for the 2s, 2p basis set not containing specially optimized $s_{1/2}$ functions for the protons.

Table 1: Energy contributions (in hartree) of various operators (see Table 1 of Ref. [2] for definitions and abbreviations) and particle combinations for the 0^- state of the $p^{+2}e^-\bar{\nu}$ deuteron system obtained by employing the 4s, 2p basis with scale factor η = 0.16, exponential damping constant A = 1.0568 a.u. and antineutrino q/m_o value of 0.527 a.u. for the XBPS Hamiltonian.

Op	p^+p^+	p^+e^-	$p^+\bar{\nu}$	$e^-\bar{\nu}$	Total
KE	286751.843(p^+)	1389897.489(e^-)	1629685.689($\bar{\nu}$)		3306335.021
C	15221.838	-11234.341	0.000	0.000	3987.496
SsO	0.000	-669587.021	105016.667	-447338.511	-1011908.865
SoO	0.000	-93.245	94.858	-893545.158	-893543.546
D	-23.567	160901.391	-1103708.083	28456.498	-914373.757
OO	0.662	-122.703	414.328	-394442.299	-394150.012
SS	0.000	-0.352	-0.205	-499287.703	-499288.260
SSδ	47.127	-0.357	-4.749	15026.997	15069.018
					-387872.905
SδI*	392749.721				392749.721
TE**					4876.816

*Strong spin-spin S increment for proton-proton interaction (see text).
**Total energy

The energy contributions for the various one- and two-particle interactions for the above two states in the 4s,2p basis are given in Table 1 (0^-) and Table 2 (1^-), respectively. These results are obtained with a slightly lower q/m_o($\bar{\nu}$)

value (0.527 a.u.) than in the $p^{+2}e^{-}\overline{\nu}$ calculations mentioned first, but correspond to very nearly the same binding energies relative to the $p^{+}e^{-}\overline{\nu}$ system of the same charge-to-mass ratios as those given above (the total energy of the latter is 44067.869 hartree, or 14505.760 hartree higher than in the other calculation detailed in Table 3 of Ref. [3]). This second series of $p^{+2}e^{-}\overline{\nu}$ calculations indicates that the $e^{-}\overline{\nu}$ complex is capable of providing a strong attraction for protons. As usual, by far the largest contributions to net binding for the system are the proton-electron and proton-antineutrino spin-same-orbit and Darwin terms. For the 0^{-} state the spin-same-orbit proton terms produce a net binding of 564570 hartree, while the corresponding Darwin term result is 942807 hartree. The corresponding results for the 1^{-} state are 441275 and 536870 hartree respectively (Tables 1 and 2). These values are 2.5 to 4.0 times greater than found in the corresponding $p^{+}e^{-}\overline{\nu}$ calculations in Table 3 of Ref. [3], again indicating that the addition of a second proton is marked by a significant contraction of the charge distribution of the system as a whole (i.e. the $p^{+2}e^{-}\overline{\nu}$ results are more than double those for the system with a single proton).

Table 2: Energy contributions (in hartree) of various operators (see Table 1 of Ref. [2]) for definitions and abbreviations) and particle combinations for the 1^{-} state of the $p^{+2}e^{-}\overline{\nu}$ deuteron system obtained by employing the 4s, 2p basis with scale factor $\eta = 0.16$, exponential damping constant A = 1.0568 a.u. and antineutrino q/m_o value of 0.527 a.u. for the XBPS Hamiltonian.

Op	$p^{+}p^{+}$	$p^{+}e^{-}$	$p^{+}\overline{\nu}$	$e^{-}\overline{\nu}$	Total
KE	290643.137(p^{+})	1341557.196(e^{-})	1512125.933($\overline{\nu}$)		3144326.266
C	7726.523	. -10467.859	0.000	0.000	-2741.336
SsO	0.000	-530003.791	88729.000	-442961.158	-884235.949
SoO	0.000	-57.868	39.310	-906688.972	-906707.530
D	0.000	178980.181	-715853.570	22920.853	-513952.535
OO	0.277	-84.456	207.748	-428116.693	-427993.124
SS	0.000	-6.087	-0.388	-491176.127	-491182.602
SSδ	0.000	-0.091	-29.955	11380.624	11350.578
					-71136.232
SδI*					3.123
TE**					-71133.109

* Strong spin-spin δ increment for proton-proton interaction (see text).
**Total energy

The fact that the total binding energies obtained for the $p^{+2}e^{-}\overline{\nu}$ system are considerably larger than observed for the deuteron experimentally, particularly when reference is made to the 0^{-} state's results, is a clear deficiency of the present theoretical treatment, but on the basis of the $p^{+}e^{-}\overline{\nu}$ computations discussed in Ref. [2, 3], it can be expected that the addition of d functions to the basis employed will probably lead to a decrease in these values. Nonetheless, a more obvious deficiency in the present results seems far less likely to be an artifact of the computational treatment considered thus far, namely that the ground state of the $p^{+2}e^{-}\overline{\nu}$ system, which is being proposed as having the composition of the deuteron, prefers singlet multiplicity by a wide margin. This result seems unavoidable so long as the interactions involving the protons are predominantly the spin-same-orbit and Darwin terms involving either the electron or antineutrino as second particle. Only the Coulomb repulsion between the two protons provides a counter-example for this type of behavior, and although this interaction does favor a triplet spin function for a two-open-shell proton configuration, it is not enough to override the decided preference of the $p^{+2}e^{-}\overline{\nu}$ system for a closed-shell structure in which only the most stable proton $s_{1/2}$ orbital is strongly occupied. The situation is thus analogous to that encountered in the electronic structure of the helium atom, which also favors a singlet ground state, and as a result there seems no question that the XBPS Hamiltonian in the form given in Table 1 of Ref. [2] *is not capable of a suitable description of the forces which bind the proton and neutron together in the ^{2}H or other nuclear systems.*

