The Binding Energy of H^3

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A calculation has been made of the constants in the meson type of potential by fitting the scattering data for the scattering of slow neutrons by protons and the binding energies of H^2 and H^3. Assuming the interaction between any two particles to be $(P_{ij}+gP_{ij}Q_{ij})(Ce^{-\lambda r_{ij}}/r_{ij}\lambda)$ one gets $C=49.54\ mc^2$, $g=0.2667$, $\lambda=1.536\ (mc^2/e^2)$. This potential gives results which will be very little different from those given by the spherically symmetrical parts of the interaction obtained from meson field theory. The use of the coordinates introduced by James and Coolidge allows sufficient simplification so that the results can be easily modified to take account of other types of spin dependence. The possibility of λ and C being different for different particle interactions may also be taken into account.

I

THE increasing importance of the potential $Ce^{-\lambda r}/r\lambda$ obtained from the meson field theory gives interest to an accurate determination of the interaction constants. Such an accurate determination has been made by Rarita and Present[1] for the potential $Ce^{-\lambda r}$. In this paper a similar determination is made for the meson type of potential, but the system of coordinates[2] used below allows considerable simplification in the calculations.

The interaction between any pair of particles (ij) is assumed to be given by

$$V_{ij}=(P_{ij}+gP_{ij}Q_{ij})Ce^{-\lambda r_{ij}}/\lambda r_{ij}, \qquad (1)$$

where P_{ij} interchanges the particle coordinates and Q_{ij} interchanges their spins. To be consistent one should use the spin dependence obtained from the meson field theory,[3] but since the spherically symmetrical parts of the interaction thus obtained will give results which differ very little from those obtained from (1) and since the non-spherically symmetrical spin-spin interaction involves an arbitrary cut-off at some distance, a practical procedure is to calculate with the type of interaction (1). There is also an ambiguity in the spherically symmetrical parts of the interaction obtained from the meson field theory, since they depend on whether one allows heavy particles to interact only with neutral mesons or whether they are also allowed to interact with charged mesons.

The use of the coordinate system introduced by James and Coolidge[2] for their discussion of the helium atom makes the calculation sufficiently simple so that these results can be easily modified when the spin dependence of the interaction becomes more definite.

II

In the interaction (1) there are three constants g, C, λ to be determined. The binding energies of H^2 and H^3 and the scattering of thermal neutrons by protons give the three conditions necessary for their determination. The interaction constants are assumed to be the same for all pairs of particles. In this paper the binding energies of H^2 and H^3 are determined by a variational calculation and the scattering is determined by numerical integration of the deuteron equation for zero energy. The scattering could also be obtained by a variational calculation but the work would be tedious.

For the S states of H^3 it is convenient to introduce the coordinates

$$\begin{aligned} x&=\lambda(r_1+r_2-r)\\ y&=\lambda(r_2+r-r_1)\\ z&=\lambda(r_1+r-r_2). \end{aligned} \qquad (2)$$

If one labels the proton particle number 1 and the neutrons 2 and 3, respectively, then r is the distance between the neutrons, r_1 is the distance between particles 1 and 2 and r_2 is the distance

[1] W. Rarita and R. Present, Phys. Rev. **51**, 788 (1937).
[2] H. M. James and A. S. Coolidge, Phys. Rev. **51**, 860 (1937).
[3] N. Kemmer, Proc. Camb. Phil. Soc. **34**, 299 (1938); J. Schwinger, Phys. Rev. **55**, 235 (1939).

between particles 1 and 3. In these coordinates the integral over the volume of a sphere of radius r_0 is

$$(1/4\lambda^6)\int_0^{2\lambda r_0}\int_0^{2\lambda r_0-x}\int_0^{2\lambda r_0-x}(x+y)(x+z)\times(y+z)dxdydz. \quad (3)$$

For the infinite sphere the upper limits become infinite.

In the coordinates (1) the wave equation for an S state of H^3 is

$$\{4/(x+y)(x+z)(y+z)\}\{\psi_{xx}(x^2y+xy^2+x^2z+xz^2+xyz)+\psi_{yy}(x^2y+xy^2+y^2z+yz^2+xyz)+\psi_{zz}(x^2z+xz^2+y^2z+yz^2+xyz)-\psi_{xy}(x^2y+xy^2)-\psi_{xz}(x^2z+xz^2)-\psi_{yz}(y^2z+yz^2)+\psi_x(-x^2+y^2+z^2+xy+xz+yz)+\psi_y(x^2-y^2+z^2+xy+xz+yz)+\psi_z(x^2+y^2-z^2+xy+xz+yz)\}+\{2b_{12}/(x+z)\}\exp\{-(x+z)/2\}P_{12}\psi+\{2b_{13}/(x+y)\}\exp\{-(x+y)/2\}P_{13}\psi+\{2b_{23}/(y+z)\}\exp\{-(y+z)/2\}P_{23}\psi+a'\psi=0; \quad (4)$$

where $a'=(EM/h^2\lambda^2)$ and b_{12}, b_{13}, b_{23} depend on the spin and are given below.

