

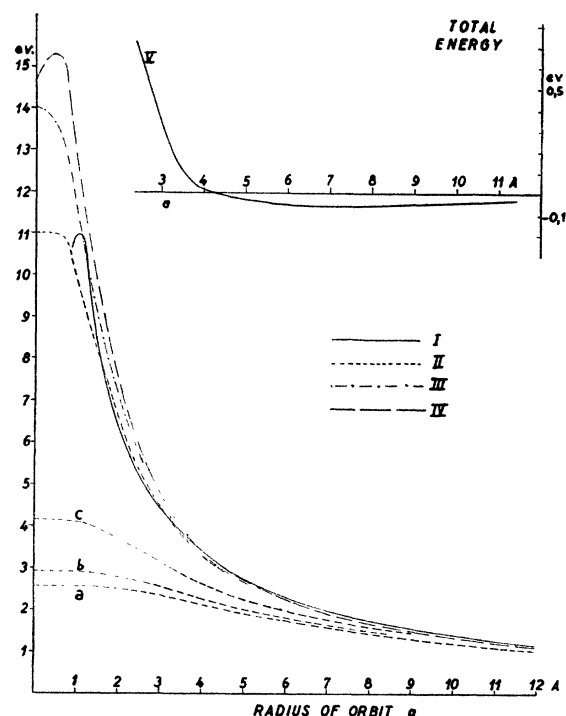


FIG. 1. (I) Negative energy of the electron bound to a free phosphorus atom. (II) Energy of the electron in the dipole field arising from the ion charge. There are contributions from the continuum of distant ($>5.16\text{\AA}$) dipoles (a), from 12 dipoles at $4.49\text{\AA}$ (b-a), from 12 dipoles at $3.38\text{\AA}$ (c-b), and from 4 dipoles at $2.27\text{\AA}$ (I-c). (III-III) Energy arising from the difference of polarizability of a P-ion with respect to a Si-atom. (IV-III) Energy in the periodic potential of the crystal. (V) Total energy $= \text{IV} - \text{I}$. The minimum is -0.065 eV at $a = 7\text{\AA}$.

28 nearest silicon atoms are considered explicitly; those farther away are treated as a continuum. The dipole moments due to the ion and the inner field are calculated making use of symmetry. For the electron-dipole field we take an approximation of the radial component of the ion-dipole field, namely,

$$F(d) = (e/d^2)\beta(d); \quad \beta(d) = \begin{cases} 1 - (d/C)^2 & \text{for } d < 5.16\text{\AA} \\ 1/\epsilon = 0.077 & \text{for } d > 5.16\text{\AA} \end{cases}; \quad C = 5.37\text{\AA}$$

and then assume that the electron-dipole field is the same expression, where d is the distance from the electron.

The method consists in minimizing the energy for the hydrogen-like wave function $\psi(r) = (\pi a^3)^{-1/2} e^{-r/a}$ with respect to the radius a .

The sum of kinetic energy $\hbar^2/2ma^2$ and potential energy $-e^2/a$ of the electron in the field of the ion must be slightly altered to give an ionization potential of 10.9 eV for free phosphorus (curve I of Fig. 1). This first energy is negative. The other energy terms are all positive. Second term: the energy of the electron in the dipole field arising from the ion charge (curve II) leaves a weak bond for $a = 7\text{\AA}$ and a stronger one for $a = 1\text{\AA}$. Third term: the energy of the electron in the dipole field arising from the electron itself is different in the bound and conducting states. Namely, the bound electron acts on the phosphorus ion, whose polarizability is taken to be smaller than that of a silicon atom by a factor $(14/15)^3$. For calculation of the resulting repulsion from the ion (III-III) cut-off radii $R_{P+} = 1.10\text{\AA}$ for a phosphorus ion and $R_{Si} = 1.17\text{\AA}$ for a silicon atom are assumed, within which there are no forces between the electron and the dipole. Incidentally, the potential energy of a conduction electron in the field of the dipoles which it induces becomes -10.0 eV , corresponding to an image-force barrier. Fourth term: it is found that a periodic potential in the crystal changes the energy only for small a (IV-III).

In the above model the minimum of the total energy is -0.065 eV for $a = 7\text{\AA}$, in essential agreement with experiment² and with the simple theory. It is only by taking all effects together that a bond with small a is excluded; but once the orbit is large, the phenomenological theory holds.

I wish to express my gratitude to Professor W. Pauli for his kind support, to Professor G. Busch for suggesting the problem, and to Dr. R. Schafroth for much helpful advice.

¹ H. C. Torrey and C. A. Whitmer, *Crystal Rectifiers* (McGraw-Hill Book Company, Inc., New York, 1948), p. 65.

² G. L. Pearson and J. Bardeen, *Phys. Rev.* **75**, 865 (1949).

