X-641-70-245
PREPRINT

NASA TM X- 63949

SIMPLIFIED MODEL FOR POSITRONIUM-HELIUM SCATTERING

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JUNE 1970

GODDARD SPACE FLIGHT CENTER
GREENBELT, MARYLAND

Simplified Model for Positronium - Helium Scattering

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Abstract

Using a local effective potential to account for electron exchange, we have analyzed the zero-energy scattering of ortho-positronium by helium atoms. The effective potential was chosen so that the results obtained in the static approximation agreed with the static-exchange results of Fraser and Kraidy. Correlation was introduced in two different approximations which agree well. We find a decrease in the scattering length $\underline{a}$ from 1.72 a_o to 1.39 a_o, and an increase of more than a factor of 2 in the quenching rate of the positronium (from $Z_{eff} = 0.042$ to 0.10), as compared with the static exchange approximation. This gives improved agreement with the experimental value $Z_{eff} \simeq 0.18$.

1. Introduction

The system consisting of one atom of helium and one of the long-lived ortho-positronium is accessible to experiment through observation of the density dependence of the annihilation rate of positrons in helium gas. The positron can be "picked off" or quenched during collision with a helium atom and this quenching rate is therefore proportional to the helium density. It measures the joint probability that the positron be at the location of one of the helium electrons and also form a singlet spin state with that electron. This pickoff probability is conventionally presented in terms of the effective number of electrons in the singlet state seen by the positron, Z_{eff}. This quantity is, in general, energy dependent, and is obtained from the scattering wave function.

More specifically, if $\Psi(\underset{\sim}{x}, \underset{\sim}{r}_1, \underset{\sim}{r}_2, \underset{\sim}{r}_3)$ is the Ps-He scattering function, $\underset{\sim}{x}$ being the coordinates of the positron and $\underset{\sim}{r}_1$, $\underset{\sim}{r}_2$, $\underset{\sim}{r}_3$ the coordinates of the electrons then one can write

$$Z_{eff} = \iiint d\underset{\sim}{x}\, d\underset{\sim}{r}_1\, d\underset{\sim}{r}_2\, d\underset{\sim}{r}_3 \sum_{i=1}^{3} \left| \Phi_i \right|^2 \delta(\underset{\sim}{x} - \underset{\sim}{r}_i) \qquad (1)$$

where Φ_i is the projection of the wave function Ψ on to the singlet spin function involving the positron and the i th electron.

Fraser and Kraidy (1966) and Fraser (1968) have calculated Z_{eff} and the scattering length $\underline{a}$ in the static exchange approximation. They assumed a trial function of the form

$$\Psi = \mathcal{A}\, \chi(R_1)\, \phi(\rho_1)\, \psi(r_1, r_2) \cdot \alpha_x \alpha_1 (\alpha_2 \beta_3 - \beta_2 \alpha_3)/\sqrt{6} \,, \qquad (2)$$

where $\underset{\sim}{R}_i = \frac{1}{2}(\underset{\sim}{x} + \underset{\sim}{r}_i)$, $\underset{\sim}{\rho}_i = \underset{\sim}{r}_i - \underset{\sim}{x}$, ϕ and ψ are the positronium and helium ground state wave functions respectively. $\mathcal{A}$ is an operator which antisymmetrizes the wave function with respect to the three electrons, and α, β represent up and down spin respectively. They determined χ by solving numerically a certain integro-differential equation obtained variationally, and with the asymptotic normalization $\chi(R) \sim \exp(i\underset{\sim}{k}.\underset{\sim}{R})$, they used (1) to compute Z_{eff}. For zero energy collisions their results were $Z_{eff} = 0.042$, and the scattering length $\underline{a} = 1.72\ a_o$.* This value for Z_{eff} is in

*These numbers are slightly different from those published by Fraser and Kraidy (1966). The change is due to a different method of treating the target wave function (Kraidy, 1969, private communication).

strong disagreement with the best experimental value of 0.180 ± 0.016, deduced by Fraser (1968) from the experimental data of Beers and Hughes (1968). Earlier experimental results for Z_{eff} range from 0.118 ± 0.011 (Duff and Heymann, 1962) to $0.25 \pm 25\%$ (Roellig and Kelly, 1967).

