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Positron-Atom Scattering by the Kohn and Harris Methods

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The S-wave scattering parameters have been calculated for the e^+-H and e^+-He systems below the positronium-formation threshold. The phase shifts were computed using the Harris variational method, while at zero energy the scattering lengths were obtained by the Kohn variational method. For hydrogen, a generalized Hylleraas wave function with three nonlinear parameters was used, giving an upper-bound scattering length $a \leq -2.10278$, agreeing with Schwartz's result $a \leq -2.10$. An extrapolation procedure gives an estimate of $a = -2.1036 \pm 0.0004$. At nonzero energies, agreement with the lower-bound results of Bhatia, Temkin, Drachman and Eiserike, to better than 0.004 rad is achieved. Since the exact atomic-helium wave function is not known, the situation for helium is less clear; various model-target wave functions are examined using a generalized Hylleraas function with two nonlinear parameters. For the exponential model used by Drachman, the scattering is in close agreement with previous results, but the annihilation-rate parameter Z_{eff} is higher by 15% in poorer agreement with experiment at zero energy.

I. INTRODUCTION

In the study of positron interaction with atoms at low energies, the positron-hydrogen system is most tractable theoretically, while the positron-helium system is much more accessible to experiment. Enough similarity between these two systems exists for the calculational techniques that succeed in the former to be expected to succeed also in the latter. It is thus useful to test proposed theoretical methods in the e^+-H system, and then to apply them to the e^+-He system.

In recent years this has been done several times, using different methods.[1-4] None of these methods was both simple enough to apply to helium and really accurate enough, as judged by comparison with the most definitive work in hydrogen. In addition, the serious problem of the inexactness of the atomic-helium wave function remained unresolved. Nevertheless, the best of these calculations[1,4] are now roughly in agreement with the best recent measurements,[5-7] and there is considerable interest in more extensive and exact calculations of cross sections and annihilation rates.

In this paper we report some new results for positron-atom scattering systems, calculated variationally. In Sec. II, the generalized Hylleraas type of scattering function is described and applied to Kohn variational calculations for zero energy and Harris calculations for higher energies. In Sec. III, S-wave scattering from atomic hydrogen below the positronium threshold is considered, and the results are compared with previous ones. In Sec. IV, the corresponding problem for helium is treated. Since the helium ground state is not known exactly, ambiguities in the formulation of scattering approximations exist. A technique is described which involves a model Hamiltonian corresponding to the approximate ground-state wave function assumed. Using this technique, the S-wave scattering parameters are computed and compared with previous results; at zero energy only, the annihila-

tion-rate parameter Z_{eff} is also evaluated.

II. VARIATIONAL METHODS

Both of the variational methods to be discussed here use trial functions of the following form:

$$\Psi_T = \psi_1 + \tan\eta_T \psi_2 + \Phi,$$
$$\psi_1 = (kx)^{-1} \sin kx \psi_0 , \qquad (1)$$
$$\psi_2 = (kx)^{-1} \cos kx (1 - e^{-\epsilon x})\psi_0,$$

where $\vec{x}$ is the positron coordinate, ψ_0 is the wave function of the atomic target, η_T is an approximate S-wave phase shift, k is the momentum of the positron in atomic units, and Φ is a closed-channel correlation function that vanishes rapidly as $x \to \infty$. (We use atomic units, with energies in rydbergs.)

In the simple case of a hydrogen target, the S-wave function depends only on the three coordinates $x, r, \rho = |\vec{x} - \vec{r}|$, where $\vec{r}$ is the atomic electron coordinate, and $\psi_0 = \pi^{-1/2} e^{-r}$. Then the generalized Hylleraas correlation function takes the form

$$\Phi = \sum_{i=1}^{N} c_i \chi_i , \qquad (2)$$

where

$$\chi_i = e^{-(\alpha\rho + \gamma r + \delta x)} x^l r^m \rho^n,$$

i represents the set of integral exponents (lmn), and the three parameters (α, γ, δ) can be adjusted to optimize the results, subject to the inequalities $\alpha + \gamma > 0$, $\alpha + \delta > 0$, $\gamma + \delta > 0$ that guarantee convergence of all integrals. (In the case of helium, not all the possible coordinates are used in Φ for simplicity; the details are given in Sec. IV.)

