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Elastic Collisions Of Positrons With Helium

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ELASTIC COLLISIONS OF POSITRONS WITH HELIUM

by

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ABSTRACT

The S-wave elastic scattering and annihilation of positrons by helium atoms in the energy region below the positronium formation threshold are studied. The correlation method has been employed in order to construct an optical potential from a set of short ranged correlation terms which represent the closed channel part of the trial function. Furthermore by applying the "method of models" of Drachman (1972b), the phase shift (scattering length) is a lower (upper) bound to the exact one of the modified Hamiltonian. The accuracy of the final results is within the reliability of the helium models. Four helium wave functions (one-parameter Hylleraas type and Hartree-Fock type) have been employed and up to 84 correlation terms are used. It has been found that the monotonicity theorem indeed applies and satisfactory convergence is obtained as the number of correlation terms is increased. However, the final results from the best model (a three-parameter Hartree-Fock wave function with correct polarizability) do differ not insignificantly from Humberston's (1973) model H5. The results are discussed in relation to those of other calculations and those of experiment.

The integro-differential equation for the radial

function was first converted into an integral equation by use of a Green's function, and the numerical functional values of the radial equation were then obtained by solving a system of linear equations. Phase shifts (scattering lengths) are hence obtained from the solution of the radial equation. The scattering wave function also has been applied to calculate the parameters of annihilation of positrons by helium atoms, i.e. the effective charge; the positron-electron cusp value and the probabilities of finding the residual He^+ ion in different ionic states after annihilation. All the numerical computations were performed on a CDC cyber/73 computer.

The four variants of Peterkop and Rabik (1971) also have been applied to the e^+-He system. The eigenvalues of the true Hamiltonian of the e^+-He system have been examined in the context of stabilization. It is found that one eigenvalue seems to be stable and this may correspond to a possible e^+-He resonance at 20.375 eV which is just below the first singlet helium excitation at 20.6 eV. However, this indication of the resonance is still yet to be confirmed.

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CHAPTER 1

INTRODUCTION

1.1 General Review

There has been some interest in using the positron in various branches of physics ever since its existence was predicted by Dirac (1928) and it was experimentally discovered by Anderson (1933). In particular, atomic physicists are interested in positron collisions with gaseous atoms. The results can provide more understanding about the processes of atomic scattering.

In calculations in scattering problems, there are some differences between the electron and positron cases. There are no exchange terms involving the incoming positron and the target electrons. Moreover, the mean static field of the atom repels a positron but the polarization force is attractive regardless of the charge of the projectile. These two forces will tend to cancel each other and hence a positron scattering calculation is very sensitive to the effective potential. Another difference is that the positronium channel will open if the energy is high enough (17.8 eV or more in helium). Positronium is a bound state of electron

and positron with a life time about 10^{-9} sec if their spins are parallel, and 10^{-10} sec if their spins are antiparallel. The virtual positronium effect or positron-electron correlation is important in low energy collisions.

Theoretically, the simplest target system is hydrogen; experimentally, positron-argon is more manageable and has been very popular. Therefore, positron-helium seems to become the compromise system between theory and experiment. There have been some review articles concerning positron atom scattering. Fraser (1968) (and references contained therein) and Massey (1971) provide a general review for positrons in gases; Bransden (1969) and Drachman and Temkin (1972) outline different theoretical methods in positron collision problems; Drachman (1972a) and McGowan (1972) gave progress reports on positron collisions in the aspects of theory and experiment respectively; Coleman, Griffith, Heyland and Killeen (1974) summarized the most recent developments, mainly in experimental work, in low energy positron interactions with gaseous atoms and molecules.

1.2 Experimental Background

Generally, two types of experiments have been carried out. The first type is the swarm experiment; the second

type is the beam experiment and has been intensively applied to gases in recent years.

The references to early experiments may be found for example in the article by Fraser (1968). The studies of annihilation (measured by Z_{eff}, the effective charge) of a free positron with a bound electron have been done by swarm experiments. The effective charge of the positron-helium† system has been determined mainly at two energies. At 77°K, they range from 3.68 by Leung and Paul (1968) to 3.96 by Roellig and Kelly (1967). At room temperature, they are ranged from 3.63 by Lee, Orth and Jones (1969) to 3.94 by Coleman, Griffith, Heyland and Killeen (1974). Tao and Kelly (1969) taking the average value between 4.2°K and 300°K, obtained an effective charge 3.84.

While swarm experiments permit studies of annihilation and indirect measurement of the cross sections for total momentum transfer at thermal energy (i.e. Leung and Paul 1968, Tao and Kelly 1969), it does not tell much of the higher energy behavior of the system. On the other hand, beam experiments in which the energy distribution is narrow

†If the positron motion were undistorted by the helium atom, the effective charge would be 2, the number of electrons in the helium atom; this leads to the so-called Dirac rate when used in equation (4.1).

and controllable, is more effective in measuring the total cross section above 2 eV. Costello, Groce, Herring and McGowan (1972) using a beam measured the total cross section up to 26 eV. There are several other groups which have been engaging in positron-helium beam experiments, e.g. the University of Toronto group (Jaduszliwer, Keever and Paul 1972; Jaduszliwer and Paul 1973, 1974; Jaduszliwer, Nakashima and Paul 1975) has measured the total cross section from 4 to 270 eV. The energy region from 2 to 400 eV has been measured by the University College group (Canter, Coleman, Griffith, and Heyland 1972, 1973). They are in relative agreement for the energy region between 20 to 30 eV, but they are in disagreement at energies below the formation threshold. Recently, the total cross section for the scattering of 50-400 eV positrons by helium has also been measured by Dutton, Harris and Jones (1975).

The measurement by Canter, Coleman, Griffith and Heyland (1973) up to 400 eV enabled Bransden, Hutt and Winters (1974) to check the consistency of the experimental results by using a sum rule based on the forward dispersion relation. They concluded that the experimental data were too low for the energy region before the Born approximation is valid. Coleman, Griffith, Heyland and Killeen (1974) presented corrected total cross sections and they are in better agreement with theoretical

estimates at high energies. Furthermore, Bransden and Hutt (1975) tested these new measurements and those by Jaduszliwer, Nakashima and Paul (1975). These authors also compared the real part of the forward scattering amplitude with some theoretical calculations.

