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Positron-Hydrogen Scattering at Low Energies*

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The complete Dalgarno-Lynn second-order adiabatic potential is used to compute the *s*-wave elastic scattering of positrons by atomic hydrogen below the threshold for positronium formation. Comparison with the definitive results of Schwartz indicates that the potential is too attractive, as expected. A simple, one-parameter modification of the potential, related to the monopole distortion term, can yield exact agreement with Schwartz's value for the scattering length. Without further adjustment of the parameter, excellent agreement is also obtained for all energies up to the positronium threshold, and fairly good results are found for higher partial waves. The results encourage one to attempt similar work with more complex atoms, for which detailed variational calculations are impractical.

I. INTRODUCTION

POSITRON–hydrogen atom scattering below the inelastic (positronium) threshold is of interest as a representative single-channel, three-body scattering problem. It is not complicated by symmetry considerations, and is unaffected by any lack of information concerning the two-particle interactions, which are simply Coulomb potentials.

Schwartz[1] has used a straightforward, extensive variational method, with many parameters, to compute what are probably the best existing values of *s*-wave elastic-scattering phase shifts and scattering length. Rotenberg[2] has used an expansion in so-called Sturmian functions, which form a complete set without continuum. An excellent general review is the paper by Burke and Smith.[3]

The main purpose of the present work is to examine the adiabatic approximation, often used for atomic scattering calculations, for a particularly simple case, in an attempt to determine whether it is accurate enough to be useful in more complex cases. In particular, previous adiabatic calculations[3] have used questionable truncations and further approximations to simplify the numerical work, and have thus obscured to some extent the errors due to the adiabatic method itself.

Section II consists of an adiabatic calculation, which makes use of the exact second-order polarization potential elegantly derived by Dalgarno and Lynn.[4] The positron is assumed to move in this potential, and the resulting *s*-wave phase shifts and scattering length are obtained numerically, and compared with those of Schwartz.[1]

In Sec. III we consider the hypothesis that the excess attraction of the Dalgarno-Lynn potential is due to its short-range part. The principal short-range contribution comes from the monopole distortion, which has no long-range part. The second-order monopole polarization potential is derived, and the *s*-wave scattering is recalculated, with a monopole suppression factor adjusted to give exact agreement with the scattering length obtained by Schwartz.[1] Without further adjustment of the parameter, excellent agreement is also obtained over the full energy range. In addition, *p*- and *d*-wave phase shifts are computed, and the problem of a position-hydrogen bound state is considered.

Section IV contains a discussion and mentions a variational extension of the present work.

II. THE ADIABATIC CALCULATION

In atomic units, with energy in rydbergs, the Hamiltonian for an electron at $\mathbf{r}$ and a positron at $\mathbf{x}$ in the field of a proton fixed at the origin is

$$H=H_r-\nabla_x^2+V(\mathbf{r},\mathbf{x}), \tag{1}$$

where

$$H_r=-\nabla_r^2-2/r$$

and

$$V(\mathbf{r},\mathbf{x})=2[x^{-1}-|\mathbf{x}-\mathbf{r}|^{-1}].$$

The total energy E equals $\mathbf{k}^2-1$, where $\mathbf{k}$ is the positron momentum, and below the threshold for positronium formation $\mathbf{k}^2<\frac{1}{2}$.

Let us consider the following reasonable adiabatic type of wave function as an approximate description of the scattering:

$$\psi_{\mathbf{k}}(\mathbf{r},\mathbf{x})=[1+G(\mathbf{r},\mathbf{x})]\Phi(r)\chi_{\mathbf{k}}(\mathbf{x}). \tag{2}$$

Here, $\Phi(r)$ is the wave function describing the ground state of the hydrogen atom, satisfying the equation

$$(H_r+1)\Phi(r)=0. \tag{3}$$

$\chi_{\mathbf{k}}(\mathbf{x})$ is a one-particle scattering function for the positron, and $G(\mathbf{r},\mathbf{x})$ is an adiabatic correlation function, which describes the effect on the ground state of

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* The main results of this paper were outlined in a talk given at the American Physical Society, 1964 Chicago meeting [Bull. Am. Phys. Soc. **9**, 626 (1964)].

[1] C. Schwartz, Phys. Rev. **124**, 1468 (1961).

[2] M. Rotenberg, Ann. Phys. (N.Y.) **19**, 262 (1962). (A long-standing discrepancy between the results of Refs. 1 and 2 seems to have been eliminated. Both Rotenberg and Schwartz have recalculated the Sturmian results, and have detected a numerical error in Ref. 2 (private communications).)