This static exchange approximation satisfies the conditions on scattering bounds (Spruch and Rosenberg, 1960) and hence the scattering length obtained is larger than the true value. Although no rigorous bound theorems for Z_{eff} are known, it is roughly correct that a large, positive scattering length must correspond to a small Z_{eff}. One expects, then, that any improvement in the trial wave function (2) leading to a decrease in $\underline{a}$ will also tend to increase Z_{eff}.

Barker and Bransden (1968, 1969) examined the effect of van der Waals' long range forces on Z_{eff}. Such forces are attractive, reduce $\underline{a}$ and are expected to increase Z_{eff}. They found, however, that an increase of only about 30% in

Z_{eff} results from this cause.

In this paper we take the view that, since the strongest force acting between the two atoms is the exchange force between the closed electron shell in helium and the electron of positronium, short-range correlation induced by this force will be the dominant correction to the trial function (2). Since Ps is much more polarizable than He, most of this correlation will affect the former, while the latter will be almost undistorted. In the next section, we outline a model embodying these considerations which, although simple, seems realistic enough to describe the system fairly well.

2. Description of the model

Consider the following model: assume the Ps electron to be distinguishable from the He electrons, and introduce an effective local interaction between the helium atom and this electron to represent the effect of the exclusion principle. Specifically we replace the exact Hamiltonian of the system (in atomic units, with energies in Rydbergs) by the following:

$$H = H_0 - \tfrac{1}{2}\nabla_R^2 + V_0 e^{-\alpha r} \qquad (3)$$

where $H_o = -2\nabla_\rho^2 - \frac{2}{\rho} + H(1,2)$

where coordinates without indices refer to electron 3, now treated as distinguishable, and H(1,2) is the Hamiltonian for the helium atom alone. The ground states, $\phi(\rho)$ of Ps, and $\psi(r_1, r_2)$ of He, satisfy the equation

$$(H - E_o)\,\phi(\rho)\,\psi(r_1, r_2) = 0 \quad , \qquad (4)$$

and the model potential depends on two parameters, V_o and α. We have omitted the electrostatic interaction with the helium charge density and, since the helium atom is not distorted in this model, no van der Waals' force occurs either; these two should have small effects which would partially compensate.

To fix the values of V_o and α appearing in(3) we use our model without distortion of the positronium, and demand that the results agree with Fraser and Kraidy (1966) and Kraidy (private communication) at zero energy. That is we assume a wave function analogous to (2):

$$\Psi = \chi(R)\,\phi(\rho)\,\psi(r_1, r_2) \qquad (5)$$

where we have suppressed the spin indices. Using the Hamiltonian of (3) in a standard variational principle and recalling (4) we obtain the equation satisfied by $\chi(R)$ in the static model approximation:

$$\left[-\tfrac{1}{2}\nabla_R^2 + U_1(R)\right]\chi(R) = 0 \qquad (6)$$

where $$U_1(R) = V_0\int d\underset{\sim}{\rho}\,\phi^2(\rho)\,e^{-\alpha\left|\underset{\sim}{R}+\frac{1}{2}\underset{\sim}{\rho}\right|} \qquad (7)$$

since $$r = \left|\underset{\sim}{R} + \tfrac{1}{2}\underset{\sim}{\rho}\right| .$$

Equation (6) was integrated numerically to give both $\chi(R)$ and the scattering length a.

Using $$\phi(\rho) = (8\pi)^{-\frac{1}{2}}\exp\left(-\tfrac{1}{2}\rho\right) \qquad (8)$$

and the approximate helium wave function

$$\psi(r_1, r_2) = z^3\pi^{-1}\exp\left[-z(r_1+r_2)\right],\ z = \frac{27}{16}, \qquad (9)$$

we compute the effective electron number Z_{eff} from the expression

$$Z_{eff} = Z^3(16\pi^2)^{-1}\iint d\underline{R}\, d\underline{\rho}\; e^{-\rho}\, e^{-2Z|\underline{R}-\frac{1}{2}\underline{\rho}|} \cdot |\chi(R)|^2 \qquad (10)$$

The parameters V_o and α were adjusted to give the values of $\underline{a}$ and Z_{eff} obtained by Fraser and Kraidy. We found $V_o = 39$ and $\alpha = 2.9$ gave sufficiently good agreement.