1.3. Theoretical Background

In one of the earlier theoretical calculations, Massey and Moussa (1958) considered positron-helium scattering in a mean static approximation using a numerical Hartree-Fock field. Kestner, Jortner, Cohen, Rice (1965) used a pseudo-potential approach in both e^- and e^+ - He scattering. Kraidy (1967) and Kraidy and Fraser (1967) considered this problem by using coupled static approximation (both helium and positronium ground state). They employed a one parameter Hylleraas target wave function. Wardle (1973) extended their work by using a Hartree-Fock wave function and found that the results are very different when different helium wave functions were used. Recently, Ho, Fraser and Kraidy (1975) qualitatively confirmed Wardle's (1973) observation by examining five helium ground state wave functions. However, their numerical results differed from those of Wardle. Furthermore, these authors pointed out that with a more elaborate helium function, the result is more qualitatively in

accord with the corresponding hydrogen problem (Cody, Lawson, Massey and Smith 1964, Chan 1972).

The effect of inexact target wave functions has been the subject of recent investigation. Peterkop and Rabik (1971) examined four variants of Kohn's variational principle in an e^- and e^+ - H scattering length calculation, and found that violently varying results could be obtained if the target wave function is inexact. Houston (1973) extended their calculation to an e^+ - He scattering length calculation and concluded that the singularities persist.

In order to recover the bound theorem, Drachman (1972b) employed an idea of Lee and Christan (1954) and suggested the "method of models" for elastic scattering problems where inexact target wave functions have to be employed and exchange plays no part. Using the method of models, Drachman (1966a) employed the adiabatic approximation to e^+ - He scattering; Houston and Drachman (1971) used Kohn's method at zero energy and the Harris method (Harris 1967) in non-zero energy calculation using five helium models. These authors considered that the target wave function which bears the correct polarizability gave the best result. Recently, Ho and Fraser (1975) considered the importance of being correctly polarizable for the target wave function. They

found that even in a method of models calculation, unrealistic results could be obtained if the target atom is over-polarizable. Furthermore, they confirmed that the target being correctly polarizable is an important consideration in low energy scattering.

Other recent positron helium calculations include Drachman's variational calculation (Drachman 1968, 1969) and semi-phenomenlogical analysis (Drachman 1971). Humberston (1973) employed the method of models and Kohn's algebraic method to an S wave e^+ - He calculation using a five parameter helium wave function which bears essentially the correct polarizability. Aulenkamp, Heiss and Wichman (1974) used Kohn's method (variant I termed by Peterkop and Rabik 1971) to calculate phase shifts up to $\ell = 3$.

A rigorous stationary upper bound of e^+ - He scattering length is 0.796 calculated by Blau, Rosenberg and Spruch (1975) and a rigorous lower bound, -0.7 is evaluated by Hahn and Spruch (1974) using the adiabatic approximation. As an example of the utilization of these bounds, we note that the scattering length of the coupled static approximation by Kraidy (1967) who used a one parameter Hylleraas wave function, is less than -0.7 and hence the lower bound is violated. A refinement of upper bound calculation, however, at this stage is difficult to implement.

1.4 The Scope and Contents of the Thesis

Humberston's (1973) zero energy calculation is an upper bound to the exact scattering length within the reliability of the helium wave function. There is no bound theorem to the phase shifts obtained from Kohn's algebraic method. Moreover, it is possible that a Schwartz (1961b) type singularity may be encountered. It is the purpose of this thesis to investigate positron-helium elastic scattering using the correlation method together with the method of models. It should be mentioned that the most rigorous positron-hydrogen elastic scattering results have been obtained by Bhatia, Temkin, Drachman and Eserike (1971) using the correlation method. These authors constructed an optical potential by a projection operator such that the correlation terms are orthogonal to the open channel part of the wave function. Following the argument of Burke and Taylor (1966), the bound principle is valid as long as the closed channel part vanishes asymtotically. Furthermore, by applying the method of models of Drachman (1972b), the bound theorem is retained and the accuracy is within the reliability of the helium models.

Four helium wave functions have been examined in this thesis. Two are one-parameter Hylleraas type wave functions

and two are of Hartree-Fock type. These wave functions are relatively simple but we believe that the present method will lead to more definitive phase shifts when more accurate helium wave functions are employed. Moreover, two of the target wave functions bear the correct polarizability. This physical parameter has been emphasized by Drachman (1966a), Houston and Drachman (1971) and Humberston (1973). Its importance in low energy collisions has been confirmed by Ho and Fraser (1975).

In Chapter 2, we present the formulations of the optical potential and bound theorem as well as the method of models. We discuss the method of solution in Chapter 3. Chapter 4 is mainly about positron annihilation with the helium atom. Results are shown in Chapter 5 where the comparison with experiments and other calculations are made. Some problems related to the present calculation are discussed in Chapter 6. For example, different variants of Peterkop and Rabik (1971) have been applied to the e^+ - He problem. The eigenvalues of the true Hamiltonian have been examined in the context of the stabilization method. A possible resonance below the first singlet helium excitation threshold is discussed. In Chapter 7, we summarize the work of this thesis. Some possible future work is discussed in the concluding remarks.

CHAPTER 2

THEORY AND FORMULATION

2.1 The Schroedinger Equation

The Schroedinger equation for the positron-helium system is

$$(H-E)\Psi = \left(-\frac{\hbar^2}{2m}\nabla_p^2 + \frac{2e^2}{r_p} - \frac{e^2}{r_{1p}} - \frac{e^2}{r_{2p}} + H_o - E\right)\Psi(\underline{r}_1, \underline{r}_2, \underline{r}_p) = 0 \quad (2.1)$$

We assume the nucleus is infinitely massive and is fixed at the origin of the coordinate system, $\underline{r}_i$ and $\underline{r}_p$ are the position vectors of electrons and positrons respectively and $r_{ip} = |\underline{r}_i - \underline{r}_p|$ with $i = 1,2$. For a scattering problem the total energy E of the system may be written as $E = E_o + \frac{\hbar^2 k^2}{2m}$ where $\frac{\hbar^2 k^2}{2m}$ is the kinetic energy of the incoming positron; H_o and E_o are the Hamiltonian and energy of the helium atom respectively.