[3] P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962).

[4] A. Dalgarno and N. Lynn, Proc. Phys. Soc. (London) **A70**, 223 (1957).

hydrogen of a fixed (or slowly moving) positron at position **x**.

Assuming that Eq. (2) represents the scattering fairly well, one inserts it into the Schrödinger equation, uses Eq. (3) and obtains

$$\begin{aligned}[][H+1-\mathbf{k}^2]\psi_{\mathbf{k}} &= \Phi(r)[1+G(\mathbf{r},\mathbf{x})][V(\mathbf{r},\mathbf{x})-\nabla_x^2-\mathbf{k}^2]\chi(\mathbf{x}) \\ &\quad +\chi(\mathbf{x})\{[H_r,G(\mathbf{r},\mathbf{x})]-\nabla_x^2G(\mathbf{r},\mathbf{x})\}\Phi(r) \\ &\quad -2\Phi(r)\nabla_xG(\mathbf{x},\mathbf{r})\cdot\nabla_x\chi(\mathbf{x})=0. \end{aligned} \tag{4}$$

In a subsequent paper this equation will be used variationally (see Sec. V), but here one simply multiplies on the left by $\Phi(r)$ and integrates over **r**. Defining

$$\langle Q(\mathbf{r},\mathbf{x})\rangle \equiv \int d^3r\Phi(r)Q(\mathbf{r},\mathbf{x})\Phi(r), \tag{5}$$

and noting that $\langle[H_r,G]\rangle=0$, one obtains the following equation for $\chi(\mathbf{x})$:

$$\begin{aligned}-(1+\langle G\rangle)(\nabla_x^2+\mathbf{k}^2)\chi+(V_1+V_2)\chi \\ -(\nabla_x^2\langle G\rangle+2\nabla_x\langle G\rangle\cdot\nabla_x)\chi=0,\end{aligned} \tag{6}$$

where $V_1\equiv\langle V\rangle$ and $V_2\equiv\langle GV\rangle$. Dalgarno and Lynn[4] have obtained the function $G(\mathbf{r},\mathbf{x})$ correct to first order in the potential V, as a solution of the differential equation:

$$[G,H_r]\Phi(r)=(V-\langle V\rangle)\Phi(r). \tag{7}$$

For a first-order wave function $\langle G\rangle$ can be taken equal to zero with no loss of generality. Hence the complete adiabatic equation, correct up to second order in V, is

$$[-(\nabla_x^2+\mathbf{k}^2)+V_1+V_2]\chi(\mathbf{x})=0. \tag{8}$$

Here, $V_1=2e^{-2x}(1+(1/x))$, while Dalgarno and Lynn[4] have obtained

$$\begin{aligned}V_2=x^{-2}[5-(4x^2+8x+10)e^{-2x}+(4x^3+7x^2+8x+5)e^{-4x} \\ -2(x+1)^2(e^{-2x}+e^{-4x})(\mathrm{Ei}[2x]-2\ln[2\gamma x]) \\ -2\,\mathrm{Ei}[-2x]([x-1]^2e^{2x}+[x^2+2x-3] \\ +4[x+1]e^{-2x})],\end{aligned} \tag{9}$$

where $\mathrm{Ei}[-z]=-\int_z^\infty e^{-y}dy\cdot y^{-1}$, and $\ln\gamma$ is Euler's constant, $0.577\cdots$. For small values of x, we have $V_1\to 2x^{-1}-2$ and $V_2\to -1$, while for large values of x, we have $V_2\to -4.5x^{-4}$. The differential equation (8) for the scattering of s waves takes the form

$$-U''+[V_1+V_2-k^2]U=0,\quad U=x\chi. \tag{10}$$

The equation was integrated numerically, using the starting approximation

$$U\sim x+x^2-\tfrac{1}{6}(1+k^2)x^3, \tag{11}$$

which can be obtained from the above behavior of V_1 and V_2 near $x=0$. For $k\neq 0$, the phase shifts are obtained easily from the large-x behavior of U and U'. For $k=0$, the scattering length requires a correction, due to the long-range polarization potential.[5] Figure 1 shows the resulting phase shifts in comparison with those of Schwartz.[1] (The scattering length is −2.54 versus Schwartz's −2.10.)