For the ^3S state of the deuteron the value of $a=(EM/h^2\lambda^2)$ for a given value of $b=(CM/h^2\lambda^2)$ is determined by minimizing a with the function

$$\phi=\sum_1^\infty C_k x^k e^{-\alpha x} \quad (x=r\lambda). \quad (5)$$

This value of a together with the known binding energy of H^2 then determines the corresponding value of λ. The value of $b(^1S)$ is then determined by numerical integration to give the proper cross section for the scattering of thermal neutrons by protons.

From the values of $b(^1S)$, $b(^3S)$ and λ for the deuteron one calculates by a variational principle the binding energy of H^3. The values of $b(^1S)$, $b(^3S)$ and λ are adjusted until the calculated binding energy of H^3 equals the experimental energy.

To determine a' of H^3 one minimizes a' with a function

$$\psi=S_A\phi_1+S_S\phi_2, \quad (6)$$

where S_A is a spin function antisymmetric for an exchange of neutron spins, ϕ_1 is a function of (xyz) symmetric for interchange of neutron coordinates and S_S is symmetric for exchange of spins and ϕ_2 is antisymmetric for exchange of coordinates. Using the same spin functions as Rarita and Present,[1] one gets after summing over the spins

	$b_{12}(h^2\lambda^2/MC)$	$b_{13}(h^2\lambda^2/MC)$	$b_{23}(h^2\lambda^2/MC)$
$\phi_1\phi_1$:	$(1+g/2)$	$(1+g/2)$	$(1-g)$
$\phi_1\phi_2+\phi_2\phi_1$:	$(g\sqrt{3}/2)$	$(-g\sqrt{3}/2)$	0
$\phi_2\phi_2$:	$(1-g/2)$	$(1-g/2)$	$(1+g)$.

For ϕ_1 and ϕ_2 one uses the variational functions

$$\phi=\sum C_{klm}x^k y^l z^m \exp[-\alpha x/2-\beta(y+z)/2], \quad (7)$$

where ϕ_1 must be symmetric for exchange of y and z and ϕ_2 correspondingly antisymmetric. The general matrix elements of a' are easily calculated (cf. appendix). One first minimizes with only the first term of ϕ_1 by varying α and β; then using these values of α and β one varies the coefficients in ϕ_1; finally using this ϕ_1 one varies the coefficients in ϕ_2. A relativistic correction calculated by the method of Feenberg[4] is also included.

The variation of the coefficients was carried out as follows: one writes

$$a'=(A/N)a_0', \quad (8)$$

where a_0' is the value of a' obtained by the previous minimizing process, A is the energy integral (cf. appendix) divided by the energy integral of the previous minimizing process and N is the normalization integral divided by the normalization integral of the previous minimization. Minimizing (8) gives

$$\frac{dA}{dC_{klm}}-\frac{A}{N}\frac{dN}{dC_{klm}}=0 \quad (klm)=0, 1, 2\cdots. \quad (9)$$

By estimating the percent reduction in energy to be obtained from varying the coefficients one can solve the set of linear equations (9) for the C_{klm}, then recalculate (A/N) and readjust the C_{klm} for the new (A/N). A small error in the estimate makes little difference in the calculated value of (A/N).

III

Using the experimental values, $E(^3S\,H^2)=-4.25(0)\ mc^2$, σ (thermal neutrons by protons $=18.3(0)\times10^{-24}$ cm^2, and $E(H^3)=-16.3(0)\ mc^2$,

[4] E. Feenberg, Phys. Rev. **50**, 674 (1936).

one obtains $C=49.54\ mc^2$, $\lambda=1.536\ (mc^2/e^2)$ and $g=0.2667$.

The variational function for the deuteron ^3S state is

$$e^{-0.9175x}(x-0.2363\,x^2+0.07266\,x^3),\quad N=0.2519$$

which gives $a(^3S)=-0.1760$. For a slightly different value of $b(^3S)$ inclusion of five terms in the series gives only 0.06 percent reduction of a below the value obtained with three terms, hence it is certainly sufficiently accurate to take $a(^3S)=-0.1761$. Inclusion of the x^2 and x^3 terms gives a reduction of 11.69 percent below the value obtained by using only the first term. Using $b(^1S)=1.505$, $b(^3S)=2.600$, $\lambda=1.536$ one gets a scattering cross section of thermal neutrons by protons of 18.30×10^{-24} cm^2.