Throughout this thesis, atomic units in which $\hbar = 2m = \frac{1}{2}e^2 = 1$ are used. The unit of length is a_o, the Bohr radius of hydrogen ($a_o = 0.53 \times 10^{-8}$ cm); the unit of energy is the rydberg ≈ 13.6 eV; cross sections are in $\pi a_o^2 = 8.8 \times 10^{-17}$ cm^2. Using these atomic units, equation (2.1) becomes

$$(-\nabla_p^2 + \frac{4}{r_p} - \frac{2}{r_{1p}} - \frac{2}{r_{2p}} - k^2 + H_o - E_o)\Psi(\underline{r}_1, \underline{r}_2, \underline{r}_p) = 0 \qquad (2.2)$$

where the true Hamiltonian for the helium atom is

$$H_o = -\nabla_1^2 - \nabla_2^2 + \frac{2}{r_{12}} - \frac{4}{r_1} - \frac{4}{r_2} \qquad (2.3)$$

When a positron collides with a ground state helium atom different channels could be open depending upon the energy of the incoming positron, e.g.:

$e^+ + He(1^1S) \rightarrow e^+ + He(1^1S)$ (elastic) (2.4a)

$\rightarrow Ps + He^+ - 17.8eV$ (positronium formation) (2.4b)

$\rightarrow e^+ + He(2^1S) - 20.6eV$ (excitation of first singlet state of helium) (2.4c)

$\rightarrow Ps(n=2) + He^+$ (excited positronium formation) (2.4d)

$\rightarrow e^+ + He^+ + e^- - 24.6eV$ (ionization) (2.4e)

with possibly $e^+ + He \rightarrow (He, e^+)$ compound state $\rightarrow He^* + e^+$ (2.4f)

Elastic scattering only, in the S-state particularly, is considered in this thesis.

2.2 Wave Function in the Asymptotic Region

For elastic scattering, the asymptotic behavior of the total wave function Ψ in equation (2.1) is

$$\Psi \underset{r_p\to\infty}{\sim} \psi_o(\underline{r}_1,\underline{r}_2)F(\underline{r}_p) \tag{2.5}$$

where $\psi_o(\underline{r}_1,\underline{r}_2)$ is the ground state of the helium atom and satisfies the following equation

$$(H_o-E_o)\psi_o(\underline{r}_1,\underline{r}_2)=(-\nabla_1^2-\nabla_2^2+\frac{2}{r_{12}}-\frac{4}{r_1}-\frac{4}{r_2}-E_o)\psi_o(\underline{r}_1,\underline{r}_2)=0. \tag{2.6}$$

The function $F(\underline{r}_p)$ is asymptotically the solution of the free particle Schroedinger equation.

$$(-\nabla_p^2-k^2)F(\underline{r}_p)=0 \tag{2.7}$$

$$\text{with} \quad F(\underline{r}_p) \underset{r_p\to\infty}{\sim} e^{i\underline{k}\cdot\underline{r}_p}+f_k(\theta)\frac{e^{ikr_p}}{r_p}. \tag{2.8}$$

For S wave scattering, we have (to a multiplicative constant)

$$F(\underline{r}_p) \underset{r_p\to\infty}{\sim} \sqrt{\frac{m}{k}}\ \frac{1}{r_p}\{\sin(kr_p)+\tan\eta_o\cos(kr_p)\} \tag{2.9}$$

where η_o is the S wave phase shift. In equation (2.8), $f_k(\theta)$ is the scattering amplitude and θ is the scattering angle, and

$$f_k(\theta) = \sum_{\ell=0} \frac{1}{2ik}(e^{2i\eta_\ell}-1)(2\ell+1)P_\ell(\cos\theta) \tag{2.10}$$

where η_ℓ is the phase shift of the ℓth partial wave. For

forward scattering in which $\theta = 0$, we have

$$\text{Re } f_k(0) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2k} \sin 2\eta_\ell \qquad (2.11a)$$

$$\text{Im } f_k(0) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2k} \sin^2 \eta_\ell \qquad (2.11b)$$

The total cross section is given by

$$\sigma_{tot} = \frac{4}{k^2} \Sigma (2\ell+1) \sin^2 \eta_\ell \qquad (\text{in } \pi a_o^2) \qquad (2.12)$$

Recently, Bransden and Hutt (1975) have carried out a study of experiments and theories for the e^+-He system. The measurements of the total cross sections (e.g. Jaduszliwer, Nakashima and Paul 1975; Canter, Coleman, Griffith and Heyland 1973) have been tested for consistency with a sum rule based on the forward dispersion relations. The real parts of the forward scattering amplitude (denoted as Re $f_k(0)$) calculated by these authors from a mixture of experimental and theoretical cross sections can be compared with theoretical calculations (equation 2.11a). It appears that Re $f_k(0)$, like the cross sections, serves as a meeting place between experiment and theory.

2.3 Optical Potential and Bound Theorem

The trial wave function is taken as

$$\Psi^t(\underline{r}_1,\underline{r}_2,\underline{r}_p) = \psi_o(\underline{r}_1,\underline{r}_2)F^t(\underline{r}_p) + \sum_i^N C_i\chi_i(\underline{r}_1,\underline{r}_2,\underline{r}_p) \qquad (2.13)$$

$$\text{with} \quad r_p F^t(r_p) \underset{r_p\to\infty}{\sim} \sqrt{\frac{m}{k}}\{\sin(kr_p)+\tan\eta_o^t\cos(kr_p)\} \qquad (2.14a)$$

$$r_p F^t(r_p) \underset{r_p\to 0}{\sim} 0 \qquad (2.14b)$$

The first term of the right hand side of equation (2.13) represents the open channel part of the wave function. The second term represents the closed channel part of the wave function and χ_i's are so-called short range correlation functions through which short range distortion effects are taken into account.