3. Consequences of the model

With the parameters of the model defined, we will next calculate, by two different techniques, the values of $\underline{a}$ and Z_{eff} which result from the Hamiltonian of (3). We will consider the zero-energy case only.

3.1 Differential Equations

To the trial function of (5) we add a closed channel term giving

$$\Psi = \left[\chi(R) + F(R)G(\underline{R},\underline{\rho})\right]\phi(\rho)\psi(r_1,r_2) \qquad (11)$$

where G is a correlation function to be chosen later. By a method like that leading to equation (5), we now obtain the pair of coupled differential equations

$$\left[-\tfrac{1}{2}D_R^2 + U_1(R)\right]\chi + U_2(R)\,F = 0$$

$$\left[-\tfrac{1}{2}N D_R^2 + W + U_N\frac{d}{dR} + U_3 + Q\right]F + U_2\,\chi = 0 . \qquad (12)$$

If we define the notation

$$\langle f \rangle = \int d\underline{\rho}\;\phi(\rho)\, f\, \phi(\rho) \qquad (13)$$

and assume, without loss of generality, that $\langle G \rangle = 0$, we can write the quantities appearing in (12) as follows:

$$U_1 = \langle V \rangle , \quad U_2 = \langle GV \rangle , \quad U_3 = \langle G^2 V \rangle ,$$

$$N = \langle G^2 \rangle , \quad W = -\tfrac{1}{2}\langle G\, D_R^2\, G \rangle ,$$

$$U_N = -\tfrac{1}{2}\frac{dN}{dR} , \quad Q = \langle G\,[H_0, G] \rangle , \qquad (14)$$

where $V = V_o e^{-\alpha r}$ is the effective potential appearing in (3). This notation is based on that used in two previous papers (Drachman 1968, 1969). Once the solution of equation (12) is obtained, Z_{eff} can be calculated by replacing χ in (10) by $(\chi + FG)$.

Guided by perturbation theory in a closure approximation, we have used an exponential form for the correlation function. If

$$g = \cosh\left[-\gamma\left|\underline{R} + \tfrac{1}{2}\underline{\rho}\right|\right]$$

we take

$$G = g - \langle g \rangle$$

which satisfies the condition $\langle G \rangle = 0$, and depends on the parameter γ. In figure 1 we show the dependence of $\underline{a}$ and Z_{eff} on γ. The best (minimum) value of $\underline{a}$ occurs at $\gamma = 0.824$, where $\underline{a} = 1.42\ a_o$ and $Z_{eff} = 0.100$.

3.2 Kohn Variational Principle

In this model scattering problem, Kohn's variational principle may be written as

$$a \leq a_V = a_T + \frac{2}{4\pi}\int \Psi_T (H - E_0)\, \Psi_T \, d\tau \qquad (15)$$

where H is given by (3) and the trial function Ψ_T has the asymptotic form

$$\Psi_T \sim R^{-1}(a_T - R)\,\phi(\rho)\,\psi(r_1, r_2) \qquad (16)$$

as $R \to \infty$. Note the factor 2 outside the integral in (15). This does not appear in Kohn's variational principle for positron-atom scattering and arises from the use of the co-ordinates $\underset{\sim}{R}$ and $\underset{\sim}{\rho}$ in place of $\underset{\sim}{x}$ and $\underset{\sim}{r}$. As already mentioned, this system satisfies the conditions for the variational approximation a_v to be an upper bound to the exact scattering length $\underline{a}$ (Spruch and Rosenberg, 1960). Using the separable form of trial function Ψ given by (5) with

$$\chi(R) = R^{-1}\left\{a_T\left(1 - e^{-\delta R}\right) - R\right\} \qquad (17)$$

where a_T is the trial scattering length and δ is a non-linear variational parameter, we found that a_v has the minimum value 1.763 a_o when $\delta = 0.6$. We then modified $\chi(R)$ by adding on terms

$$e^{-\delta R} \sum_{i=0}^{N} a_i R^i$$

until a_v converged. This was with N = 4 and then a_v was 1.722 a_o which is in agreement with the value obtained by numerical integration in the previous section and thus with Fraser and Kraidy. Furthermore when Z_{eff} is calculated using (10), with the parameters a_T and a_i determined by the variational calculation, we obtain the value $Z_{eff} = 0.042$, thus verifying that our model reproduces the static exchange results of Fraser and Kraidy.