At zero energy ($k = 0$), the Kohn variational principle gives an upper bound[8] on the true scattering length a. In this limit, Eq. (1) becomes

$$\Psi_T = [1 - (a_T/x)(1 - e^{-\epsilon x})]\psi_0 + \Phi , \qquad (3)$$

and the quantity a_V is stationary with respect to variations of all the parameters including a_T. Here we have

$$a \leq a_V = a_T + (4\pi)^{-1} \int \Psi_T [H - E_0] \Psi_T d\tau , \qquad (4)$$

E_0 is the ground-state energy of the target, and $d\tau$ represents integration over the coordinates of the positron and all the electrons.

The Harris method[9] was introduced to overcome a defect in the Kohn variational method at nonzero energies. Schwartz[10] found that, since the method does not give bounds for $k \neq 0$, variation on the nonlinear parameter could yield unreasonable values of the phase shifts. Nesbet[11] has examined the entire question in detail and concludes that the Harris method is a Hulthén variational method, adjusted to eliminate the unsatisfactory phase-shift values. [There has been some confusion concerning this point: The identity with the Hulthén method must be demonstrated by a limiting process as the energy approaches a Harris eigenvalue λ_β (see below), since *at* such an eigenvalue an indeterminate situation occurs.]

The first step in the Harris technique is to diagonalize the Hamiltonian in the space spanned by the N approximating functions defined in Eq. (2). That is, we solve the finite matrix equation

$$[\tilde{H} - \lambda \tilde{S}]\tilde{c} = 0, \qquad (5)$$

where $H_{ij} = \langle \chi_i | H | \chi_j \rangle$ and $S_{ij} = \langle \chi_i | \chi_j \rangle$. The N eigenvectors $\tilde{c}^{(\beta)}$ with corresponding eigenvalues λ_β define N functions Φ_β. If we require Ψ_T to satisfy the Schrödinger equation in the space defined by the N functions Φ_β then

$$\langle \Phi_\beta | [H - E] | \Psi_T \rangle = 0, \qquad (6)$$

and if we further choose $E = \lambda_\beta$, then it follows that the phase shift at that energy satisfies

$$\tan\eta = -\langle \Phi_\beta | [H - \lambda_\beta] | \psi_1 \rangle / \langle \Phi_\beta | [H - \lambda_\beta] | \psi_2 \rangle . \qquad (7)$$

Equation (7) thus gives the phase shift in terms of quadratures, but only for those energies that are determined by the matrix equation (5). By varying the nonlinear parameters in Eq. (2) we can effectively cover the energy region of interest.

III. POSITRON-HYDROGEN SCATTERING

A. $k^2 = 0$

For zero energy, we have repeated Schwartz's calculation,[10] but with the more flexible trial function of Eq. (2), which contains three nonlinear parameters; Schwartz's function corresponds to the case $[\alpha = 0, \ \delta = \gamma = \epsilon]$. The results are summarized in Table I, and show the dependence of a_V on N when $\alpha = 0$, $\gamma = 0.8$, and the other nonlinear parameter is optimized. (We follow the tradition of reporting results at only certain values of N; these correspond to including all non-negative exponents l, m, n, in χ_i such that $l + m + n \leq \omega$, where ω is an integer.) Even for $N = 84$ ($\omega = 6$) the calculation had not converged well enough, and we improved the convergence[10,12] by adding one more term to represent the long-range dipole polarization of the form

$$\chi_{N+1} = c_{N+1}(1 - e^{-\epsilon x})^3 x^{-2}(r + \tfrac{1}{2}r^2) P_1(\hat{x} \cdot \hat{r}) \psi_0(r) . \qquad (8)$$

This strikingly accelerated the convergence, although further addition of an analogous quadrupole term of the form

$$\chi_{N+2} = c_{N+2}(1 - e^{-\epsilon x})^4 x^{-3}(\tfrac{1}{2}r^2 + \tfrac{1}{3}r^3) P_2(\hat{x} \cdot \hat{r}) \psi_0(r) \qquad (9)$$

TABLE I. Convergence of the e^+-H scattering length with increase in N: $\alpha = 0$, $\gamma = 0.8$, optimum δ (near 0.3).

N	4	10	20	35	56	84
$-a_V$	1.0297	1.5279	1.7881	1.8989	1.9635	1.9933

TABLE II. Convergence of the e^+-H scattering length with increase in N; dipole $(N+1)$ and quadrupole $(N+2)$ terms included. The nonlinear parameters used were essentially optimized. The consistency parameter Δ is defined in the text.