From the Kohn variational principle applied to the trial wave function Ψ_t

$$\delta[\langle\Psi_t|H-E|\Psi_t\rangle - \tan\eta_o^t] = 0 \qquad (2.15)$$

where the variation is taken with respect to F^t and C_i, we obtain the following coupled integro-differential and algebraic equations

$$\langle\psi_o(\underline{r}_1,\underline{r}_2)|H-E|\psi_o(\underline{r}_1,\underline{r}_2)F^t(\underline{r}_p)+\sum_i^N C_i\chi_i(\underline{r}_1,\underline{r}_2,\underline{r}_p)\rangle=0 \qquad (2.16a)$$

$$\langle\chi_j(\underline{r}_1,\underline{r}_2,\underline{r}_p)|H-E|\psi_o(\underline{r}_1,\underline{r}_2)F^t(\underline{r}_p)+\sum_i^N C_i\chi_i(\underline{r}_1,\underline{r}_2,\underline{r}_p)\rangle=0 \qquad (2.16b)$$

In order to establish a bound theorem on $\tan \eta_0$, following Gailitis (1965), we define projection operators P and Q=1-P, such that $P\Psi \underset{r_p \to \infty}{\sim} \psi_0 F(r_p)$. We take $P=|\psi_0><\psi_0|$, where ψ_0 is the ground state wave function. From the asymptotic behavior of the projection, one could say that P projects out the open part of a wave function and Q, the closed.

The Schroedinger equation for the exact Ψ may be written as

$$P(H-E)(P+Q)\Psi=0 \tag{2.17}$$

$$Q(H-E)(P+Q)\Psi=0 \tag{2.18}$$

We obtain, by eliminating $Q\Psi$,

$$P(H-E+V_{opt})P\Psi=0 \tag{2.19}$$

where $$V_{opt}=P(H-E)Q\frac{1}{Q(E-H)Q}Q(H-E)P \tag{2.20}$$

If E is less than the lowest eigenvalue of the operator QHQ, V_{opt} is negative and hence phase shifts increase from the lower bound static approximation ($V_{opt}=0$).

In practice we use an incomplete Q, Q^t, to construct an approximate potential. We introduce an operator

$$M=|\psi_0><\psi_0|+\sum_i |\xi_i><\xi_i| = P + Q^t \approx 1 \tag{2.21}$$

where ξ_i is an orthonormal set which can be constructed from the linearly independent set χ_i of equation (2.13). By requiring Ψ satisfy

$$M(H-E)M\Psi=0, \tag{2.22}$$

instead of obtaining equations (2.19) and (2.20), we get

$$P(H-E+V_{opt}^{t})P\Psi=0 \tag{2.23}$$

with $$V_{opt}^{t}=P(H-E)QM\frac{1}{MQ(E-H)QM}MQ(H-E)P. \tag{2.24}$$

Gailitis (1965) has proved that $V_{opt}^{t} \geq V_{opt}$ if E is less than the lowest eigenvalue of QHQ, hence $\eta_o^t < \eta_o^{exact}$, and the bound theorem is established. Furthermore, following the argument of Burke and Taylor (1966), χ_i need not be made orthogonal to the open channel space. As long as they vanish asymptotically and do not affect the asymptotic behavior of $F(r_p)$, the bound theorem is retained. Equation (2.23) is equivalent to equation (2.39) which is obtained later in this chapter as a rewriting of equations (2.16).

2.4 The Method of Models

The bound theorem is valid if the target wave function is exact, i.e. $\psi_o(\underline{r}_1,\underline{r}_2)$ is the solution of equation (2.7). In reality ψ_o cannot be obtained exactly for target systems other than hydrogenic. The effect of an inexact target

function has been investigated recently and it has been found that unrealistic results could be due to inexact target wave functions (Peterkop and Råbik 1971, Houston 1973). To preserve a version of the bound theorem, the method of models (Drachman 1972b) has been employed in this thesis.

The method is to replace the target Hamiltonian and energy H_o and E_o of equation (2.2) by H_o^M and E_o^m respectively. The approximate target wave function becomes an eigenstate of H_o^m, i.e.

$$H_o^m \psi_o = E_o^m \psi_o \tag{2.25}$$

H_o^m is given by

$$H_o^m = T_t + E_o^m - \frac{1}{\psi_o}(T_t \psi_o) \tag{2.26}$$

where T_t is the kinetic energy part of the target Hamiltonian and in the last term T_t operates only on ψ_o and nothing following. As noted by Drachman (1972b), there may be difficulty if ψ_o has nodes. The full (H-E) operator for the system then becomes, with T_p the projectile kinetic energy operator and V_{int} the interaction energy

$$H-E \rightarrow T_p + T_t - \frac{1}{\psi_o}(T_t \psi_o) + V_{int} - k^2 \tag{2.27}$$

With a trial wave function of the form of equation (2.13), we have to calculate, among other terms,

$$[T_t - \frac{1}{\psi_o}(T_t\psi_o)]\chi_i \qquad (2.28)$$

The practicality of a trial function of the form of equation (2.13) then depends on whether or not matrix elements of $\{\frac{1}{\psi_o}(T_t\psi_o)\}$ are readily calculated. Such is not difficult if ψ_o is separable. For example, if ψ_o is a one parameter Hylleraas type wave function, the matrix elements of $\frac{1}{\psi_o}(T_t\psi_o)$ can be evaluated analytically; if ψ_o is a three parameter Hartree-Fock type wave function, $\frac{1}{\psi_o}(T_t\psi_o)$ can be simplified into a function of single variable, and the matrix elements can be calculated semi-numerically (Ho and Page 1975). It would generally become impractical for non-separable ψ_o, and we should then use the product form for the trial function, i.e.

$$\Psi^t(\underline{r}_1,\underline{r}_2,\underline{r}_p)=\{F(\underline{r}_p) + \sum_i C_i\chi_i'(\underline{r}_1,\underline{r}_2,\underline{r}_p)\}\psi_o(\underline{r}_1\underline{r}_2) \qquad (2.29)$$

where χ_i' are also short range correlation functions. It has been implied in the literature that it is necessary that to use the method of models, the trial function must have form of equation (2.29), but this is not so (Ho, Fraser and Kraidy 1975).

We should point out that equation (2.28) is equivalent to Drachman's (1972b) original presentation in terms of a trial function like (2.29), which we show in the context of a one electron target. In this case $T_t \rightarrow -\nabla_1^2$, equation (2.28) becomes

$$\{-\nabla_1^2 + [\frac{1}{\psi_o}(\nabla_1^2\psi_o)]\}\chi_i \tag{2.30}$$

This is identical to the quantity

$$\psi_o\{-\nabla_1^2 - 2(\nabla_1 \log \psi_o)\cdot\nabla_1\}\chi_i \tag{2.31}$$

which arises in Drachman's (1972b) paper, taking $\chi_i' = \chi_i/\psi_o$.