III. The Spin-Dependence of the interaction between nucleons

The failure of the above calculations to account for certain basic aspects of the structure of the deuteron is most easily overcome by looking for additional interactions which would not be expected to play a role in either the particle-antiparticle binary computations discussed in Refs. [4, 5] or those for the $p^{+}e^{-}\overline{\nu}$ resonance associated with the neutron in Refs. [2, 3]. This approach is certainly not inconsistent with the accepted theory of nuclear structure, which has long emphasized that a non-electromagnetic interaction must be assumed between any two nucleons in order to provide a plausible explanation for observed characteristics of the structure of nuclei [9, 12, 13]. Although it is generally believed that such forces involve spin-orbit coupling akin to the terms in the Breit-Pauli approximation [14], it has also been shown [15] that the coupling constants associated with the interactions between nucleons must be far greater than would be expected based on consideration of electromagnetic effects alone. As an example from experiment, one may consider the energy splittings between the ground and excited states of the ^{11}B and ^{11}C nuclei. According to the nuclear-shell model [16, 17], these quantities should give an accurate reflection of the $p_{3/2}$-$p_{1/2}$ spin-orbit splittings of a nuc1eon in these systems, but their magnitudes (2.14 and 1.85 MeV, respectively) are far larger [18] than can be explained on the basis of Breit-PauIi interactions [14]. Observations of the scattering of polarized nucleons from ^{4}He and ^{12}C nuclei lead to much the same conc1usions [19].

There have been a number of concrete proposals for the form of the nucleonic spin-orbit coupling operator [13, 20, 21],

but there is unfortunately no consensus on this point. If one goes through the list of Breit-Pauli terms with the goal of finding an interaction which is capable of influencing the relative stability of the singlet and triplet deuteron states, one discovers that most of them will have no effect on this situation by virtue of the fact that the proton orbitals which are strongly occupied in the corresponding wavefunctions are exc1usively of $s_{1/2}$ type. Neither of the spin-orbit terms, nor the spin-spin tensor force or the orbit-orbit interaction has any non-vanishing matrix elements when only such spin-orbitals are involved. Moreover, the Darwin term is completely independent of spin [14] and is therefore also totally ineffective for this task.

A clear exception to this pattern still remains, however, namely the spin-spin δ-function term. It is both spin-dependent and capable of producing a non-vanishing interaction between particles occupying $s_{1/2}$ orbitals. In order to obtain a suitably large effect from such an operator when applied to a pair of protons (nucleons), it is c1early necessary to change the value of the coupling constant relative to those of Table 1 of Ref. [2], however, as can be seen from the results of Tables 1 and 2.

It is thus proposed to augment the XBPS Hamiltonian with a term of spin-spin δ-function type in which the q/m_o values for the proton particles are replaced by much larger coupling constants of the order of their electronic counterparts; for concreteness, a value of unity (1.0 bohr magneton) will be taken for this purpose. Otherwise, the previous description of the XBPS Hamiltonian is simply retained and full CI calculations are carried out as in the last section for both the 0^- and 1^- $p^{+2}e^-\overline{\nu}$ states, employing the same values for the damping constant A (1.0567 a.u.), the q/m_o ratio for the antineutrino (0.527) and exponents for the Gaussian basis functions as in the treatment whose results are given in Tables 1 and 2. It is found that the 1^- state is virtually unaffected by this change, with a total energy of -71133.109 hartree (-1.936 MeV) having been obtained. This result is only 3.123 hartree above the value shown in Table 2 without including the spin-spin δ-function term. On the other hand, the total energy of the $p^{+2}e^-\overline{\nu}$ singlet (0^-) state is changed dramatically to +4876.816 hartree, an increase of 392749.721 hartree relative to the treatment without the new spin-spin δ-function term for proton-proton interactions. As a result the lowest state of the $p^2e^-\overline{\nu}$ system has triplet multiplicity, with a binding energy relative to the proton and $p^+e^-\overline{\nu}$ system of 2.719 MeV = 71133 + 28781 hartree (compared to the experimental value of 2.22452 MeV).

Examination of the above findings shows that the anti-symmetry of the proton wavefunction is a crucial factor in obtaining this result. The simplest representation of the triplet wavefunction is:

$$\Psi_T = 2^{-1/2} [s_1(1)s_2(2) - s_1(1)s_2(2)] \alpha(1)\alpha(2).$$

The expectation value of the spin-spin δ-function term for this function has the familiar form of the difference of a Coulomb and exchange integral, but since the δ-function has equal values for these two quantities, unlike the case for the electrostatic interaction, the result is of vanishing magnitude. On the other hand, the simplest representation of the 0^- state whose energy contributions are listed in Table 1 is:

$$\Psi_S = 1/2 [s_1(1)s_2(2) + s_1(1)s_2(2)] [\alpha(1)\beta(2) - \alpha(2)\beta(1)]$$

The expectation value in this case is:

$$\langle\Psi_S| -\frac{8\pi}{3}\pi\alpha^2\delta(1,2)\,\mathbf{s_1}\cdot\mathbf{s_2}\,|\Psi_S\rangle = 2\alpha^2\pi \langle s_1(1)\, s_1(2)\, \delta(1,2)\, s_1(1)\, s_2(2)\rangle,$$

a large positive energy contribution. Adding this term to the Hamiltonian produces a destabilizing effect on the closed-shell configuration of Ψ_S. A significantly different wavefunction is obtained for the lowest 0^- root from the corresponding 4s,2p full CI treatment than with the original XBPS Hamiltonian, with much more emphasis on the open-shell configuration analogous to that dominating the triplet wavefunction.

