The Coulomb Energy of He³

The assumption^{1, 2} that, except for the Coulomb repulsion between protons, the neutron-neutron and protonproton attractions may be taken as equal leads to the conclusion that the difference in binding energies of H³ and He³ should be due entirely to the Coulomb repulsion. This statement is tested here by evaluating the Coulomb energy of He³ using the variational wave-function

$$\psi = \psi_0 + \lambda H \psi_0, \tag{1}$$

where $\psi_0 = N e^{-(\nu/2)(r_{12}^2 + r_{13}^2 + r_{23}^2)}$. (2)

The Hamiltonian used was the symmetrical form

$$H = -\frac{1}{2}(\Delta_1 + \Delta_2 + \Delta_3) - \frac{2}{3}A_{II}(e^{-\alpha r_{12}^2} + e^{-\alpha r_{13}^2} + e^{-\alpha r_{23}^2})$$

the A_{II} being taken from Table I of reference 2. The λ and ν were determined in (1) by varing ν so that the best value of the energy E was obtained using the method described in the appendix of the above reference. Then

$$\lambda = -\frac{(0|H|0) - E}{(0|H^2|0) - E(0|H|0)}$$

The Coulomb energy is, after normalization of ψ ,

$$E_{c} = \frac{(2\pi)^{\frac{1}{2}}}{8} \int \psi \frac{1}{r_{23}} \psi d\tau_{1} d\tau_{23},$$

where r_{23} is the distance between the two protons. The integration gives

$$E_{c} = \frac{1}{8[1+2\lambda(0|H|0)+\lambda^{2}(0|H^{2}|0)]} \Big\{ (12\alpha\rho)^{\frac{1}{2}} + 2\lambda \Big[(12\alpha\rho)^{\frac{1}{2}} \frac{63\alpha\rho^{2}+42\alpha\rho-12A_{II}\rho}{12\rho+8} - 12A_{II} \Big(\frac{6\alpha}{(2\rho+1)} \Big)^{\frac{1}{2}} \frac{\rho^{2}}{3\rho+2} \Big] \\ + \lambda^{2} \Big[(12\alpha\rho)^{\frac{1}{2}} \frac{531\alpha^{2}(27\rho^{5}+72\rho^{4}+60\rho^{3}+16\rho^{2})+48A_{II}^{2}(9\rho^{3}+12\rho^{2}+4\rho)-8A_{II}\alpha(567\rho^{4}+1242\rho^{3}+628\rho^{2})}{16(27\rho^{3}+72\rho^{2}+60\rho+16)} \\ + \Big(\frac{6\alpha}{2\rho H} \Big)^{\frac{1}{2}} \frac{24A_{II}^{2}(18\rho^{6}+33\rho^{5}+20\rho^{4}+4\rho^{3})-36A_{II}\alpha(63\rho^{7}+173\rho^{6}+171\rho^{5}+70\rho^{5}+10\rho^{3})}{54\rho^{5}+171\rho^{4}+210\rho^{3}+125\rho^{2}+36\rho+4} \\ + 6A_{II}^{2} \Big(\frac{12\alpha}{\rho+1} \Big)^{\frac{1}{2}} \frac{6\rho^{4}+8\rho^{3}+\rho^{2}}{9\rho^{3}+24\rho^{2}+19\rho+4} \Big] \Big\}$$

in which $\nu = \alpha \rho$. The Coulomb energy E_c^0 given by the wave-function (2) was also calculated, the ν being chosen in this case to make

$E^0 = \int \psi_0 H \psi_0 d\tau_1 d\tau_{23}$

a minimum. The results are summarized in Table I.

It is seen that E_c and E_c^0 vary much more slowly than $\sqrt{\alpha}$. This is because the wave-functions are forced out of the potential well as the range of forces is decreased. Interpolation gives $E_c = 1.37mc^2$ for $\alpha = 16(1/\sqrt{\alpha} \sim 2.3 \times 10^{-13} \text{ cm})$. The experimental difference in the binding energies of H³ and He³ is $1.58 \pm 0.18 mc^2$.³ It should also be mentioned that at $\alpha = 16$, $A_{\nu\nu} < (1 - g/2)A_{\nu\pi}$ and thus the actual Hamiltonian is not quite completely symmetrical. Unlike particles will on the average be a little closer together than like particles and therefore the Coulomb energy calculated from the correct slightly unsymmetrical Hamiltonian would possibly be slightly smaller. This effect is probably negligible at $\alpha = 16$. There may thus be a slight discrepancy between the calculated Coulomb energy and the experimental difference in the binding energies of H3 and He3 which is however very small compared to the Coulomb energy itself. The results, then, support the view that aside from the Coulombian interaction the proton-proton and neutron-neutron forces are equal. Interpolation gives $E = -14.2mc^2$ for the energy of H³ (experimental value

TABLE I. Calculated Coulomb energies. Energy units $mc^2 = 0.510$ MEV, length units $\hbar/c(Mm)^{\frac{1}{2}} = 8.97 \times 10^{-13}$ cm.

-		Using	ψo	*****	Using ψ						
α	A_{11}	ν	$-E^0$	E_{c^0}	ν	λ	-E	Ec	-E'		
10 20 30	65 98 129	7.9 10.8 12.6	16.37 10.08 5.30	1.22 1.42 1.54	7.0 9.2 10.4	$-0.0145 \\ -0.00884 \\ -0.00689$	$17.62 \\ 12.72 \\ 9.27$	1.25 1.44 1.55	17.9 14.3 11.6		

 $-16.8mc^2$). The agreement is rather good and the wavefunction (1) may be considered as a fairly close approximation to the correct H³ normal state eigenfunction. The values given in the last column of Table I are taken from Table I of reference 2 and are given for comparison of the variational with the corrected "equivalent two-body" calculations of the H³ binding energy.