2.5 The Radial Equation

Equation (2.16) can be simplified to

$$(\nabla_p^2 + k^2)F^t(r_p) = U(r_p)F^t(r_p) + \sum_{i=1}^{N} C_i V_i(r_p) \tag{2.32a}$$

$$\sum_i (EN_{ji} - H_{ji})C_i = \int d\underline{r}_p \, V_j(r_p)F^t(r_p) \tag{2.32b}$$

where $$U(r_p) = \langle\psi_o|\frac{4}{r_p} - \frac{2}{r_{1p}} - \frac{2}{r_{2p}}|\psi_o\rangle \tag{2.33}$$

is the static potential for the incoming positron and helium atom, and

$$V_i(r_p) = \langle \psi_o | H-E | \chi_i \rangle \tag{2.34a}$$

$$H_{ji} = H_{ij} = \langle \chi_j | H | \chi_i \rangle \tag{2.34b}$$

$$N_{ji} = N_{ij} = \langle \chi_j | \chi_i \rangle \tag{2.34c}$$

It should be emphasized that in the method of models calculation, the (H) and (H-E) operators in equation (2.34) are those of equation (2.26). Explicitly, we have,

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_p^2 + \frac{4}{r_p} - \frac{2}{r_{1p}} - \frac{2}{r_{2p}} + V^m(r_1, r_2) \tag{2.35}$$

$$\text{where } V^m(r_1, r_2) = E_o^m + \frac{(\nabla_1^2+\nabla_2^2)\psi_o}{\psi_o} \tag{2.36}$$

$$\text{with } E_o^m = - \left. \frac{(\nabla_1^2+\nabla_2^2)\psi_o}{\psi_o} \right|_{\substack{r_1 \to \infty \\ r_2 \to \infty}} \tag{2.37}$$

After solving the eigenvalue problem

$$\sum_{i=1}^{N} (H_{ji} - \varepsilon^{\lambda} N_{ji}) a_i^{\lambda} = 0 \tag{2.38}$$

equation (2.32) can be converted to

$$(\nabla_p^2+k^2)F^t(\underline{r}_p)=U(r_p)F^t(\underline{r}_p)+\sum_\lambda \frac{V^\lambda(r_p)}{E-\varepsilon^\lambda}\left[\int d\underline{r}_p' V^\lambda(r_p')F^t(\underline{r}_p')\right] \quad (2.39)$$

where $$V^\lambda(r_p) = \sum_i a_i^\lambda V_i(r_p) \quad (2.40)$$

with a_i^λ the eigenvectors of equation (2.38).

For S wave scattering, i.e. the orbital angular momentum state of Ψ is zero, we can write the radial function as

$$F^t(\underline{r}_p) = \frac{f^t(r_p)}{r_p} \quad (2.41)$$

We finally obtain an integro-differential equation for the scattering problem

$$\left(\frac{d^2}{dr_p^2} + k^2\right) f^t(r_p)=U(r_p)f^t(r_p)+\sum_{\lambda=1}^{N} \frac{W^\lambda(r_p)}{E-\varepsilon^\lambda}\int W^\lambda(r_p')f^t(r_p')dr_p' \quad (2.42)$$

where $$W^\lambda(r_p) = r_p V^\lambda(r_p) \quad (2.43)$$

and the boundary conditions for $f^t(r_p)$ are

$$f^t(0) = 0 \quad (2.44a)$$

$$f^t(r_p) \underset{r_p\to\infty}{\sim} \sqrt{\frac{m}{k}}\{\sin(kr_p)+\tan \eta_o^t \cos(kr_p)\} \quad (2.44b)$$

CHAPTER 3

CALCULATIONS AND METHOD OF SOLUTIONS

3.1 Helium Atom Models

In this thesis, four helium wave functions have been used. They are all product type wave functions, namely HY1, HY2, HF1 and HF2. HY and HF represent "Hylleraas" and "Hartree-Fock" respectively. The index 1 denotes a minimum variational energy type wave function and index 2 indicates that the wave function bears the correct polarizability (we take the polarizability to be $\alpha = 1.376\ a_o^3$). These wave functions are described as follows:

One-parameter Hylleraas: models HY1 and HY2

$$\psi_o(r_1,r_2) = N\ e^{-a(r_1+r_2)} \qquad (3.1a)$$

Analytic Hartree-Fock: models HF1 and HF2

$$\psi_o(r_1,r_2) = N\ (e^{-ar_1} + c\ e^{-br_1})(e^{-ar_2} + c\ e^{-br_2}) \qquad (3.1b)$$

The parameters of these models with various physical properties are listed in table 3.1. The function HY2 has been introduced by Drachman (1966a) in which he chose to adjust

Table 3.1 Various properties of helium atom models

model	N	a	t (b=ta)	c	Energy (Rydbergs)	Dipole polarizability (a_o^3)	$\langle r^2 \rangle$ (a_o^2)
HY1	1.52961	1.6875			-5.6953	1.1099	1.0535
HY2†	1.30184	1.5992			-5.6797	1.376	1.1730
HF1††	0.70122	1.455799	2.0	0.6	-5.7233	1.4792*	1.1818
HF2*	0.73842	1.481102	2.0	0.6	-5.7216	1.376	1.1417
Exact					-5.8074‖	1.383§	1.1935‖

† Drachman (1966a)
‖ Pekeris (1959)
†† Green, Mulder, Lewis and Woll (1954)
* Ho, Fraser and Kraidy (1975)
§ Schwartz (1961a), Thomas and Humberston (1972). The experimental values range from 1.376 to 1.395 (see Houston and Drachman 1971 for references).

the parameter a to give a polarizability $\alpha = 1.376\ a_o^3$. The experimental values reported range from $1.376\ a_o^3$ to $1.395\ a_o^3$ (see Houston and Drachman 1971 for references), while the most elaborate theoretical calculations give $1.383\ a_o^3$ (Schwartz 1961a, Thomas and Humberston 1972). For comparison purposes, Ho, Fraser and Kraidy (1975) constructed HF2 by keeping $\alpha = 1.376\ a_o^3$. The method of obtaining the wave function HF2 has been discussed by these authors in which some further references to polarizability calculations are also mentioned.