Another encouraging result of the computations with the augmented XBPS Hamiltonian is the finding that the next three most stable states after the 1^- species are nearly degenerate and correspond to the symmetries expected for the translationally excited counterpart of the above ground state. Such a translational function would be expected to have 1^- symmetry itself and thus exchanging it for the 0^+ species of lowest energy as a factor multiplying the 1^- internal wavefunction would lead to new solutions of 0^+, 1^+ and 2^+ symmetry, with these expected to be very nearly equal in energy to one another. This expectation is fulfilled, with total energies of -31260.220 (0^+), -31265.499 (1^+) and -31265.715 (2^+) hartree being found for the most stable states of each of these three symmetries.

This example serves as a reminder that the XBPS Hamiltonian contains translational energy contributions as well. As a consequence, the excited states obtained with this method may differ from the corresponding ground state in the amounts of either their internal or translational energies or both. This introduces an additional complication into the present theoretical treatment which is clearly not present when the center-of-mass motion is factored out (or when the **P**= 0 condition is imposed), but the present example shows how symmetry characteristics can be employed to distinguish between the two distinct types of excited states. In essence one obtains a discrete representation of the translational continuum in the present treatment of nuclear motion, whereby the density of states obtained is clearly dependent on the number and type of basis functions employed in explicit calculations.

One can summarize the present results for the ground state of the $p^{+2}e^-\overline{\nu}$ system as follows. With the addition of a spin-dependent term for the proton-proton interaction having a coupling constant of the order of the electronic bohr magneton, it is possible to obtain a state of lowest energy from the XBPS treatment in the 4s, 2p basis which has triplet multiplicity and a binding energy relative to the proton-$p^+e^-\overline{\nu}$ dissociation products which is at least on the order of the experimental deuteron value. The attractive central potential which is responsible for this result is provided by the $e^-\overline{\nu}$ complex of 0^- symmetry which is analogous to the e^+e^- ground state associated with the photon in the present model. The spin-dependent proton-proton adjunct to the XBPS Hamiltonian has virtually no influence on the total energy eigenvalue and associated eigenfunction

for the triplet ground state itself, but plays a key role in destabilizing the corresponding singlet spin combination of the protons, particularly the helium-like closed-shell configuration which otherwise is so favored when this term is absent.

These results are obtained with relatively small basis sets and thus it is difficult to make a more quantitative assessment of the accuracy of the present model on this basis alone, but there at least seems justification for pursuing this approach further, both at higher levels of computational accuracy and also for the description of other nuclear systems. There is another comparison with experimental data which is also encouraging, namely for the mean radius of the two nucleons in the deuteron system, estimated [7] to be 4.32 fm or 1.5 α^2 bohr on the basis of scattering observations. The value of the Coulomb proton-proton repulsion of 7726.523 hartree (Table 2) allows a straightforward estimate of this radius for the 1^- state, namely 2.43 α^2 bohr. While the agreement between these two results can hardly be described as quantitative, it at least shows that the range of the forces described by the XBPS Harniltonian is physically reasonable.

Since the present calculations have been carried out without the *ad hoc* introduction of parametric inter-nucleon potentials, it can be argued that their results speak in favor of the major assumptions underlying the present model, especially the insistence upon treating the electron and antineutrino as being physically present in the deuteron nucleus. Again, the results of Table 2 appear reasonable on this point, showing kinetic energies for the electron and antineutrino of 36.50 and 41.14 MeV. Under the assumption of a deuteron radius of 1.5 α^2 bohr, an estimate based on the approximation $p \cong r^{-1}$ can be made of 46.68 MeV ($pc = 1.5^{-1}\alpha^{-2}c = 1.5^{-1}\alpha^{-3}$ hartree) for each of these quantities.

It also should be noted that the addition of d functions to the basis set employed in the XBPS calculations should also favor the triplet state of the deuteron over that of the singlet. This is because a ds proton configuration can have a J = 1 multiplet but not one with J = 0. It has long been thought [13] that the deuteron ground state contains a small d-function component because of the observation that its magnetic moment deviates by a significant amount (2.6%) from the sum of the proton and neutron moment values. The small but non-zero value of the deuteron's electric quadrupole moment is also consistent with this conclusion. The extent of the present 4s,2p calculations for the $p^{+2}e^-\overline{\nu}$ system precludes the addition of d functions to the basis set at the present time, so it has not been possible to verify this effect explicitly, but the above arguments at least make it seem plausible that such a result would occur.