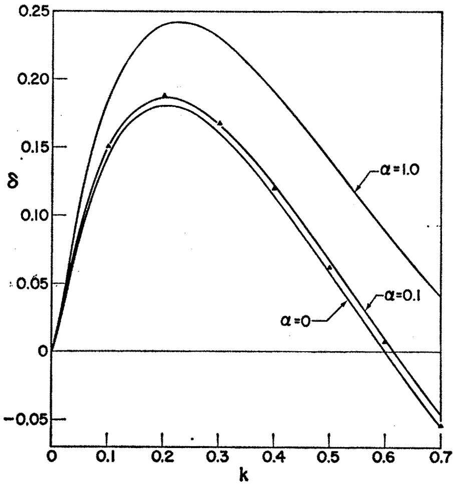

FIG. 1. Phase shifts in radians for s-wave scattering. The curve marked $\alpha=1$ corresponds to the full Dalgarno-Lynn adiabatic potential (Ref. 4), while $\alpha=0$ corresponds to full monopole suppression. The triangles indicate Schwartz's results (Ref. 1).

Notice that the adiabatic results indicate an effective interaction which is more attractive than that of Schwartz.[1] This is expected, since the adiabatic potential assumes that the hydrogen atom can rearrange itself to follow exactly the motion of the positron. This is clearly not true even for zero energy, since the positron accelerates toward the atom during part of its [classical] trajectory, but it becomes even less true as k increases. These qualitative expectations are borne out by the results of Fig. 1.

In fact, the adiabatic potential is likely to be least accurate close to the nucleus, and any attempt to improve the results of Fig. 1 must involve ways of modifying the form of the potential for small x.

III. THE MODIFIED ADIABATIC CALCULATION

The derivation of V_2 by Dalgarno and Lynn uses elliptical coordinates to solve Eq. (7) is closed form. It is also possible, however, to expand $G(\mathbf{r},\mathbf{x})$ in Legendre polynomials,

$$G(r,x,\theta)=\sum_{m=0}^{\infty} G_m(r,x)P_m(\cos\theta), \tag{12}$$

where θ is the angle between **r** and **x**. It can be easily shown that for $m>0$ the leading term for large x falls off like some inverse power of x. For $m=0$, however, only short-range contributions occur. Nevertheless, the monopole ($m=0$) contribution to V_2 is not negligible, since it is *entirely* responsible for the short-range parts of the potential V_2.

The monopole correlation function satisfies the equation

$$[G_0,H_r]\Phi(r)=[V_0-\langle V_0\rangle]\Phi(r), \tag{13}$$

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[5] A. Temkin, Phys. Rev. Letters **6**, 354 (1961).

where

$$V_0=0, \qquad x>r$$
$$=2(x^{-1}-r^{-1}), \quad x<r.$$

Inserting the appropriate forms for each of the potentials as well as $\Phi=e^{-r}/\pi^{1/2}$, one finds

$$d^2G_0/dr^2+2(1/r-1)dG_0/dr=V_0-V_1. \tag{14}$$

This inhomogeneous equation can be solved by quadratures for both $r\gtrless x$, and using the corresponding homogeneous equation one obtains a complete solution in both regions, continuous and with continuous derivative called $F_{>,<}$:

$$F_<=\tfrac{1}{4}[Q(r)+2\,\mathrm{Ei}(2x)-e^{2x}/x]V_1 \\ +[1-x^{-1}][\ln x-\tfrac{1}{2}x]-1, \tag{15a}$$

$$F_>=[\tfrac{1}{2}V_1-x^{-1}+1][\ln r-1/2r]+[\tfrac{1}{2}V_1-x^{-1}]r, \tag{15b}$$

where

$$Q(r)=[e^{2r}-1]r^{-1}+2r+2[\ln r-\mathrm{Ei}(2r)]. \tag{15c}$$

However, $\langle F\rangle\neq 0$, so the full solution is

$$G_0=F-\langle F\rangle,$$
$$V_{20}=\langle V_0F\rangle-V_1\langle F\rangle. \tag{16}$$

The modified adiabatic calculation uses a parameter α to specify how much of the monopole correlation term G_0 is to be retained in Eq. (12). That is, the modified potential

$$V_1+V_2+(\alpha-1)V_{20} \tag{17}$$

is used in a Schrödinger equation which replaces Eq. (8). Clearly $\alpha=1$ corresponds to no suppression and $\alpha=0$ to full suppression of the monopole part of G. The higher multipoles are assumed to require no modification.