A Scattering Approximation

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SCATTERING of a plane wave by a square well potential has been treated in an approximation comparable in simplicity to the Born approximation but with the added feature of being exact at low energies as well as high.

One proceeds from the integral formula for the scattering amplitude:

$$f(\theta) = (mV_0/2\pi\hbar^2) \int \exp(-ik'\cdot r)\psi(r)dr; \quad (1)$$

V_0 is the depth of the well, m is the reduced mass, and the integral is over the domain $r < a$, where a is the radius of the well; and $\psi(r)$ is the exact wave function inside the well, i.e.,

$$\psi(r) = \sum_l a_l (2l+1) i^l j_l(\alpha r) P_l(\cos\theta), \quad (2)$$

where α is the interior wave number and the coefficients a_l are found as usual by matching logarithmic derivatives:

$$a_l^{-1} = x^2 \{ [j_l(y)n_l'(x) - (y/x)j_l'(y)n_l(x)] - i[j_l(y)j_l'(x) - (y/x)j_l'(y)j_l(x)] \}, \quad (3)$$

where $x = ka$; $y = \alpha a$.

It is now observed that the series (2) is summable if one substitutes for the spherical bessel functions in Eq. (3) their asym-

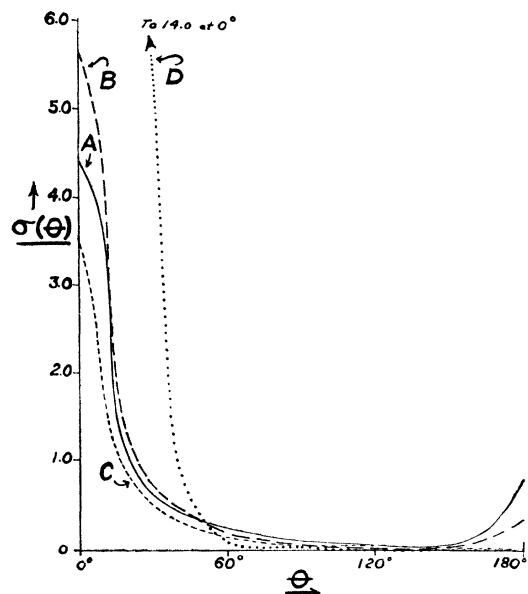


FIG. 1. Differential cross section in barns per steradian: A, exact; B, approximation based on Eq. (5); C, approximation based on Eq. (5) with $a_1 = a_0$; D, Born approximation.

ptotic forms¹ valid for $x, y \gg l$. The result is

$$a_{2n} = a_0 = e^{-i\alpha} [\cos y - i(x/y) \sin y]^{-1},$$

$$a_{2n+1} = a_1 = e^{-i\alpha} [(x/y) \cos y - i \sin y]^{-1},$$

and

$$\psi(r) = \frac{1}{2}(a_0 + a_1) \exp(i\alpha \cdot r) + \frac{1}{2}(a_0 - a_1) \exp(-i\alpha \cdot r). \quad (4)$$

This approximation is exact only for $l=0$ and becomes progressively less accurate as l increases. However, since partial waves for which $l \gg x$ do not contribute appreciably to the scattering, the inaccuracy will be slight for all but a few partial waves in the transition region $l \approx x$.

Now whereas the Born approximation makes use of the incident plane wave as the trial function in Eq. (1), we prefer at this point to use the approximate wave function (4), which, inserted into Eq. (1) and integrated, yields

$$f(\theta) = \frac{1}{2}(a_0 + a_1)g(\theta) + \frac{1}{2}(a_0 - a_1)g(\pi - \theta). \quad (5)$$

The function $g(\theta)$ is just a modified Born approximation for the scattering amplitude, starting with the function $\exp(i\alpha \cdot r)$ instead of $\exp(i\mathbf{k} \cdot \mathbf{r})$. For a square well one has

$$g(\theta) = (2mV_0 a^2 / \hbar^2) j_1(Ka) / Ka,$$

which is the familiar Born result² except now

$$K = [(\alpha - k)^2 + 4\alpha k \sin^2 \frac{1}{2}\theta]^{1/2}.$$

As an example, the case $V_0 = 30$ Mev, $a = 4.26 \times 10^{-13}$ cm, an incident energy of 18.26 Mev, and mass m equal to a nucleon mass was worked out using Eq. (5) and compared with the exact solution³ as shown in Fig. 1. Also shown is the Born approximation and a simplified form of Eq. (5) in which a_1 is set⁴ equal to a_0 .

Finally, the total cross sections were computed to be as follows: A. Exact: 2.7 barns; B. Approximation based on Eq. (5): 3.0 barns; C. Approximation based on Eq. (5) with $a_1 = a_0$: 1.7 barns; D. Born approximation: 12.1 barns.