Before concluding this section it is well to return to a key point which has wide-ranging consequences regarding the qualitative interpretation of nuclear interactions in terms of neutrons and protons. To obtain a sound basis on which to discuss heavier nuclei, it seems inescapable that proton orbitals appear in pairs of nearly equal energy, one set to be associated with neutrons in the conventional model, the other with the corresponding protons themselves. Such a development seems unlikely when reference is made to the electronic structure of atoms and molecules, according to which the lowest two s orbitals are of greatly different energy, for example. The form of the potential employed in the XBPS Hamiltonian suggests that the situation may well be different in the present case, however. Unlike the Coulomb potential, whose r-dependence is monotonic in character, the damped Breit-Pauli counterparts possess an extremum similar to that shown in Fig. 2 of Ref. [5], which is essential in the present model to avoid variational collapse and hence to suitably describe bound nucleons. Consequently there are equi-potential points on either side of the minima in the variation of the damped Breit-Pauli terms with inter-particle distance which conceivably could lead to orthogonal orbitals of contrasting radial dependence but very nearly equal stability. Once this possibility is assumed, it is not difficult to imagine how the results of calculations for larger nuclei could be formulated in terms of the nuclear-shell model of Goeppert-Mayer [16] and Jensen [17], or even more simply in terms of distinct neutrons and protons serving as the nuclear constituents.

IV. Structure of The Lightest Nuclei

It was recognized by Wigner [22] in 1933 that the binding energies of the simplest nuclides increase very rapidly with atomic mass number, and that this phenomenon is very strong evidence for the short range of the forces involved. Even if one allows for the quadratic increase in the number of nuclear bonds as nucleons are added, one still finds that the binding energy trends are notably different than one observes in the study of atomic and molecular structure. In the present model, in which the electron and antineutrino are treated explicitly in the theoretical calculations, the next simplest system after the deuteron is the ^{3}He nucleus, with a total of five elementary constituents. The experimental total energy of the ^{3}He nucleus relative to that of its separated protons, electron and antineutrino is -254966 hartree, which corresponds to a binding energy of 201993 hartree relative to the stable deuteron plus proton fragments. In view of the $\varphi_a\varphi_b$ configuration assumed for the deuteron in the last section, the simplest assumption is that the additional proton occupies one of these two orbitals with opposite spin. Since the potential in Fig. 2 of Ref. [5] has only one extremum, it seems plausible that a third orbital φ_c would not be sufficiently stabilized by the $e^-\overline{\nu}$ complex to make a proton configuration with three open shells advantageous. Because of the 0^- character of the $e^-\overline{\nu}$ unit, the overall symmetry of such a $\varphi_a^2\varphi_b$ ground state would be $1/2^-$.

In order to investigate these possibilities a series of calculations has been carried out for the $p^{+3}e^-\overline{\nu}$ system employing the 4s, 2p basis introduced in Sect. 2 of Ref. [3]. It was not possible to solve the secular problem corresponding to a full CI treatment in this case, however. Instead a multiple reference CI [23] common in molecular calculations has been employed, which should be capable of approximating the corresponding full CI eigenvalues and wavefunction to a satisfactory approximation. The CI space considered is generated by taking all possible single and double excitations relative to a series of 42 reference configurations chosen on the basis of the magnitude of their coefficients in the final eigenvectors. The Hamiltonian employed is again that of Table 1 of Ref. [2] augmented with the spin-spin δ-function term for the proton-proton interaction discussed in Sect. III. The same q/m_o value (0.5375 a.u) for $\overline{\nu}$ is assumed as yields the experimental neutron (negative) binding energy for the $p^+e^-\overline{\nu}$ system (see Sect. V of Ref. [2]). The same value of the exponential damping constant A (1.0567 a.u.) is also employed as in the

latter treatment. The exponents of the most compact two s-type functions were optimized specifically for the $p^{+3}e^{-}\overline{\nu}$ system in the $1/2^{-}$ state, and it was found that these values are about 30% larger than those which produce minimal energy for the $p^{+2}e^{-}\overline{\nu}$ system, i.e. $\alpha_1 = 0.338 \times 10^{9}\ a_o^{-2}$ and $\alpha_2 = 0.8 \times 108\ a_o^{2}$).

The total energy obtained in the optimum 4s,2p treatment is found to be -212334.852 hartree. Optimization of the above exponents from their original $p^{+2}e^{-}\overline{\nu}$ values brought an energy lowering of 14562 hartree, indicating a substantial contraction of the charge distribution of the protons in the larger $p^{+3}e^{-}\overline{\nu}$ system. The resulting total energy is thus 42631 hartree (1.16 MeV) higher than the experimentally deduced value for the ^{3}He nucleus mentioned above. The computed binding energy relative to the $p^{+2}e^{-}\overline{\nu}$ 1^{-} state (see Table 2) and a free proton is 141202 hartree. Although this is a substantial amount, it is still only 69.9% of the experimental energy difference between the ^{3}He nuc1eus and the deuteron plus proton system. The spin-spin δ-function proton-proton interaction is quite important in this determination, having a value of 127952 hartree, as compared to virtually zero magnitude for the corresponding $p^{+2}e^{-}\overline{\nu}$ expectation value in the 1^{-} state.