Since the wave-functions (1) and (2) give practically the same Coulomb energies it was thought desirable to plot, Fig. 1, the expressions

$$f(r_{23}) = \int \psi^2 d\tau_1,$$

$$f_0(r_{23}) = \int \psi_0^2 d\tau_1.$$



FIG. 1. Functions $f(r_{23})$ and $f_0(r_{23})$ plotted against r_{23} .



FIG. 2. Functions $r_{23}f_0(r_{23})$ and $r_{23}f(r_{23})$ plotted against r_{23} .

These functions represent the probability of various separations of the two protons in the two cases. Except for the large r_{23} , which contribute only small amounts to the Coulomb energy, the larger region of integration in which $f_0(r_{23}) > f(r_{23})$ is sufficient to practically balance the bigger contribution of f for small r_{23} . In Fig. 2 the quantity $r_{23}f(r_{23})$ is plotted as a function of r_{23} . The areas under the curves are proportional to the Coulomb energies since $E_c = \int 1/r_{23}$ $\times f(r_{23})d\tau_{23}$ and the angle integrations merely introduce a factor 4π . (The curves for $\alpha = 10, 20, \text{ and } 30$ are very similar and only those for $\alpha = 20$ are included.) The writer wishes to express his gratitude to Dr. Eugene Feenberg for suggesting these calculations and for the advice and suggestions which he gave while they were being made.

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University of Wisconsin, August 4, 1936.

¹ Feenberg and Knipp, Phys. Rev. **48**, 906 (1935). ² Feenberg and Share, Phys. Rev. **50**, 253 (1936). ³ This value was given by Professor H. Bethe in a private com-munication to Dr. Feenberg. Bethe and Bacher give the value 0.76 ± 0.14 MEV ($1.49 \pm 0.27mc^2$) in Rev. Mod. Phys. **8**, 147 (1936). alue 0.76

On the Intensity of X-Rays Reflected from Zinc

The senior author has recently investigated theoretically the temperature dependence (usually represented by the factor e^{-2M}) of the intensity of x-rays reflected from anisotropic crystals.1 He found that in crystals with hexagonal symmetry M has the form

$$M = (a \cos^2 \psi + b \sin^2 \psi) \sin^2 \theta / \lambda^2, \tag{1}$$

where ψ is the angle between the normal to the reflecting plane and the principal axis. The constants for Zn and Cd were calculated from the known elastic constants, using the simple Debye model of a solid. The constants for Zn are

TABLE I. Constants at $T = 298^{\circ}K$.

	a	b	
Simple Debye Model	0.75 A ²	0.42 A	
Brindley	1.295	0.51	
Jauncey and Bruce	2.34	0.68	
Modified Debye Model	1.06	0.595	

given in the first row of Table I (the original calculations must be corrected by factors of 1.27 and 1.30 for Zn and Cd. respectively).

During the publication of this paper an article by Brindley appeared on the intensity of x-rays reflected from Zn.² In a second paper³ he has compared these and further experimental results with formula (1). He finds that a better fit with the experiments is obtained by using the semi-empirical constants in the second row of Table I.

In this laboratory Jauncey and Bruce have investigated Zn by the method of diffuse scattering of x-rays.⁴ In the third row of Table I are given the values of a and b which they find best fit their experiments, and which also give an excellent fit with Brindley's experiments. These disagree still more with the theoretical constants of the first row.

One possible source of this discrepancy has been suggested by Brindley. In interpreting the experiments all anisotropy of the atoms has been neglected. A second possible source of error lies in the assumptions of the simple Debye model. In this letter the authors report the modifications introduced by partially taking into account the discrete structure of a solid.

In a linear lattice with atoms of only one mass, the relation between frequency and wave-length is given by5

$$\nu = (c/\pi d) \sin (\pi d/\lambda). \tag{2}$$

Here d is the lattice spacing, and c is the velocity of waves long compared with d. If this relation is used in the three-dimension lattice in place of the usual relation

$$\nu = c/\lambda, \tag{3}$$

the factor $(2/\pi) \int_0^{\pi/2} (x/\sin x)^2 dx = 1.42$ is introduced into

the expression for both a and b when $T > \Theta$. It is interesting to note that a decision between (2) and (3) cannot be made from specific heat data.6

The values of the constants obtained by using (2) in place of (3) are given in the last row of Table I. A further improvement was sought by taking the integration in wave number space over the region appropriate to a hexagonal close packed lattice, in place of over a spherical region. This introduced no appreciable change in either a or b.

Although this change in the theoretical value of the constants is in the right direction, it is not sufficient to obtain agreement with the experiments as interpreted by the assumption of isotropic atoms. The decision as to whether the source of the remaining discrepancy lies in the assumption of atomic isotropy or in the model for a solid used in the theoretical calculations, can only be made by experiments at different temperatures.

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Wayman Crow Hall of Physics, St. Louis, Missouri, June 23, 1936.

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 ⁴ Jauncey and Bruce 50, 408 (1936).
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 ⁶ Eucken, Handbuch der Experimental Physik, Vol. VIII/1, 256.