By repeating the zero-energy calculation for various values of α, it is found that agreement with Schwartz's[1] scattering length is obtained at $\alpha=0.1$. Figure 1 shows the phase shifts for this value of the parameter, as well as those for $\alpha=0$. It is clear that this latter value, which corresponds to $V_2(0)=0$, is also not seriously in error,[6] yielding a scattering length of -2.07.

It is now straightforward to calculate the scattering for higher partial waves. One simply adds the centrifugal potential term and solves the equation

$$-U_l''+[V_1+V_2+(\alpha-1)V_{20} \\ +l(l+1)x^{-2}-k^2]U_l=0, \tag{18}$$

with the starting conditions near $x=0$

$$U_l\sim x^{l+1}+(l+1)^{-1}x^{l+2} \\ -[k^2+\alpha+2l(l+1)^{-1}](4l+6)^{-1}x^{l+3}. \tag{19}$$

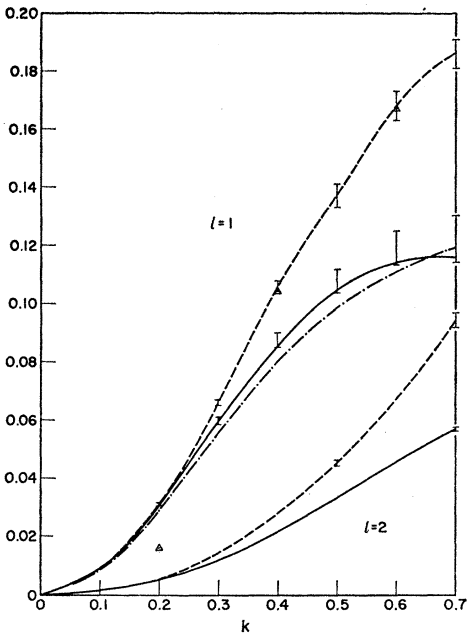

FIG. 2. Phase shifts in radians for p- and d-wave scattering. The solid curves are for $\alpha=0.1$, and the vertical bars indicate $\alpha=1.0$ and $\alpha=0$ limits. The triangles are Bransden's p-wave values (Ref. 7); the lower bound given by Kleinman *et al.* (Ref. 8) is shown, for $l=1$, by the broken curve, and, for $l=2$, is almost indistinguishable from the $\alpha=0.1$ curve, while their extrapolated values are shown (with estimated errors) by the dashed curves.

The results are shown in Fig. 2 for the value of $\alpha=0.1$ determined above, and the error quoted represents the extreme values obtained for $\alpha=1$ and $\alpha=0$. Notice the insensitivity of the higher phase shifts to α, especially for small k. This is due to the fact that the centrifugal potential keeps the positron so far away that the short-range potential becomes unimportant. The results are to be compared [for $l=1$] with those of Bransden,[7] obtained by including a virtual positronium term. Kleinman, Hahn, and Spruch[8] have reported lower bounds and extrapolated values for $l=1$ and 2, which are also shown.

There has been some recent interest[9] in the question of the possible existence of a bound state of the system e^+-e^--P. There is no evidence for such a state, and the present calculation gives a nodeless $k=0$ wave function, which supports the idea that no such state exists. For some more massive positive particle a bound state must occur, since the H_2^+ ion is bound. Handler[10] has used a Hylleraas trial function with up to 20 terms, and has shown that a positive particle of mass m is bound to the hydrogen atom if $m\geq 3m_e$. (The variational nature of the calculation does not rule out the existence of a bound state for a still lower mass.) The

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[6] The desirability of having $V_2(0)=0$ has been indicated by V. D. Ob'edkov, Opt. i Spectroskopiya 17, 189 (1964) [English transl.: Opt. Spectry. (USSR) 17, 101 (1964)].

[7] B. H. Bransden, Proc. Roy. Soc. (London) A79, 190 (1962).

[8] C. J. Kleinman, Y. Hahn, and L. Spruch, Bull. Am. Phys. Soc. 9, 39 (1964), and private communication.

[9] C. Fronsdal and A. Ore, Physica 19, 605 (1953); M. R. Baker and G. S. Handler, Bull. Am. Phys. Soc. 8, 631 (1963).