The most important configuration in the $p^{+3}e^{-}\overline{\nu}$ wave function is of the $\varphi_a^2\varphi_b$ type, so that the simplest interpretation is that that the more compact s-type orbital corresponds to that occupied by the two ^{3}He protons in the conventional description. The magnitude of the Coulomb repulsion for the three protons is 35369.772 hartree, nearly five times the value found for the $p^{+2}e^{-}\overline{\nu}$ 1^{-} system. Since there are three times as many pair-wise interactions in the heavier system, this result is also evidence for a general contraction of the $p^{+3}e^{-}\overline{\nu}$ system relative to its two-proton counterpart (see Table 2). This result is understandable with reference to the nature of the XBPS Hamilonian employed in the present treatment. As a new proton is added to the $p^{+2}e^{-}\overline{\nu}$ system, one has both an increase in the total kinetic energy of these heavy particles and an enhancement of their net attractive interactions for the $e^{-}\overline{\nu}$ complex of lighter elements, thereby disturbing the equilibrium prevailing for the original nuclide. Because the changes in the short-range attractive interactions are greater, this leads to a drawing of the entire system together and a greater increase in total binding energy than would be possible by simply occupying the original proton orbitals of the lighter system. Under these circumstances one must be wary of making a strict correspondence between the $s_{1/2}$ orbitals occupied in the deuteron and ^{3}He respectively. The fact that only one electron and antineutrino are present inevitably leads to the designation of only one of the nucleons as a neutron (open-shell occupation) and the remaining pair as protons (closed-shell).

This line of argumentation leads to an interesting question, however, namely what happens when still another proton is added to the system. On the basis of what has been said above, it is tempting to think that the resulting (^{4}Li) nuc1eus would be bound by a rather large margin, possessing a c1osed-shell $\varphi_a^2\varphi_b^2$ proton configuration. A Li isotope of this mass number is not stable, which raises the specter of a breakdown in the above model, or at least unusually high Coulomb repulsion effects that make such extrapolations very inaccurate. This need not be the case, however, because the ^{4}Li system is more likely unstable because it is prone to electron capture and the subsequent formation of the highly stable alpha particle ^{4}He (E=-982528.11 hartree), rather than because it is subject to spontaneous decomposition itself.

Calculations similar to those discussed above have thus also been carried out for a system with four protons and a single $e^{-}\overline{\nu}$ unit. The closed-shell $\varphi_a^2\varphi_b^2$ proton configuration mentioned above corresponds to a 0^{-} $p^{+4}e^{-}\overline{\nu}$ state. The most stable state of this symmetry in the present treatment does not have a significant contribution from this configuration, however. Instead, proton p orbitals show significant occupation, which according to the nuclear-shell model are the next available to the hypothetical ^{4}Li nucleus. The total energy of this 0^{-} state is -219926.758 hartree, some 7600 hartree lower than that of the $p^{+3}e^{-}\overline{\nu}$ $1/2^{-}$ ground state.

The lowest energy obtained for the four-proton system is for the 0^{+} state (-313119.128 hartree). There is also a 1^{+} state of only slightly higher energy (-310409.680 hartree) and a 1^{-} species lying just above it (-303091.067 hartree). In the first two cases the preferred configuration is $\varphi_a^2\varphi_b\varphi_c$, i.e. three-fold $s_{1/2}$ occupation corresponding to the $p^{+3}e^{-}\overline{\nu}$ ground state discussed earlier and having the remaining proton located in the lowest p shell. Since there is no spin-orbit term of the type foreseen in the nuclear-shell model [16,17] in the Hamiltonian employed, there is essentially no splitting computed between the corresponding $p_{1/2}$ and $p_{3/2}$ sub-shells. Even with such a specific proton-proton interaction, however, it seems clear that the lowest of such states would be quite unstable with respect to the electron capture process required to form the ^{4}He nucleus. The experimental total energy of the latter's 0^{+} ground state is still more than 18 MeV lower than any of the calculated results for the $p^{+4}e^{-}v$ system associated with the ^{4}Li nucleus in the present model, and so it seems plausible that such states could not exist for sufficient time to be observed prior to their decay. Hence, no contradiction exists between the present computed results and experiment. The lifetime [24] of the ^{5}Li isotope is only 10^{-21} s and this species should be considerably more stable than the lighter ^{4}Li system, in agreement with this assessment.

As a result, it seems best to terminate the present discussion of systems formed by adding still more protons to a single $e^{-}\overline{\nu}$ binary and turn instead to the far more interesting possibility that as the number of protons continues to increase in a nucleus, there is a strong attraction for additional electrons and antineutrinos. The fact that a $\overline{\nu}$ species is also required in electron capture is consistent with the inevitable appearance of a departing neutrino as well (see Sect. 3 of Ref. [1]), both of which come from the same mass-less $\nu\overline{\nu}$ binary according to the present model. Such considerations lead one naturally into a discussion of the weak interaction in theoretical physics, but this is best deferred until a general discussion of nuclei heavier than the α particle. Instead, a second nuclear series will be considered which results from the addition of successive protons to a pair of $e^{-}\overline{\nu}$ units.

A system of two protons and two $e^{-}\overline{\nu}$ singlets can best be thought of in the present model in terms of a deuteron interacting with a single electron-antineutrino unit. The spatial orbitals which comprise the latter's wavefunction must be different than those employed for the first $e^{-}\overline{\nu}$

complex because according to the XBPS calculations of Ref. [2], every conceivable spin combination other than that for the lowest-lying 0^- state is quite unstable. It therefore follows that the next best two-particle $e^-\overline{\nu}$ function is probably somewhat less stable than the first. In essence, the calculations indicate that one proton must make up for deficiencies related to the electron's pairing with a particle of a significantly smaller charge-to-mass ratio than that of its antiparticle. A proton has the capacity for doing this because it has a net attraction for both the electron and antineutrino (see Tables 1-3 of Ref. [3] and Tables 1-2) and it has relatively small kinetic energy in the required short inter-particle distance range. Nonetheless it can't quite achieve net binding with an $e^-\overline{\nu}$ unit on a one-to-one basis. This result amounts to concluding that a bound system of two neutrons does not exist, as is well known experimentally, even though the simplest view of nuclear structure holds that the nn interaction is of quite similar strength as that for pn.