N	4	10	20	35	56	84
$-a_V(\alpha=0)$	1.3267	1.9195	2.0544	2.0920	2.1006	2.1027
$\Delta\ (\alpha=0)$	−0.022	0.061	0.077	0.048	0.054	0.048
$-a_V(\alpha\neq0)$	1.9682	2.0621	2.0939	2.10138	2.10229	2.10278
$\Delta\ (\alpha\neq0)$	0.057	0.130	0.069	0.066	0.043	0.034

had no effect except when N was small.

In Table II the results for $\alpha = 0$ and $\alpha \neq 0$ including χ_{N+1} and χ_{N+2} are shown. The convergence in the latter case is faster, but the final result is seen to be about the same: The best value we obtain is $a_V = -2.10278$ (for $\alpha = 0.35$, $\gamma = 0.9$, $\delta = 0.15$) to be compared with Schwartz's value of -2.10. A measure of internal consistency in Kohn variational calculations is $\Delta = (a_V - a_T)/a_T$, which in some sense measures the over-all accuracy of the wave function. A necessary, but not sufficient, condition for an exact result is the vanishing of this quantity. The convergence of Δ with increasing N is also shown in Table II. Besides giving us experience in handling the generalized Hylleraas function which will be useful in computing the scattering length for helium, this calculation confirms the result obtained by Schwartz for hydrogen with a less general trial function.

With the additional speed of convergence afforded by the inclusion of the nonlinear parameter α, we

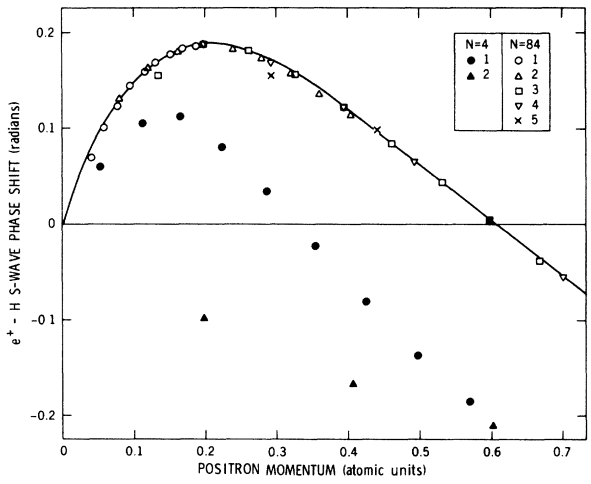

FIG. 1. Positron-hydrogen phase shifts η calculated by the Harris method. Results are shown for the two extreme cases $N=4$ and $N=84$, with $\alpha=0$, $\gamma=1$, and δ varied to vary the energy. For a given value of δ several eigenvalues fall within the elastic scattering range; the various symbols identify their ordering. Lower eigenvalues give more reliable phase shifts than higher ones. The curve represents the result of Ref. 15.

TABLE III. Convergence of a typical e^+-H phase shift η as a function of α: $k=0.4$.

N	20	35	56	84
$\alpha=0$	0.110	0.113	0.115	0.116
$\alpha=0.25$	0.123	0.123	0.123	0.123
$\alpha=0.50$	0.129	0.127	0.127	0.126

can hope to extrapolate the entries in Table II to $N=\infty$ and obtain more significant figures in the scattering length. We used the two difference-fitting formulas

$$a_V(\omega) - a_V(\omega-1) = c\omega^{-p}, \tag{10a}$$

$$a_V(\omega) - a_V(\omega-1) = cp^{\omega}, \tag{10b}$$

where c,p in each case are fitted to the last three entries in Table II. The extrapolated values are $a(\infty) = -2.1038$ and -2.1034, respectively, and we feel justified in quoting a final result $a = -2.1036 \pm 0.0004$.

B. $0 < k^2 < \frac{1}{2}$

We applied the Harris method[9] to the S-wave elastic scattering of positrons from hydrogen at nonzero energies. The wave function used was the same as that in Eqs. (1) and (2), with the minor difference that ϵ appearing in ψ_2 was kept fixed and equal to unity. We first explored the general behavior of the phase shift as a function of δ with $\alpha = 0$ and $\gamma = 1$, which gave a fairly smooth dependence on energy when $N > 20$. Since $E = k^2 - 1$, only those eigenvalues $\lambda \leq -\frac{1}{2}$ were in the elastic scattering region; for each value of δ about five eigenvalues lay in this range. (No stabilization of eigenvalues was found,[13] confirming the conclusion[14,15] that no e^+-H resonances exist below the positronium threshold.)