[10] G. S. Handler (unpublished).

nonvariational method described here can be easily modified to examine this question. One simply calculates the zero-energy scattering length for various values of the mass m in the equation

$$-U''+m[V_1+V_2+(\alpha-1)V_{20}]U=0. \qquad (20)$$

A change of sign of the scattering length indicates the appearance of the bound state. For $\alpha=0.1$, the critical mass is $3.6m_e$, while for $\alpha=1$ it is about $3.1m_e$. Both of these results are reasonable, but one expects α to increase with m as the adiabatic model improves. In any case, as m increases, the effective attraction would increase for other reasons (as the H_2^+ limit is approached) and these results should be considered as suggestive only.

IV. DISCUSSION AND CONCLUSIONS

1. The adiabatic method has been considered of interest for some time. Its appeal lies in simplicity and concreteness. Nevertheless, a general recognition of the incompleteness of the method has apparently prevented one from taking it quite seriously. The philosophy behind the approach reported here is to use the exact second-order adiabatic potential and then to seek modifications. Earlier work usually began with rough approximations to this potential,[11] a procedure which prevents an easy evaluation of deviations from adiabaticity.

The second-order potential used here is evidently somewhat too attractive for s waves, and the excess can be traced to the monopole or short-range part, and corrected effectively by adjustment of a single energy-independent parameter. This is, in itself, a significant fact, and it remains significant although the adjustment is only empirical.

2. One may question the great reliance placed upon the second-order potential; surely higher corrections might be significant and could change the qualitative situation. In particular, the complete adiabatic potential is known[12] and gives the potential-energy curve for the H_2^+ ion.

An answer can be given as follows: The complete adiabatic problem assumes two fixed positive particles, in whose field one electron moves quantum-mechanically. The electron can spend as much time in the vicinity of the incoming particle as the target. This evidently would be realistic for low-energy p-H scattering. For e^+-H scattering, however, the small reduced mass of the positronium system suppresses, to a large extent, the exchange of the electron between the proton and the positron. It is this necessary suppression which rules out the use of the H_2^+ potential and favors low-order perturbation theory. Nevertheless, these arguments weaken considerably as the positronium threshold $k^2=\frac{1}{2}$ is approached, and some additional positronium contribution to the wave function may be required for $l>0$, as Bransden's work[7] (Fig. 2) indicates. In the present context, additional positronium corresponds to a closer approach to the H_2^+ potential and a consequent increase in attraction. This question is presently under investigation.

As the mass of the incoming positive particle increases, also, one expects that the H_2^+ potential should become increasingly realistic. Since this potential gives greater attraction than does the second-order potential (except at $x=0$ and $x\rightarrow\infty$), the results of Sec. III must overestimate the critical mass m necessary to produce a bound state.

3. The wave function assumed in this work [Eq. (2)], with the monopole part suitably suppressed or the short-range part suitably modified, is applicable as well to a strict variational calculation. This will be discussed in a subsequent paper. It suffices here to note that an effective one-particle equation will have to be solved which contains (besides V_1 and V_2) a third-order potential, a "normalization factor," and two terms which give nonadiabatic effects, including a velocity-dependent term discussed previously by Mittleman and Watson.[13] Separate variational parameters can be used to measure suppression and other short-range modifications of the higher multipoles. The detailed calculations are rather complex, but a simplified three-parameter variation has already produced the rigorous upper bound[14] to the scattering length of -1.62.

4. Since it is at present too difficult to use the rigorous variation methods of Schwartz[1] for several-electron atoms, the adiabatic approximation for positron-atom scattering should prove useful. Since there is no clear way to determine the parameter α, one probably must be satisfied with using complete monopole suppression,[6] $\alpha=0$. The simple shielded hydrogenic approximation is now being employed in an attempt to compute the low-energy scattering of positrons from helium.

ACKNOWLEDGMENTS

All the numerical calculations reported here were programmed for the Goddard Theoretical Division IBM 7094 electronic computer by Edward Monasterski, to whom I am greatly indebted. I wish also to thank Dr. Aaron Temkin for many essential conversations concerning the positron-scattering problem.

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[11] For example, the method of polarized orbitals [A. Temkin and J. C. Lamkin, Phys. Rev. 121, 788 (1961)] uses a wave function essentially equivalent to the present Eq. (2), but restricts the detailed evaluation to the region $r<x$ and a limited number of multipole terms. For the electron-scattering problem the former restriction introduces very little error due to the requirement of antisymmetrization of the wave function of the electrons.

[12] E. A. Hylleraas, Z. Physik 71, 739 (1931).

[13] M. H. Mittleman and K. M. Watson, Phys. Rev. 113, 198 (1959).

[14] L. Spruch and L. Rosenberg, Phys. Rev. 117, 143 (1960).