The situation seems likely to improve when an excess of protons is available, especially because the inter-proton distances can become smaller because of the net increase in the spin-same-orbit and Darwin term attraction to the $e^-\overline{\nu}$ species. A system with three protons and two such binaries corresponds to one proton and two neutrons in the conventional accounting, i.e. the tritium nucleus ^{3}H. Experimentally this system is found to be only 0.4935 MeV (18136 hartree) less stable than the ^{3}He nucleus. Considering that their respective total energies are on the order of -250000 hartree relative to their separated (stable) particles, this is a comparatively small difference. As before with ^{3}He, two configurations come into question to describe the ground state, namely $\varphi_a^2\varphi_b$ and $\varphi_a\varphi_b^2$. Because the number of particles increases to seven in the ^{3}H calculations in the present model, it has not yet been possible to carry out explicit calculations to study this point. One can speculate that the relative stability of the φ_a and φ_b proton orbitals must depend fairly strongly on the number of $e^-\overline{\nu}$ units present in a given system, however. It may even be that the designation of each of these $s_{1/2}$ species as either of proton or neutron type is different for ^{3}H, so that the composition of the doubly occupied orbitals of the two systems are actually fairly similar to one another.

In any event, the true ground-state wavefunctions of both ^{3}He and ^{3}H can be expected to consist of heavy mixtures of the above two configurations in a CI sense. What of the low-lying excited states of complementary structure which are indicated in each case, however? It seems conceivable that whenever either system occupies the state of lesser stability that it rapidly either loses or gains an $e^-\overline{\nu}$ unit to become the corresponding ground state of the other system without greatly altering the original occupation of its two most stable proton orbitals φ_a and φ_b. In fact, only one of the four possible configurations is truly stable, since the ^{3}H ground state is known to undergo beta decay with a half-life of 12.4 years to form the ^{3}He ground state [24]. In other words, ^{3}He is weakly repelled by a second $e^-\overline{\nu}$ species but this effect can be minimized by altering its proton charge distributions.

The situation may also in some way be similar to a phenomenon which often occurs in molecular physics [25], according to which two iso-electronic systems have *mutually inverted ground and excited states* with correspondingly distinctive nuclear conformations. For example, ozone prefers to doubly occupy the $4b_2$ orbital which tends to give it an open-chain structure, whereas cyclopropane [26] prefers the $2b_1$ species instead, which in turn allows it to have a triangular ring conformation. Both molecules have excited states with the opposite occupations, however, whose nuclear conformations are quite different as a result, corresponding to an open-chain form of cyclopropane and a ringed isomer of ozone. In this case the numbers of electrons are equal for the two systems but the nuclear environment is quite different. In the present comparison of ^{3}H and ^{3}He, the number of protons is equal according to the present model (corresponding to the mass number in standard usage), but the two systems differ in the number of $e^-\overline{\nu}$ units combined with them in each case.

Another important characteristic of the $e^-\overline{\nu}$ complex which it shares with the e^+e^- massless system is that the Darwin repulsion between the two constituent particles is very small (see Tables 1-3 of Ref. [3] and Tables 1-2)). The expectation value for the un-damped Darwin term vanishes exactly for the e^+e^- 0^- prototype system. In both cases this result indicates that the particles avoid each other so completely that they never (or only rarely in the $e^-\overline{\nu}$ case) reside in the same region of space (with or without the same spin). This result strongly implies that a definite region of space must be reserved to accommodate each electron-antineutrino pair within a given nucleus. Analysis of Table 3 of Ref. [5] shows that this situation arises primarily because it allows for maximum advantage to be taken of the attractive Breit-Pauli interactions between the two particles. In e^+e^-, for example, any change in the respective charge distributions which leads to a non-zero δ-function expectation value must result in a net increase in total energy because a variational minimum is involved. The situation is not quite as severe for $e^-\overline{\nu}$, but nonetheless the absolute magnitude of the Darwin term in this instance is only 5% of that of the corresponding spin-same-orbit expectation value. At the same time the calculations indicate that the proton and electron charge distributions are not similarly restricted, as a rather large Darwin interaction is invariably computed between them (178980.181 hartree in Table 2, for example).

These results are very reminiscent of the experimental observations mentioned in Sect. IV of Ref. [1] which indicate that the nuclear volume is essentially directly proportional to the number of its constituent nucleons. According to the present calculations, it appears somewhat more precise to say that the nuclear volume is proportional to the number of constituent $e^-\overline{\nu}$ units, which arithmetically amounts to essentially the same relationship. In other words, because each electron must avoid each antineutrino, one can expect a fixed volume to be reserved for every such pair of light particles to insure maximum stability for the nucleus as a whole. The protons are much freer to move in a small volume because their rest masses are so much greater, but even as they shrink in orbital size with increased binding, the corresponding $e^-\overline{\nu}$ charge distributions remain relatively unaffected. This observation is also consistent with the form of the exponential damping factors in the spin-same-orbit and Darwin terms (Table 1 of Ref. [2]), which as mentioned before allow a closer approach to the lighter particles to maximize the attractive forces as each proton is added to the system. The exponential operators are strongly dependent on the momentum (and consequently the orbital compositions) of the electron and antineutrino,

however, so that the volume occupied by them is relatively independent of the number of protons in their environment. Only if the proton occupation drops below or rises above a critical level necessary to support a given number of $e^-\overline{\nu}$ units is a volume change advantageous, which is to say a β interaction occurs to either decrease or augment the number of electron-antineutrino pairs within the confines of the nucleus.