The phase shifts are shown in Fig. 1, where the individual points were obtained for different values of δ and N as well as different eigenvalues; for small N only the lowest eigenvalue gave reasonable results. A smooth curve representing the phase shifts of Bhatia *et al.*[15] is also shown, and the agree-

TABLE IV. Positron-hydrogen S-wave phase shift η as a function of k.

k	Present work	Schwartz[a] (±0.001)	Bhatia *et al.*[b] (±0.0002)
0.1	0.149	0.151	0.1483
0.2	0.189	0.188	0.1877
0.3	0.169	0.168	0.1677
0.4	0.123	0.120	0.1201
0.5	0.065	0.062	0.0624
0.6	0.008	0.007	0.0039
0.7	−0.049	−0.054	−0.0512

[a]Reference 10.
[b]Reference 15.

ment is quite good.

To make a more direct comparison with other results which are conventionally given at intervals $\Delta k = 0.1$, it is desirable to keep k fixed while increasing the expansion length N. For each value of α it was possible to adjust δ, so that k remained constant to at least three decimal places over the full range $k = 0.1-0.7$. We consider the best value of α to be the one producing the best convergence with N. To illustrate, we show the results for $k = 0.4$ in Table III for three values of α: 0.0, 0.25, and 0.50. Notice that the phase shift remains almost constant for $\alpha = 0.25$, while it converges from below and above for $\alpha = 0.0$ and $\alpha = 0.5$, respectively. We have adopted the values obtained at $\alpha = 0.25$ and $N = 84$ as our best. In Table IV we give these optimum phase shifts along with those of Schwartz[10] and Bhatia *et al.*[15] for comparison. These latter are extrapolated to $N = \infty$ from rigorous lower bounds and are the most accurate e^+-H phase shifts obtained to date. The present results are seen to deviate from the others in the third significant figure, but we consider this sufficiently accurate for the application to helium to be considered below.

IV. SCATTERING BY HELIUM

Since the Kohn variational method at zero energy and the Harris method for positive energies have given satisfactory results for scattering by hydrogen, we would like to apply these methods directly to scattering by helium. However, we cannot follow exactly the same procedure because the ground-state wave function $\psi_0(\vec{r}_1, \vec{r}_2)$ for helium is not known exactly. This means that the Kohn approximation to the scattering length is no longer an upper bound and it is also not clear that we would obtain reliable phase shifts from the Harris method.

Instead we have used a certain technique previously employed by Drachman.[1,4] It restores the zero-energy bounds and the good convergence at nonzero energies by assuming that whatever approximate target wave function we use is an eigenfunction of the atomic-helium Hamiltonian. Formally, we are replacing the true Hamiltonian of the helium system by a model Hamiltonian

$$\bar{H}_0 = -\nabla_1^2 - \nabla_2^2 + U(\vec{r}_1, \vec{r}_2), \tag{11}$$

where the equation

$$(\bar{H}_0 - \bar{E}_0)\psi_0(\vec{r}_1, \vec{r}_2) = 0$$

determines the model potential U in terms of the approximate wave function ψ_0. Then the complete Hamiltonian of the model scattering system is

$$H = \bar{H}_0 - \nabla_x^2 - 2/\rho_1 - 2/\rho_2 + 4/x, \tag{12}$$

where $\rho_i = |\vec{x} - \vec{r}_i|$, and the index $i = 1, 2$ denotes the two atomic electrons.

In principle, one envisions a program consisting of ever more accurate models eventually converging to the true ground state of helium, with the scattering parameters eventually approaching the exact ones. In practice, computational difficulties forced us to use fairly crude models defined by the following five functions in two classes:

Class I:

$$\psi_0(\vec{r}_1, \vec{r}_2) = \mathcal{A} u(r_1)u(r_2),$$

Class II:

$$\psi_0(\vec{r}_1, \vec{r}_2) = \mathcal{A}[u(r_1)v(r_2) + u(r_2)v(r_1)].$$

Three models of class I were examined:

Models A (Ref. 16) and B (Ref. 4):

$$u(r) = e^{-zr}, \quad z_A = 1.6875, \quad z_B = 1.5992;$$

Model C (Ref. 17):

$$u(r) = e^{-zr} + ce^{-2zr}, \quad z = 1.4558, \quad c = 0.6.$$

Two models of class II were examined:

Models D (Ref. 18) and E:

$$u(r) = e^{-pr}, \quad v(r) = e^{-qr}, \quad p_D = 2.1832, \quad q_D = 1.1886;$$

$$p_E = 1.9007, \quad q_E = 1.3457.$$

Functions of class I may be called Hartree-Fock or product functions, while those of class II are known as open-shell functions. Model A gives the lowest variational energy of any exponential form, while model B gives a good value of the helium polarizability[19] ($\alpha = 1.376$). Model C is also determined variationally and fits the numerical Hartree-Fock function well. The parameters in model D minimize the variational energy while permitting the two electrons to occupy different single-particle orbitals. The parameters in model E were chosen by a different procedure, discussed below. It is probable, at least for low positron energies, that the polarizability is the single ground-state property that is most important for obtaining accurate scattering results.

Accordingly, we would like to emphasize those functions giving good values of α; model B gives α exactly, while model A is in error by about 25%. For the other three models, the value of $\langle r^2 \rangle$ is easier to evaluate and is related to α (For A and B one can show that $\langle r^2 \rangle = \alpha^{1/2}$.) In Table V we collect data concerning the five models. On the basis of $\langle r^2 \rangle$ alone, we expect models A and D to be poor, while models B, C, and E should give similar (and better) scattering results; model E was adjusted to give $\langle r^2 \rangle$ exactly.

The last entry in Table V gives the value of k_0^2, the positron energy at the first inelastic threshold *as predicted by the model*. The lowest such threshold for the real positron-helium system is for posi-

TABLE V. Various properties of the five helium-atom models (energies are in rydbergs, polarizabilities in units of $e^2 a_0^3$, and $\langle r^2 \rangle$ in units of a_0^2)

Model	A	B	C	D	E	Exact
Variational energy	−5.695	−5.680	−5.723	−5.751	−5.717	−5.807[a]
Polarizability	1.110	1.376	...	...	...	1.376–1.395[b]
$\langle r^2 \rangle$[c]	1.053	1.173	1.180	1.238	1.19	1.193[a]
Inelastic threshold energy	2.14	1.92	...	0.91	1.31	1.31

[a]C. L. Pekeris, Phys. Rev. 115, 1216 (1959).
[b]Reference 19.
[c]Y. K. Kim and M. Inokuti, Phys. Rev. 165, 39 (1968).

tronium formation, occurring at $k^2 = 1.31$. If we take the model potential seriously, we can let one electronic coordinate approach infinity and compute the ground-state energy $\overline{E}_+$ of the model He^+ ion containing the remaining electron. Then we have

$$k_{Ps}^2 = \overline{E}_+ - \overline{E}_0 - \tfrac{1}{2}, \tag{13}$$

where the true threshold is obtained from $E_0 = -5.807$ and $E_+ = -4$. [Notice that $\overline{E}_0$ is not generally the same as E_0, the variational (Rayleigh-Ritz) energy corresponding to the given wave function and the true Hamiltonian.] For models of class I we have $\overline{E}_+ = \frac{1}{2}\overline{E}_0$, since the two electrons are independent and hence $k_{Ps}^2 = z^2 - \frac{1}{2}$. For models D and E, one electron is more weakly bound than the other; one finds $k_{Ps}^2 = q^2 - \frac{1}{2}$. For models A and B (and probably C) the positronium threshold lies above the first atomic excitation energy $k_{ex}^2 = \frac{3}{4}z^2$, and this lower energy appears in the table. For model D the positronium threshold lies below the true threshold and we cannot expect reasonable results between these two energies. The parameter q in model E was adjusted to give k_{Ps}^2 exactly, leaving p free to give $\langle r^2 \rangle$ correctly as mentioned above.

A. $k^2 = 0$

We have used essentially the same trial function as in Sec. III with the exceptions that ψ_0 was replaced by one of the approximate forms for helium, the short-range correlation functions χ_i given by Eq. (2) were made symmetric with respect to the coordinates r_1 and r_2 of the helium electrons, and

TABLE VI. Zero-energy positron-helium results for five different models. For each model, the convergence of a_V vs N is shown, and for some cases Z_{eff} and Δ are also given. Note especially the improved convergence of a_V when the long-range polarization term is added and the similarity between models B, C, and D. Quantities marked (*) were computed without the long-range polarization term [Eq. (15)], those marked (+) included this term, and those marked (‡) also took account of the x^{-2} term of Eq. (17). This last term only improved Δ but did not affect a_V or Z_{eff}.