¹ Recently Robert W. Hart, J. Acoust. Soc. Am. 23, 323 (1951), independently observed that the exterior solution could be summed in this way. He interprets his approximation directly to find the cross section. We, however, shall require of ours only that it be a good initial trial function in the integral formula.

² See L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), first edition, p. 167.

³ We wish to thank Dr. R. E. LeLevier for supplying us with the exact calculations, which involved seven partial waves significantly.

⁴ The comparison suffers somewhat in this example from the fact that the $l=4$ wave is nearly in resonance.

π^- Absorption in D_2 and the $n-n$ Force*

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WATSON and Stuart¹ have recently published detailed theoretical calculations concerning the gamma-ray spectrum from the process $\pi^- + D \rightarrow 2n + \gamma$ previously observed.² The resultant spectrum is clearly sensitive to the $n-n$ interaction at low energies. Since the analysis was based on unpublished data, it appears advisable here to state the experimental status concerning this spectrum. The present data allow considerable latitude regarding the $n-n$ interaction parameters. It is clear, however, that a not immeasurable improvement of the data could lead to quite conclusive evidence concerning the stability of the di-neutron.

When the curves of Watson and Stuart¹ are "folded" into the resolving power of the pair spectrometer used in the absorption experiments,³ the resultant curves for various values of the $n-n$ interaction show a negligible difference in shape but are effectively displaced along the energy scale. Figure 1 shows a curve of this effective displacement plotted against the binding energy of a hypothetical di-neutron, real or virtual. Figure 2 shows the theo-

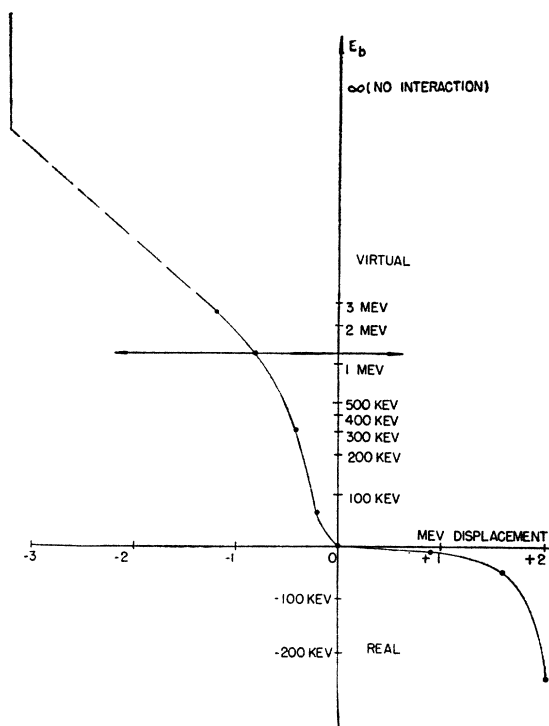


FIG. 1. Plot of effective displacement of theoretically computed spectra (see reference 1) resulting from the process $\pi^- + D \rightarrow 2n + \gamma$, as a function of the binding energy E_B of the lowest level of the $n-n$ system.

retical spectrum, with the resolution folded in, of the curve corresponding to zero binding. Marked on the abscissa is the value of $E_0 = [(\pi^- + p)^2 - n^2] / 2(\pi^- + p)$; here π^- , p , and n are the rest energies of the particular particles. E_0 is thus the expected value of the gamma-ray from the process $\pi^- + p \rightarrow n + \gamma$. Measurement of the gamma-ray process in H on the same spectrometer will thus determine the value of E_0 without specific reference to the π^- mass. Plotted on Fig. 2 also is the theoretical shape of the gamma-ray line from $\pi^- + p \rightarrow n + \gamma$, i.e., the resolution of the instrument. The value of the binding energy will then simply result by comparing the separation of the gamma-ray peaks of the two processes with that plotted in Fig. 2 and then reading E_B

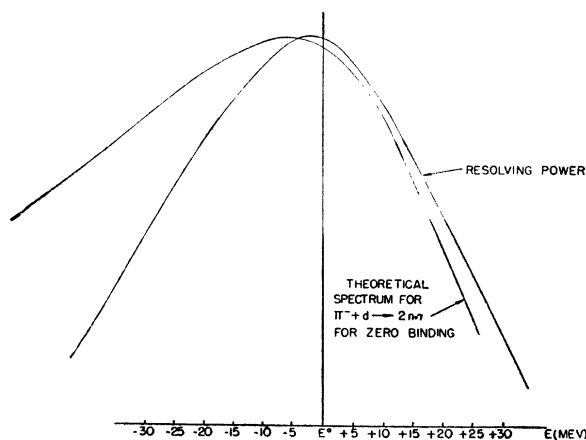


FIG. 2. Theoretical γ -spectra of the processes: $\pi^- + D \rightarrow 2n + \gamma$ and $\pi^- + H \rightarrow n + \gamma$; these spectra include the resolution.