3.2 Correlation Terms and Eigenvalue Problem

The correlation functions in equation (2.13) have been taken as

$$\chi_i(r_1,r_2,r_p) = r_p^{\ell_i} e^{-\gamma_i r_p} (r_1^{m_i} r_{1p}^{n_i} e^{-\alpha_i r_1 - \beta_i r_2} + r_2^{m_i} r_{2p}^{n_i} e^{-\beta_i r_1 - \alpha_i r_2}) \qquad (3.2)$$

where α_i, β_i and γ_i are non-negative constants and $\ell_i + m_i + n_i \leq \omega$, with $\omega = 1,2,3,4,5,6$ which correspond to N=4,10,20,35,56,84 respectively. These are explicitly symmetric in the spatial coordinates of the two electrons.

If we recall the bound theorem from Chapter 2, the phase shift η (strictly tan η) calculated using correlation terms (equation 3.2) is a lower bound to the exact phase shift for

the modified Hamiltonian. Furthermore, it has also been shown (Gailitis 1965) that as the number of correlation terms increases, the phase shifts do not decrease; i.e. $\tan\eta^t_{N+1} \geq \tan\eta^t_N$, where η^t_{N+1} and η^t_N are the phase shifts from two sets of correlation terms ε_{N+1} and ε_N respectively and ε_{N+1} includes all the members of ε_N. The bound theorem further means that the non-linear parameters α_i, β_i, and γ_i may be optimized to give the highest $\tan\eta$ and we know the exact value will not be exceeded. (Because of a sign change in the definition of scattering length - see equation (3.10) -, the calculations give upper bounds to the scattering length, etc.)

The method of calculating the matrix elements H_{ij} and N_{ij} of equations 2.34 b,c) are those of Perkins (1968). In the case of the HF wave functions, the matrix elements involving the form of $(\frac{1}{\psi_o}\nabla^2\psi_o)$ of equation (2.30) are integrated semi-numerically (see section 2.4). The formalism and some numerical examples have been discussed by Ho and Page (1975). This method is also applied to do the necessary integrals to construct the optical potential.

The matrix form of the eigenvalue problem, equation (2.38), is as follows

$$HA = NA\Lambda \qquad (3.3)$$

where A is a matrix of eigenvectors and Λ is a diagonal matrix of eigenvalues.

Two methods have been tested to solve the eigenvalue problem. The first method is the Cholesky-Wilkinson decomposition (see for example Reinsch and Wilkinson 1971). Since N is symmetric and positive definite, N can be decomposed as $N=LL^T$ where L is a lower triangular matrix, and equation (3.3) becomes

$$(L^{-1}H(L^{-1})^T)(L^TA) = (L^TA)\Lambda \qquad (3.4)$$

Equation (3.4) can then be solved by Jacobi's method. The second method is to solve a generalized matrix eigenvalue problem using the Householder reduction. It has been found that the two methods gave the same result and hence provided a partial check to the accuracy of the subroutines involved. In the final calculations of this thesis, the Householder reduction method has been employed.

3.3 Green's Function and Integral Equation

Having solved the eigenvalue problem, and the necessary integrals for $V_i(r_p)$ (Ho and Page 1975), the optical potential is readily obtained. Dropping the superscript t, equation (2.42) can be rewritten as

$$\left(\frac{d^2}{dr_p^2} + k^2\right) f(r_p) = U(r_p) f(r_p) + \int V_{opt}(r_p, r_p') f(r_p') dr_p' \quad (3.5)$$

where $$V_{opt}(r_p, r_p') = \sum_{\lambda=1}^{N} \frac{W^\lambda(r_p) W^\lambda(r_p')}{E - \varepsilon^\lambda} \quad (3.6)$$

with $W^\lambda(r_p) = r_p V^\lambda(r_p)$ and $V^\lambda(r_p) = \sum_i a_i^\lambda V_i(r_p)$, where a_i^λ are the eigenvectors of the eigenvalue problem (2.38).

The boundary conditions on the scattering function are

$$f(0) = 0 \quad (3.7a)$$

$$f(r_p) \underset{r_p \to \infty}{\sim} \sin(kr_p) + \tan \eta_0 \cos(kr_p). \quad (3.7b)$$

Note that the boundary conditions are similar to equation (2.44) with a trivial change in normalization.

The integro-differential equation can be converted into an integral equation by the use of Green's function:

$$f(r_p) = \sin(kr_p) + \int G(r_p, r_p') U(r_p') f(r_p') dr_p' + \iint G(r_p, r_p') V_{opt}(r_p', r_p'') f(r_p'') dr_p'', \quad (3.8)$$

where $$G(r,r') = \begin{cases} -\frac{1}{k} \sin(kr)\cos(kr') & (r \le r') \quad (3.9a) \\ -\frac{1}{k} \sin(kr')\cos(kr) & (r \ge r') \quad (3.9b) \end{cases}$$

3.4 Scattering Length Calculation

We define the scattering length a by

$$a = \lim_{k\to 0}\left(-\frac{\tan\eta_0}{k}\right). \qquad (3.10)$$

The scattering length can be determined by introducing a new function $g(r_p) = \left.\frac{f(r_p)}{k}\right|_{k\to 0}$ into equation (3.8) (see for example Fraser 1961), the integral equation becomes

$$g(r_p) = r_p + \int dr_p' G(r_p, r_p') U(r_p') g(r_p') dr_p'$$

$$+ \iint G(r_p, r_p') V_{opt}(r_p', r_p'') g(r_p'') dr_p'' dr_p' \qquad (3.11)$$

with the boundary conditions

$$g(0) = 0 \qquad (3.12a)$$

$$g(r_p) \underset{r_p\to\infty}{\sim} r_p - a. \qquad (3.12b)$$

The Green's function, equation (3.9) then becomes

$$G(r,r') = \begin{cases} -r & (r \le r') \qquad (3.13a) \\ -r'. & (r \ge r') \qquad (3.13b) \end{cases}$$