We now introduce correlation into the calculation by replacing $\chi(R)$ by a function $\chi'(R,\rho,r)$ thus:

$$\chi'(R,\rho,r) = R^{-1}\left\{q_T(1-e^{-\delta R}) - R\right\} + e^{-\delta R}e^{-\beta\rho}e^{-\gamma r}\sum_{i=1}^{N} a_i R^{l_i}\rho^{m_i}r^{n_i} \quad (18)$$

where β, γ are additional non-linear parameters and l_i, m_i, $n_i \geq 0$. This is a generalized Hylleraas type expansion in the coordinates R, ρ and $r = |\underset{\sim}{R} + \underset{\sim}{\rho}|$ and is anologous to using the coordinates (r_1, r_2, r_{12}) in, for example, a positron-hydrogen atom scattering problem. (See, for example, Schwartz, 1961.) This is an effective way of including the distortion of the Ps atom.

The number of terms N was chosen to include all terms such that

$$0 \leq \ell_i + m_i + n_i \leq \omega$$

where ω took the values 1 to 6. This corresponded to N taking the values 4, 10, 20, 35, 56, 84. At this stage of the calculation all the integrals were carried out analytically.

With N = 35, the three non-linear parameters δ, β, γ, were varied until the minimum value of $1.389\ a_o$ was obtained for a_v. This was with $\delta = 0.7$, $\beta = -0.2$, $\gamma = 0.8$. This is close to the value of $1.42\ a_o$ obtained by the differential equation method, but is lower because a more general correlation function was used. Increasing the number of terms N to 84 did not reduce a_v below this value, and furthermore, with N = 84, the value for a_v was insensitive to small changes in the non-linear parameters. We conclude that $1.389 a_o$ is the least upper bound obtainable for the scattering length with this type of trial function. Table I shows the convergence of a_v as N is increased.

We now substituted this variationally determined 35-term wave function into equation (10) and calculated Z_{eff}. We now used numerical integration and the value obtained

for Z_{eff} was 0.098, again in good agreement with the result of Section 3.1.

We could only have calculated the Z_{eff} integrals analytically by taking $\gamma = 0$ and restricting n_i to be even. In this case we found that a_v did not converge even after 80 terms (corresponding to $\omega = 7$) and was still as large as 1.463 a_o. We abandoned this line of enquiry. However, this point has an interesting analogy in positron-hydrogen atom scattering. In the present coordinate system, (R, ρ, r), r corresponds to the "interelectronic" coordinate r_{12} used in Hylleraas-type wave functions for positron-hydrogen scattering and it is well known that an expansion which includes all powers of r_{12} converges much faster than an expansion in Legendre polynomials of the cosine of the angle between $\underset{\sim}{r}_1$ and $\underset{\sim}{r}_2$. This polynomial expansion essentially restricts the power of r_{12} to even values. We have seen this demonstrated again in the present problem.

4. Conclusions

Within the restricted framework of our simple model we have examined the zero-energy scattering of ortho-positronium by helium. Short-range correlation terms representing distortion of the Ps atom were effective in bringing about a large improvement in the pickoff annihilation rate, as

compared with experiment. At the same time, the scattering length was significantly reduced.

A model of this kind serves only to indicate a direction for future work. In this case, it suggests that a variational calculation with short-range correlation terms should prove successful in treating the fundamental Ps-He problem, as an extension of the earlier work of Fraser and Kraidy (1966).

We emphasize the importance of the Ps-He system: it is the next step in complexity after the e^+-He system, and is both experimentally and theoretically tractable. Measurements of the quenching rate are already available, as noted above, and the interesting experiments on cavities in liquid helium (Roellig and Kelly, 1967) offer the possibility of measuring the scattering length. We hope that the results reported here will encourage others to examine both theory and experiment more fully.

Acknowledgments

The numerical calculations described in Section 2 and Subsection 3.1 were programmed for the IBM 360 computer by Edward Monasterski.