N	4	10	20	35	56	84
			Model A ($z = 1.6875$)			
a_V(*)	−0.025	−0.226	−0.277	−0.313	−0.327	−0.340
a_V(‡)	−0.236	−0.376	−0.396	−0.401	−0.402	−0.402
Z_{eff}(‡)	2.203	3.326	3.621	3.809	3.843	3.878
Δ(‡)	−0.006	0.043	0.002	0.006	0.000	0.003
			Model B($z = 1.5992$)			
a_V(*)	−0.165	−0.288	−0.413	−0.444	−0.473	−0.485
a_V(+, ‡)	−0.302	−0.488	−0.516	−0.522	−0.524	−0.524
Z_{eff}(*)	2.242	2.677	3.583	3.745	4.112	4.126
Z_{eff}(+, ‡)	2.323	3.695	4.039	4.251	4.289	4.326
Δ(+)	0.347	0.107	0.114	0.084	0.077	0.063
Δ(‡)	0.067	0.035	−0.003	0.008	−0.002	0.005
			Model C (Hartree-Fock)			
a_V(*)	−0.157	−0.303	−0.435	−0.471	...	...
			Model D (Open shell)			
a_V(*)	−0.186	−0.399	−0.516	−0.559	−0.580	...
Z_{eff}(*)	2.182	2.766	3.740	3.969	4.347	...
			Model E (New open shell)			
a_V(*)	−0.199	−0.349	−0.446	−0.481	−0.499	...
Z_{eff}(*)	2.192	2.671	3.493	3.679	4.016	...

we omitted the $e^{-\alpha\rho}$ factor to simplify the integrals. In the first instance we used

$$\chi_i = e^{-\delta x} x^l (e^{-\beta r_1} r_1^m \rho_1^n + e^{-\beta r_2} r_2^m \rho_2^n) \psi_0(\vec{r}_1, \vec{r}_2). \quad (14)$$

Later we made this slightly more general by including factors like r_{12}^ν where $r_{12} = |\vec{r}_1 - \vec{r}_2|$, but this did not make any significant difference to the final result.

Various explorations were made at zero energy of the five models described above. We discuss them in general here and give the results in Table VI. Most thorough work was done on models A and B; models C and E were indeed very similar to B as we anticipated while model D seemed to be less satisfactory (see Table V). The following describes the sequence of calculations:

(i) Keeping the parameter β fixed at zero, we varied δ with up to 84 terms in the trial function and found slow convergence of a_T as in the case of hydrogen (Table I).

(ii) We then added a term to represent the long-range dipole polarization of the form [see Eq. (8)]

$$\chi_{N+1} = c_{N+1}(1 - e^{-\epsilon x})^3 x^{-2}[(r_1 + b r_1^2) P_1(\hat{x} \cdot \hat{r}_1) + (r_2 + b r_2^2) P_1(\hat{x} \cdot \hat{r}_2)] \psi_0(\vec{r}_1, \vec{r}_2), \quad (15)$$

where perturbation theory gives $b = \frac{1}{2} z$ for models A and B. Including this term again accelerated the convergence to a satisfactory degree.

(iii) We also calculated Z_{eff}, an effective electron number which is proportional to the annihilation rate of zero-energy positrons in helium. This parameter is more easily measured experimentally than the scattering length (or cross section) so we compute Z_{eff} in order to compare with experiment.

Z_{eff} essentially measures the probability that the positron and one of the electrons are at the same point and is given by

$$Z_{eff} = \int |\Psi_T(\vec{x}, \vec{r}_1, \vec{r}_2)|^2 [\delta(\vec{x} - \vec{r}_1) + \delta(\vec{x} - \vec{r}_2)] d\tau. \quad (16)$$

These are also listed in Table VI and are seen to converge from below to values close to 4.