The cross section is given by

$$\sigma = 4a^2 \qquad (\text{in } \pi a_o^2) \qquad (3.14)$$

3.5 Numerical Method of Solution

The method of solution for the scattering function $f(r_p)$ is non-iterative. The functional values of $f(r_p)$ were determined at Gaussian integration points. Equation (3.8) is approximated by

$$f_i = s_i + \sum_j \omega_j G_{ij} U_j f_j + \sum_{kj} \omega_j \omega_{ik} G_{ik} (V_{opt})_{kj} f_j \qquad (3.15)$$

where ω and ω' are Gaussian integration weights, f_i represents the functional value $f_i(r_p)$ at the ith Gaussian point and $s_i \equiv (\sin kr_p)_i$ etc. Equation (3.15) can be written in a matrix form

$$\bar{F} = \bar{S} + \bar{Y}\,\bar{F} \qquad (3.16)$$

where $\bar{F}$ and $\bar{S}$ are column matrices and $\bar{Y}$ is an N by N matrix with

$$\bar{Y}_{ij} = \omega_j (G_{ij} U_j + \sum_k \omega'_{ik} G_{ik} (V_{opt})_{kj}) \qquad (3.17)$$

After solving the system of linear equations, phase shifts can be determined by the asymptotic form (equation 3.7b) i.e.

$$\tan \eta_o = \frac{f(r_a)-\sin(kr_a)}{\cos(kr_a)} \qquad (3.18)$$

where r_a denotes a value of r_p in the asymptotic region. Since f satisfies

$$f(r) = \sin(kr) + \int_o^\infty dr'\, G(r,r')\{Uf + \int V_{opt} f\} \qquad (3.19a)$$

$$\text{with } G(r,r') = -\frac{1}{k}\cos(kr)\sin(kr'), \text{ for } r>r', \qquad (3.19b)$$

we can see that the value of $\tan\eta_o$ given by (3.18) would be the same as that obtained from the integral expression

$$\tan \eta_o = -\frac{1}{k}\int_o^\infty dr' \sin(kr')\{Uf + \int V_{opt} f\} \qquad (3.20)$$

Furthermore, by checking the consistency of the phase shifts obtained at several values of r_a in the asymptotic region, we are able to make sure the asymptotic region is reached. It also implies that the range of the Gaussian points is long enough to represent $f(r_p)$.

Similar to equation (3.18), the scattering length is determined by

$$a = r_a - g(r_a) \qquad (3.21)$$

Throughout this thesis, $f(r_p)$ has been represented at 40 Gaussian integration points. We used 16 Gauss-Legendre.

points to cover the range from the origin to r_p=R and 24 Gauss Laguerre points to cover the remaining region which extended to $(81+R)a_o$ approximately. The value of R ranged from $4a_o$ to $6a_o$. The independence of the results on changes in R (since the final result should be independent of the Gaussian points chosen provided that the range is long enough as discussed before) served as one of the criteria for accuracy of the program. By "independent" we mean that they are consistent to three to four digits.

In approximating the integral numerically, due note has been taken of the discontinuities of the slope of the Green's functions. For example, the integral over r_p' in the last term of the RHS of equation (3.8) is broken down into two parts, from 0 to $r_p' = r_p$ and from r_p to ∞. The Gaussian weight ω_{ik}' of equation (3.15) is consequently dependent on the value of r_p of the LHS of equation (3.8). This numerical technique has been employed for example by Chan (1972) and Chan and Fraser (1973).

CHAPTER 4

POSITRON ANNIHILATION WITH THE HELIUM ATOM

4.1 Introduction

A positron can annihilate with an electron when they are within a Compton wavelength $\lambda\!\!\!^{-}_c = \hbar/mc = (1/137)a_o$ of each other. According to selection rules, a positron and an electron with opposite spin can annihilate into two gamma quanta; with parallel spin, they produce three gamma quanta. The probability that the later process will take place is in the order of 1/137 of the former.

Experimentally, one measurable quantity is the annihilation rate or its inverse, the lifetime τ. Theoretically, a quantity which can be calculated is Z_{eff}, the effective number of electrons per atom (or molecule) felt by the incoming positron. The direct relation between annihilation rate R_s and Z_{eff} is

$$R_s = \pi r_o^2 \, c \, \eta_A \, Z_{eff} \qquad (4.1)$$

where $r_o = e^2/(m c^2) = 2.82 \times 10^{-13}$ cm is the classical radius of the electron; c is the velocity of light and η_A is the number density of atoms or molecules. A discussion of equation (4.1) can be found for example in Fraser (1968).

4.2 Effective Charge Calculation

The effective charge for the positron-helium system is given by

$$Z_{eff} = 2 \int d\underline{r}_1 d\underline{r}_2 d\underline{r}_p \, |\Psi(\underline{r}_1, \underline{r}_2, \underline{r}_p)|^2 \, \delta(\underline{r}_1 - \underline{r}_p) \qquad (4.2)$$

The free part of the wave function in equation (4.2) must have unit amplitude at infinity, i.e. it has the asymptotic form

$$\Psi(\underline{r}_1, \underline{r}_2, \underline{r}_p) \sim \psi_o(r_1, r_2)\left(e^{i\,\underline{k}\cdot\underline{r}_p} + f_k(\theta)\frac{e^{ikr_p}}{r_p}\right). \qquad (4.3)$$

The S wave part of equation (4.3) is

$$\Psi \sim \psi_o(r_1, r_2)\, e^{i\eta_o} \sin(kr_p + \eta_o)/(kr_p). \qquad (4.4)$$

The S state trial wave function Ψ^t must therefore be modified to be

$$\Psi^t \sim \psi_o(r_1, r_2)\, e^{i\eta_o}\left(\frac{\cos\eta_o}{k}\right) f(r_p)/r_p \qquad (4.5)$$

with $$f(r_p) \sim \sin(kr_p) + \tan\eta_o \cos(kr_p) \qquad (4.6)$$

The effective charge from the S-wave contribution is

$$Z_{eff} = 2\left(\frac{\cos \eta_o}{k}\right) \int |\psi_o(\underline{r}_1, \underline{r}_p) \frac{f(r_p)}{r_p}$$

$$+ \Sigma\, C_i \chi_i\, (\underline{r}_1, \underline{r}_p, \underline{r}_p)|^2\, d\underline{r}_1\, d\underline{r}_p \qquad (4.7a)$$

for k=0, we have

$$Z_{eff} = 2 \int |\psi_o(\underline{r}_1, \underline{r}_p) \frac{g(r_p)}{r_p}$$

$$+ \sum_i C_i\, \chi_i(\underline{r}_1, \underline{r}_p, \underline{r}_p)|^2\, d\underline{r}_1\, d\underline{r}_p \qquad (4.7b)$$

Since ψ_o and χ_i decay exponentially, we can see from equations (4.7) that the largest contribution to Z_{eff} is from the inner part of the scattering wave function. The effective charge can be regarded as another meeting place between theory and experiment which probes the adequacy of the inner part of the wave function.