For H^3 the variational functions are

$$\phi_1=[1-0.1087x-0.07112(y+z)+0.03669\times x(y+z)]\exp[-0.8333x-0.7500(y+z)],$$

$$\phi_2=[0.04222(y-z)-0.004793x(y-z)]\times\exp[\cdots],\quad N=0.6284.$$

Adding further second degree terms and third degree terms in ϕ_1 gives only about 0.05 percent reduction in the energy, and adding other terms in ϕ_2 gives a negligible reduction.

The exponential term alone gives $a'=-0.6293$; further terms in ϕ_1 produce a reduction of 1.81 percent; the inclusion of ϕ_2 causes a reduction of 3.74 percent; and the relativistic correction ($0.267\ mc^2$) produces 1.75 percent reduction, giving $a'=-0.6752$ compared to the experimental value of $-0.675(6)$.

The difference in the binding energies of He^3 and H^3, determined by considering the Coulomb interaction as a perturbation, is

$$E(He^3)-E(H^3)=1.671\ mc^2.$$

The experimental value of this difference is uncertain, values of $1.35\ mc^2$ and $2.35\ mc^2$ having been obtained.[5]

The above value of λ gives the mass of the meson as 211 m. The fact that the above value of λ is considerably different from that determined by Share, Hoisington and Breit[6] from proton-proton scattering has been discussed elsewhere,[7]

Use of the spherically symmetrical parts of the potential obtained from meson field theory can cause but little modification in the above values since one would get the same results as above if the wave function $\psi(H^3)$ had the same dependence on x, y and z. The small deviation which one has from this symmetry condition cannot cause more than a few percent change in the calculated energy of H^3. The spin-spin terms of the meson field theory which give rise to a quadripole moment of the deuteron will modify the above values, but one could not calculate the modification in an unambiguous manner because of the arbitrary cut-off necessary to get convergence. From the calculations of Bethe[8] on the quadripole moment of the deuteron it seems likely that the singular spin-spin terms would make the value of λ even less than that given in this paper.

The accuracy of the above results is also dependent on the accuracy of the experimental values used. As an indication of the modifications caused by a change in the binding energy of H^3 or in the scattering cross section, it may be stated that for $E(H^3)=-16.48\ mc^2$ one would have

$$C=50.49\ mc^2,\quad \lambda=1.552(mc^2/e^2),\quad g=0.2643,$$

and for $\sigma=13.1\times10^{-24}$ cm^2 one would have (approximately)

$$C=55.4\ mc^2,\quad \lambda=1.64(mc^2/e^2),\quad g=0.264.$$

In conclusion the author wishes to express his appreciation for being allowed the use of the facilities of the California Institute of Technology.

Appendix

Matrix elements of the H^3 energy terms.

If one puts $a'=A/N=(A_k-b_{12}A_{12}-b_{13}A_{13}-b_{23}A_{23})/N$ one gets for the matrix elements $[(\alpha x)^\kappa(\beta y)^\lambda(\beta z)^\mu|(\alpha x)^k(\beta y)^l(\beta z)^m]$, taking account of the exchange operations

$$P_{12}: x\rightleftarrows z\quad y\rightleftarrows y$$
$$P_{13}: x\rightleftarrows y\quad z\rightleftarrows z$$
$$P_{23}: y\rightleftarrows z\quad x\rightleftarrows x,$$

[5] L. H. Rumbaugh, R. B. Roberts and L. R. Hafstad, Phys. Rev. **54**, 675 (1938).

[6] S. S. Share, L. E. Hoisington and G. Breit, Phys. Rev. **55**, 1130 (1939).

[7] F. W. Brown and M. S. Plesset, Phys. Rev. **56**, 841 (1939).