(iv) The computation of Z_{eff} requires detailed knowledge of the wave function. Although the addition of χ_{N+1} gives excellent convergence for a_T, the wave-function quality parameter Δ is not as satisfactory. We therefore added the long-range open-channel term

$$f = d(1 - e^{-\epsilon x})^3 x^{-2} \psi_0(\vec{r}_1, \vec{r}_2) \quad (17)$$

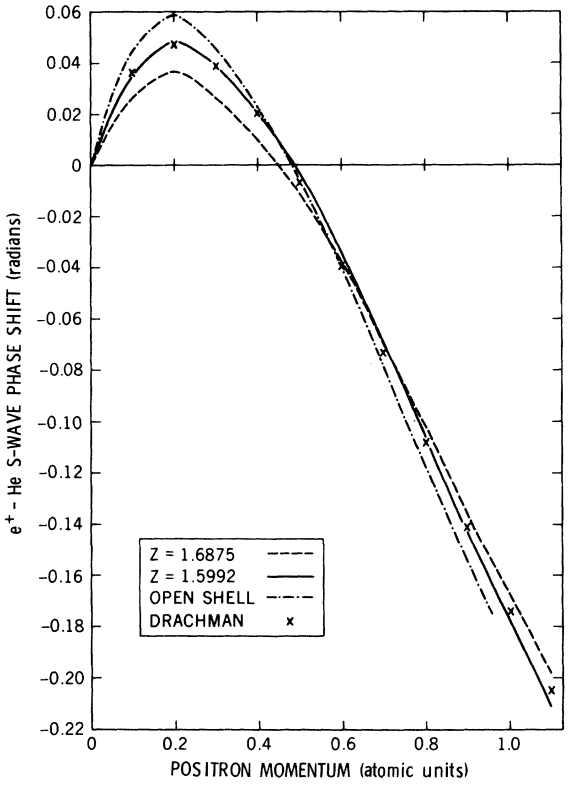

FIG. 2. Positron-helium phase shifts η calculated by the Harris method, for the following three models: A ($z = 1.6875$), B ($z = 1.5992$), D (open shell). The crosses are the results of Ref. 4 for model B. No results are given above the spurious threshold for model D, while model E was omitted for clarity; it is very similar to model B.

TABLE VII. Comparison at $k^2 = 0$ of the present positron-helium results for model B with previous variational and nonvariational results. The experimental value of Z_{eff} also appears.

	Nonvariational	Variational[a]	Present	Expt[b]
a	-0.659[a]	-0.511	-0.524	...
Z_{eff}	6.3[c]	3.7	4.3	3.677 ± 0.025

[a] Reference 4.
[b] Reference 5 (see also Refs. 6 and 7).
[c] R. J. Drachman, Phys. Rev. 150, 10 (1966).

TABLE VIII. Positron-helium S-wave phase shifts for model B, compared with previous results (Ref. 4).

k	Present	Variational	Nonvariational
0.1	0.035	0.036	0.050
0.2	0.049	0.047	0.072
0.3	0.039	0.039	0.071
0.4	0.020	0.020	0.056
0.5	−0.003	−0.007	0.032
0.6	−0.034	−0.039	0.002
0.7	−0.069	−0.073	−0.031
0.8	−0.106	−0.107	−0.066
0.9	−0.143	−0.141	−0.100
1.0	−0.177	−0.174	−0.133
1.1	−0.211	−0.205	−0.166

and obtained much better convergence of Δ towards zero. No change was observed in a_V or Z_{eff} when this term was added. c_{N+1} and d were treated as free variational parameters and the fact that they turned out very close to the perturbation values is another indication of consistency.

(v) We then permitted the parameter β of Eq. (14) to take nonzero values, but found the minimum a_V to differ only in the fifth significant figure from its value at $\beta = 0$. As mentioned above, inclusion of factors like r_{12}^{ν} changed a_V very little.

We have already indicated that we consider model B to be the most satisfactory of those treated here, at least for low energies. Drachman has previously examined this model both nonvariationally[1] and by a less extensive variational method.[4] In Table VII we show comparisons between these methods and the present method for the scattering length and Z_{eff}; a good recent experimental value of the latter is also shown.[5] (Notice too that model A gives Z_{eff} in better agreement with experiment.)

B. $k^2 \neq 0$

We applied the Harris method[9] to models A, B, D, and E in the manner described in Sec. III B, using the function of Eq. (14) with $\beta = 0$. The results are given in Fig. 2 and Table VIII and compared with those of Ref. 4. When we examined the values of λ obtained, we found one stabilized eigenvalue,[13] representing a resonance at $k = 1.05$ for model D; this lies between the exact and model thresholds (see Table VII) and is to be disregarded. For models A and B, one resonance appeared just below the inelastic threshold. This represents the first of the well-known hydrogenic resonances[20] which lie below the $n = 2$ states; here they are of academic interest only, since the models distort the level structures considerably.