To conclude this section, the result of adding a fourth proton to the double $e^-\overline{\nu}$ complex will be discussed. The product is clearly the relatively stable ^{4}He nucleus, originally named the alpha particle a century ago [27]. It has a closed-shell ground state corresponding to the $\varphi_a^2\varphi_b^2$ proton configuration and represents an optimal proportion between the number of protons and electrons for such light nuclei. The experimental binding energy of the last proton (compared to ^{3}He) is 728212 hartree. Relative to two neutrons and protons this represents a binding energy of 1.04 megahartree, or in excess of 250000 hartree per proton (nucleon). The latter result is about 2.5 times larger than the corresponding value for ^{3}He and ^{3}H. The indication is that the proton φ_a, φ_b orbitals shrink markedly as the last proton is added, which is quite consistent with the closed-shell configuration characterizing this system. The fact that ^{4}He is the only stable nucleus with this mass number indicates that the number of $e^-\overline{\nu}$ units is similarly optimal, however, as already discussed in connection with the hypothetical ^{4}Li system.

V. Conclusion

Within the present model of a triatomic $p^+e^-\overline{\nu}$ composition for the neutron, one expects the deuteron to consist of two protons, one corresponding to the neutron and the other to the proton in the conventional description. The XBPS calculations for the neutron indicate that the $e^-\overline{\nu}$ complex in the neutron wavefunction should retains the 0^- character preferred by both e^+e^- and the isolated system, and as such is unlikely have an effect on the angular momentum of such a four-particle system. In analogy to the electronic structure of the two-electron He atom, one would therefore be led to the conclusion that the two proton orbitals in the deuteron would prefer to doubly occupy a closed shell orbital φ_a, so that the lowest-energy configuration has singlet multiplicity (J=0). Experiment is not consistent with such an interpretation, however, but rather demands that two (orthogonal) proton orbitals (φ_a and φ_b) must be occupied with triplet multiplicity (J=1).

Experimental values of the relevant atomic masses show that the deuteron has a total energy of -52972.813 hartree, which corresponds to 2,22452 MeV binding energy relative to the separated proton and neutron. Using a small 2s2p basis for the XBPS calculations, the total energy of the lowest singlet state is -254512 hartree, which is far different than the above value. At the same time, the lowest triplet state has a much higher energy of +21956 hartree. Employing a larger 4s2p basis leads to significantly lower energies. This shows that the additional s orbitals are quite important for achieving an optimum charge distribution, and is thus an indication that the protons prefer relatively more compact charge distributions in the two-proton system than for the neutron $p^+e^-\overline{\nu}$. The results of Tables 1 and 2 show that the spin-same-orbit and Darwin term interactions between the protons and the respective e^- and $\overline{\nu}$ particles are quite strong. The fact that the lowest energy is obtained for a singlet state, however, is clear evidence that the XBPS Hamiltonian is not capable of giving a satisfactory description of the deuteron ground state.

The failure of the above calculations with the electromagnetic XBPS Hamiltonian can be overcome by taking a cue from the accepted theory of nuclear structure. It emphasizes that a non-electromagnetic interaction must be involved in order to explain observed characteristics of nucleonic structure. In particular, it is generally held that something akin to spin-orbit coupling must be involved, but that the coupling constants in such operators must be far greater than one expects on the basis of strictly electromagnetic interactions. For example, the known energy splittings between the ground and excited states of the ^{11}B and ^{11}C nuclei are far greater (2.14 and 1.85 MeV, respectively) than would be expected on the basis of the assumption of a conventional $p_{3/2}$-$p_{1/2}$ Breit-Pauli spin-orbit coupling interaction with standard couplings. Nonetheless, the nuclear-shell model of Goeppert-Mayer and Jensen assumes that

the above splitting must be due to an interaction between a $p_{3/2}$ and a $p_{1/2}$ shell. Observations of the scattering of polarized nucleons from ^{4}He and ^{12}C lead to the same conclusion.

The next step in the theoretical treatment is therefore to find other Breit-Pauli-like operators that can have a significant influence on the XBPS results for the deuteron singlet and triplet states. Since the only proton orbitals with significant occupation are of s-type, most of the Breit-Pauli terms can be safely ignored in such a search. The spin-spin δ operator (see Table 1 of Ref. [2]) is a clear exception, however. It is both spin-dependent and capable of producing a significant interaction between two $s_{1/2}$ orbitals, but to have a useful impact it is clearly necessary to alter the value of its coupling constant. For concreteness, the q/m_0 values for protons have been replaced by much larger values on the order of their electronic counterparts; specifically a value of 1.0 bohr magneton has been chosen. This interaction has thus been added to the exponentially damped Breit-Pauli Hamiltonian operator used in the previous calculations of the 0^- and 1^- $p^{+2}e^-\overline{\nu}$ states. The results are given in Tables 1 and 2. It is found that the spin-spin-δ operator with the unit coupling constant has virtually no effect on the results for the 1^- triplet state. A total energy of -71133 hartree is obtained. On the other hand, there is a very large effect on the lowest singlet state, causing its total energy to be +4877 hartree. Consequently, the lowest $p^{+2}e^-\overline{\nu}$ state now has triplet multiplicity with a binding energy of 2.719 MeV compared to the experimental value of 2.224 MeV. In summary, the addition of the spin-spin δ operator with unit coupling constants for interactions between two protons allows one to obtain a triplet ground state for the deuteron with a reasonably accurate binding energy relative to its proton and neutron constituents.