[8] H. A. Bethe, Phys. Rev. **55**, 1261 (1939).

$$A_k=(1/\beta^4)\{2(131)+2(113)+2(122)-(213)-(231)-(222)+4k[(131)+(113)+(122)]-4k^2[(031)+(013)+(022)]\}+(1/\alpha\beta^3)\{2(221)+2(212)+4(122)+(231)+(213)-(321)-(312)-(132)-(123)+4k[(221)+(212)-\tfrac{1}{2}(131)-\tfrac{1}{2}(113)]+4l[-\tfrac{1}{2}(221)+\tfrac{1}{2}(113)+\tfrac{1}{2}(122)+(121)]+4m[-\tfrac{1}{2}(212)+\tfrac{1}{2}(131)+\tfrac{1}{2}(122)+(112)]-4k^2[(121)+(112)]-4l^2[(112)+(103)]-4m^2[(121)+(130)]+4kl(121)+4km(112)+4lm[(121)+(112)]\}+(1/\alpha^2\beta^2)\{4(221)+4(212)-2(311)-2(222)+(321)+(312)-(231)-(213)+4k[(211)-\tfrac{1}{2}(221)-\tfrac{1}{2}(212)]+4l[(221)+(212)-\tfrac{1}{2}(311)]+4m[(221)+(212)-\tfrac{1}{2}(311)]-4l^2[(211)+(202)]-4m^2[(211)+(220)]+4kl(211)+4km(211)\}+(1/\alpha^3\beta)\{4(311)-(321)-(312)+4l(311)+4m(311)-4l^2(301)-4m^2(310)\},$$

$$N=(1/\alpha\beta^5)[(132)+(123)]+(1/\alpha^2\beta^4)[(231)+(213)+2(222)]+(1/\alpha^3\beta^3)[(321)+(312)],$$

where $(123)=\Gamma(\kappa+k+1)\Gamma(\lambda+l+2)\Gamma(\mu+m+3)$;

$$A_{12}=(\alpha/\gamma)^{\kappa+k}(\beta/\gamma)^{\mu+m}\{(1/\beta\gamma^4)2(212)+(1/\beta^2\gamma^3)2[(221)+(122)]+(1/\beta^3\gamma^2)2(131)\},$$

where $\gamma=(\alpha+\beta+1/2)$ and $(123)=\Gamma(\kappa+m+1)\times\Gamma(\lambda+l+2)\Gamma(\mu+k+3)$;

$A_{13}=A_{12}$ with μ replaced by λ and m replaced by l;

$$A_{23}=(\beta/\delta)^{\lambda+\mu+l+m}\{(1/\alpha\delta^4)2(122)+(1/\alpha^2\delta^3)2[(221)+(212)]+(1/\alpha^3\delta^2)2(311)\},$$

where $\delta=(\beta+\frac{1}{2})$ and $(123)=\Gamma(\kappa+k+1)\Gamma(\lambda+m+2)\Gamma(\mu+l+3)$. Their numerical evaluation for given values of α and β is a matter of simple arithmetic.

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The Spectra of Y V and Zr VI

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The Br I isoelectronic sequence has been extended to Y V and Zr VI. Spectrograms covering the region from 150A to 1000A were obtained with a three-meter grazing incidence vacuum spectrograph having a dispersion of 1.0A/mm at 500A. The separations of the ground doublets $4s^24p^5$ were predicted by the regular doublet law and observed to be 12,068 cm^{-1} for Y V and 15,600 cm^{-1} for Zr VI. With the aid of the irregular doublet law and Moseley diagram curves, most of the expected $4s4p^6$, $4s^24p^44d$ and $4s^24p^45s$ levels with $j\leq 5/2$ were found. Forty-two lines of the spectrum of Y V and forty-six lines of the spectrum of Zr VI have been classified. The absolute term values of the $^2P^0_{3/2}$ ground levels of Y V and Zr VI were estimated to be 620,000 cm^{-1} and 798,000 cm^{-1}, respectively.

THE spectra of Br I,[1] Kr II,[2] Rb III[3] and Sr IV[3] have been analyzed to the extent that in each case the term values for nearly all the important lower lying levels are known. The ground state of a member of this sequence is determined by the configuration $4s^24p^5$ which gives rise to two odd levels: $^2P^0_{1\frac{1}{2}}$ and $^2P^0_{\frac{1}{2}}$, of which the former lies the deeper. The strongest emission lines in this sequence should arise from transitions between the ground state doublet and the configurations $4s4p^6$, $4s^24p^44d$ and $4s^24p^45s$. These lines should exhibit, except when j is $\geqslant 2\frac{1}{2}$, a constant frequency difference equal to the doublet separation of the ground state.

The analysis of Rb III and Sr IV was based on spectrograms made with a vacuum spectrograph covering the extreme ultraviolet region from 250A to 1200A. Only transitions into the ground doublet were considered. In the present

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[2] De Bruin, Humphreys and Meggers, Nat. Bur. Stand. J. Research **11**, 409 (1933).
[3] D. H. Tomboulian, Phys. Rev. **54**, 350 (1938).