Table 1. a_v and Z_{eff} for different values of N

N	4	10	20	35	56	84
a_v	1.448	1.396	1.391	1.389	1.389	1.389
Z_{eff}	0.090	0.096	0.096	0.098		

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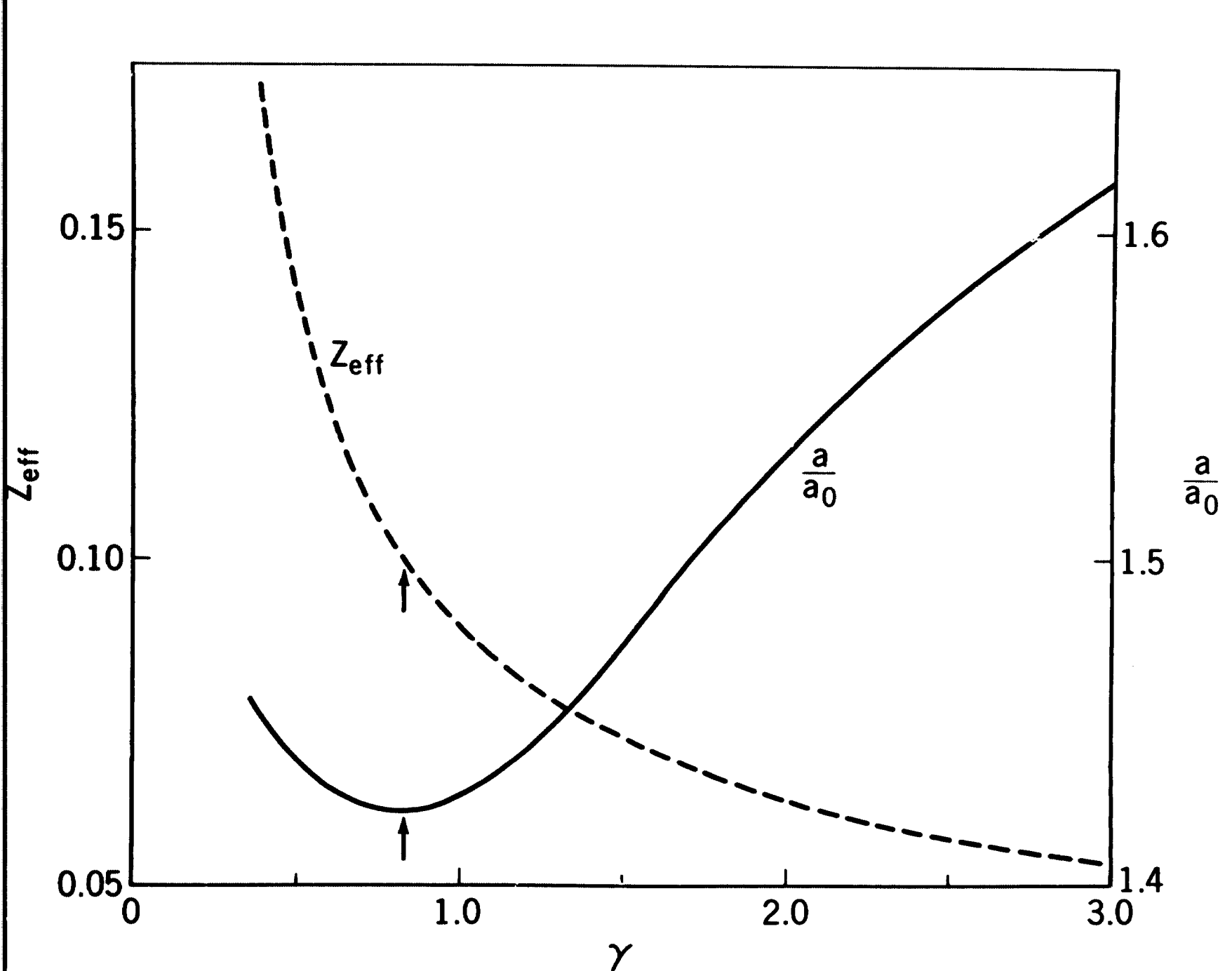
Caption for Figure 1

$\underline{a}$ and Z_{eff} as a function of γ, calculated by the differential equations method.


0.15
0.10
0.05
Z_{eff}
Z_{eff}
$\frac{a}{a_0}$
1.6
1.5
1.4
$\frac{a}{a_0}$
0
1.0
2.0
3.0
γ