There is another comparison with experiment which is encouraging as well. It is found that the mean radius of the two nucleons is estimated to be 4.32 fm = 2.43 α^2 bohr. The corresponding theoretical value is obtained from the proton-proton Coulomb repulsion in Table 2 to be 6.8488 fm, 1.58 times larger, showing at least that the computed range of the forces is reasonable. It also can be noted that the form of the potential in the XBPS model, with its equi-potential points

on either side of the minimum, suggests that there may be two orbitals of different radial dependence but approximately the same energy in the manifold of accessible states, contrary to the case for electronic orbitals. One can be associated with a proton and the other with a neutron, for example.

Calculations for heavier atoms such as ^{3}He verify Wigner's observation that the binding energies of the lightest nuclides increase very rapidly with atomic mass number. According to the XBPS model, ^{3}He contains three protons plus a single $e^- \overline{\nu}$ unit. Based on the deuterium $\varphi_a\varphi_b$ ground state configuration, it would be expected that the corresponding ^{3}He configuration

should have one closed-shell and one open-shell orbital, i.e. $\varphi_a^2\varphi_b$, with $1/2^-$ symmetry rather than require a third proton $s_{1/2}$ orbital. The calculated total energy is -212334 hartree, corresponding to a deuterium-proton binding energy of 141202 hartree (3.842 Mev), 69.9 % of the experimental value. The contribution of the proton-proton spin-spin δ operator is +127952 hartree (3.482 MeV), a substantial amount, as compared to the nearly zero value for the 1^- deuterium state. As expected the leading configuration is of $\varphi_a^2\varphi_b$ type, so the simplest interpretation is that the more compact (φ_a) orbital corresponds to that occupied by the two ^{3}He protons.

The value of the Coulomb repulsion for the three protons is 35370 hartree, which is nearly five times that found for the 1^- deuterium state (Table 2). Since there are only three times as many pair-wise interactions for ^{3}He than is the case for deuterium, this is evidence for a contraction of the $p^{+3}e^- \overline{\nu}$ system relative to $p^{+2}e^- \overline{\nu}$. Since there is still only one $e^- \overline{\nu}$ component, the conclusion is that the open-shell orbital (φ_b) is occupied by the neutron and the remaining closed-shell pair (φ_a) is occupied by the two protons. Adding a fourth proton to the $e^- \overline{\nu}$ complex does lead to a minor lowering in energy. This result is not necessarily contradicted by experiment, however, since such a nucleus would be quite unstable to electron capture that produces the very stable α particle with the same number of protons, i.e. two protons and two neutrons, in addition to two $e^- \overline{\nu}$ complexes.

In order to have a second $e^- \overline{\nu}$ complex occupied in the presence of three or more protons, it is necessary for its wavefunction to be quite different than that of the first complex. Experiment shows that ^{3}H, which has three protons and two $e^- \overline{\nu}$ units, has very nearly the same energy as ^{3}He. Adding a fourth proton leads to a large lowering in total energy, producing ^{4}He. Since a second $e^- \overline{\nu}$ complex is required for this to occur, it is perfectly consistent with the present model for a neutrino to appear from a $\nu \overline{\nu}$ mass-less binary, in addition to a positron, as observed experimentally for the formation of the α particle from ^{3}He.

The calculations indicate that further protons can cause a stable environment for two or more

$e^- \overline{\nu}$ units in which the inter-proton distances become ever smaller. An increase in the spin-same-orbit and Darwin term net attractions for protons has benefits for both the electron and antineutrino. As before with ^{3}He, two configurations seem likely to be occupied in the ^{3}H nucleus, namely $\varphi_a^2\varphi_b$ and $\varphi_a\varphi_b^2$. In both cases, adding an extra proton leads to the formation of a close-shell ground state with the $\varphi_a^2\varphi_b^2$ occupation favored by the ^{4}He particle. Since the ^{3}H nucleus is known to undergo β decay with a half-life of 12.4 years to form ^{3}He, the evidence is that the latter is weakly repelled by a second $e^- \overline{\nu}$ unit, but that the effect can be all but eliminated by altering the charge distributions of the proton constituents.

An important characteristic of the $e^- \overline{\nu}$ complex is shared with the e^+e^- mass-less particle. In both cases the value of the Darwin term is relatively small. It vanishes exactly for e^+e. The e^- and $\overline{\nu}$ particles avoid each other so completely that they hardly ever reside in the same region of space. As a consequence, it is necessary that a definite region must be reserved to accommodate each such complex within a given nucleus. The charge distributions of the protons are not similarly restricted, so their positions can be altered significantly in order to minimize the total energy of the system, The calculations accordingly indicate that there is a large Darwin term interaction between the proton and electron (see Table 2).

The experimental binding energy of the fourth proton to the ^{3}He nucleus, i.e. the binding energy of the second neutron, is 728212 hartree (19.8 MeV). This represents a binding energy of 250000 hartree per nucleon. It is 2.5 times larger than the value for either ^{3}He or ^{3}H. This indicates that the proton orbitals φ_a and φ_b shrink markedly as the fourth proton is added. The fact that there is no other stable nucleus with this mass number indicates that the number of $e^- \overline{\nu}$ units is similarly optimal, which places the α particle in a unique position among the light nuclides.

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