The argument favoring model B (or C) at low energy may not hold at higher energy. Nevertheless, model E is very similar to B at all energies up to the positronium threshold, and there is no indication of any unusual behavior; for clarity we have omitted the results from Fig. 2. We consider that the envelope of the curves shown in Fig. 2 should be considered to be the result of the present calculation at the higher energies above the point where the curves cross the horizontal axis.

V. SUMMARY AND CONCLUSIONS

The Kohn and Harris methods have been applied successfully to the problems of positron scattering from hydrogen and helium atoms at low energies. In hydrogen, good agreement with previous results was found, and an improved scattering length was obtained.

In helium, the problem of the inexact target wave function was approached by introducing a sequence of model atomic Hamiltonians corresponding to certain simple variationally obtained wave functions. Those functions whose polarizability is close to the correct value are expected to give good low-energy scattering results. At higher energies, the excitation spectrum may also be important.

We note that our scattering results for the helium model previously treated in Refs. 1 and 4 are in very close agreement with the variational treatment rather than the nonvariational method. Although we have treated the S-wave phase shifts only, this result reduces the low-energy cross section by a factor of about $\frac{2}{3}$ and raises the high-energy cross section significantly, compared to those reported in Ref. 1. Nevertheless, the model is crude, and better ones become progressively more difficult to handle.

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Total Cross Sections for Inelastic Scattering of Charged Particles by Atoms and Molecules. VI. Metastable Helium†

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Sum rules for the asymptotic Born cross sections have been applied to the evaluation of various inelastic-scattering cross sections of metastable He ($2\,^1S$ and $2\,^3S$). The ionization cross sections for the two species are similar in magnitude, and each constitutes only a small part of the total cross section for inelastic scattering. Although the first Born approximation is inappropriate for the scattering of slow charged particles, the energy dependence exhibited in the recent experiment by Long and Geballe for the ionization of He ($2\,^3S$) by low-energy electrons (≤ 16 eV) is compatible with the high-energy behavior predicted by the theory. The exchange correction evaluated from the Mott formula has been included in the ionization cross section by electron impact. Optical oscillator strengths for the first three transitions to doubly excited states [$2\,^1S \rightarrow (2lnl')^1P$] are also given.

I. INTRODUCTION

Rigorous applications of the Bethe procedure[1-3] to obtain various inelastic-scattering cross sections so far have been restricted to one- and two-electron atoms in the ground state.[4] The theory is not restricted to the ground state, and in this paper we present an example of its application to metastable He in the $2\,^3S$ and $2\,^1S$ states. Moreover, these metastable species have open-shell structure, and serve as a prototype for the application of the theory to complex atoms.

The Bethe procedure in its extended form[4] provides an asymptotic expression for the total cross section for inelastic scattering

$$\sigma_{\text{tot}} = A\,(\ln T)/T + B/T + C/T^2 + \cdots , \qquad (1)$$

where A, B, and C are constants determined solely from the properties of the target atom and T is proportional to the square of the incident particle velocity. The constants A and C are readily calculated from the initial-state wave function of the atom. To determine B, however, the oscillator-strength distribution (OSD) must be known, in addition to the initial-state wave function.[1,3] When the cross section is given in the form of Eq. (1) with only two constants A and B, we shall refer to it as the Bethe cross section.

For metastable He, various wave functions and expectation values derived from them are available in the literature.[5] We have used the correlated wave functions determined by Weiss.[6] As was shown earlier,[7] the Weiss wave functions are in many ways as reliable as the Pekeris wave functions.

The OSD of metastable He, however, has many uncertainties. Theoretical or experimental data on the OSD of higher continua such as $(\text{He}^* \rightarrow \text{He}^{++} + 2e)$ are not available. The data for the autoionizing states are very scarce.[8] On the other hand, there are many qualitative aspects which are shared by the $2\,^3S$ and $2\,^1S$ states of He, particularly in the OSD. These features. including the uncertainties in the OSD's, are expected to be common in complex atoms, and the experience gained in the present investigation should provide a valuable guide for future applications.

Individual cross sections can also be written in the form of Eq. (1) with three constant – we shall call such expressions the Born asymptotes – which are determined from the generalized oscillator strength (GOS).[7,9] By subtracting the sum of the Born asymptotes for the discrete excitations from the total cross section, we get the Born asymptote for ionization. The ionization cross section thus obtained represents a simple sum of cross sections for all events leading to ionization and is known as the counting ionization cross section. The Born asymptotes for ionization have been further improved by adding the correction for electron