In order to estimate the contribution of higher partial waves ($\ell > 0$) to Z_{eff}, we subtract the S wave contribution of the undisturbed free wave from the Dirac rate, $Z_{eff} = 2$ i.e.

$$Z_{eff}(\ell > 0) = 2 - 2 \int \psi_o^2(\underline{r}_1, \underline{r}_2)\left\{\frac{\sin(kr_1)}{k\, r_1}\right\}^2 d\underline{r}_1\, d\underline{r}_2. \qquad (4.8)$$

For the one-parameter helium wave function $\psi_o = N\, e^{-a(r_1+r_2)}$ we have

$$Z_{eff}(\ell > 0) = \frac{2k^2}{a^2+k^2} \qquad (4.9)$$

4.3 Excitation of the Residual He^+ Ion

We assume the annihilation takes place instantaneously when an electron is at the position of a positron. The times involved are very rapid compared with atomic times, and the spectator electron of the He^+ ion will be found in different ionic state of the new Hamiltonian after the annihilation is completed. The probability P_n of finding the residual He^+ ion in a state whose wave function is ϕ_n is given by: (Drachman 1966b)

$$P_n = \int d\underline{r}_p |A_n(\underline{r}_p)|^2 / \sum_n \int d\underline{r}_p |A_n(\underline{r}_p)|^2 \qquad (4.10)$$

where $$A_n(\underline{r}_p) = \int d\underline{r}_1 \, \phi_n^*(\underline{r}_1) \Psi(\underline{r}_1, \underline{r}_p, \underline{r}_p) \qquad (4.11)$$

is the coefficient in the expansion of the parent wave function (the scattering wave function with electron 2 and positron coalesced) in the ionic eigenstates; i.e.

$$\Psi(\underline{r}_1, \underline{r}_p, \underline{r}_p) = \sum_n A_n(\underline{r}_p)\phi_n(\underline{r}_1) \, . \qquad (4.12)$$

By using the closure relation for ionic eigenstates,

the denominator in equation (4.8) is equal to $\frac{1}{2}Z_{eff}$ and P_n becomes

$$P_n = \int d\underline{r}_p |A_n(\underline{r}_p)|^2 / \tfrac{1}{2}Z_{eff} \qquad (4.13)$$

Drachman(1966b) suggested that if the probability for being found in excited states other than the ground state is not too small, there may be a possibility of observing the radiative de-excitation of the residual He^+ ion, following annihilation. No experiment for this process has yet been done, but the present calculation hopefully will provide some guidance for future investigation.

4.4 Cusp Values

To test the accuracy of the wave function, Kato's cusp condition (Kato 1957) may be employed here. The cusp condition, or coalescence condition, states that the exact wave function Ψ for a system of particles interacting through coulombic force must satisfy

$$\left.\frac{\partial \log \Psi}{\partial r_{ij}}\right|_{r_{ij}=0} = q_i\, q_j\, \mu_{ij} \equiv \nu_{ij} \qquad (4.14)$$

where q_i and q_j are the charges in units of e of particles i and j, and μ_{ij} is their reduced mass; ν_{ij} (measured in a_o^{-1})

is defined as the cusp value between particles i and j.

Since annihilation properties are point properties between the electron and positron, it is useful to judge the goodness of Z_{eff} by comparing the calculated cusp values to the exact one. This has been particularly emphasized by Schrader (e.g. Lebeda and Schrader 1969). The exact cusp value of electron and positron, ν_{1p} is -0.5 (from $q_p = -q_1 = +1$ and $\nu_{1p} = \frac{1}{2}$). Taking the average of equation (4.14) for a trial function Ψ, Chong and Schrader (1969) obtained explicitly

$$\nu_{1p} = \langle\Psi|\delta(\underline{r}_1 - \underline{r}_p)\frac{\partial}{\partial r_{1p}}|\Psi\rangle / \langle\Psi|\delta(\underline{r}_1 - \underline{r}_p)|\Psi\rangle \qquad (4.15)$$

where the denominator is equal to $\frac{1}{2}Z_{eff}$.

CHAPTER 5

RESULTS

5.1 Optimization of Non-Linear Parameters

Throughout this thesis, up to 84 correlation terms were used. The first step is to optimize the non-linear parameters α_i, β_i and γ_i of equation (3.2). Guided by the bound theorem, the non-linear parameters were chosen such that the calculation gave the highest phase shifts. Similarly, for zero energy calculation, the non-linear parameters were chosen to give the lowest scattering lengths. The results should be optimized for each k and each N for each helium model. However, this is economically impractical. On the other hand, there is some evidence that the non-linear parameters that gave the best scattering lengths did not necessarily give the best phase shifts. Therefore, we have used two sets of non-linear parameters for each model. The first set is applied to the energy region $k \leq 0.1$ and the second set is applied to $k > 0.1$ up to $k = 1.0$. They have been optimized at N=10 terms and k=0.0 and 0.2 respectively.

The non-linear parameters are shown in table 5.1 with $\alpha = \alpha_i$ for all i, etc. It should be noted that the two values of γ, the non-linear parameter for the positron coordinate

Table 5.1 Non-linear parameters for different models (Optimized at N=10)

models	α		β		γ	
	I	II	I	II	I	II
HY1	1.395	1.402	1.702	1.705	0.5195	0.660
HY2	1.322	1.320	1.614	1.617	0.503	0.606
HF1	1.212	1.225	1.675	1.679	0.488	0.622
HF2	1.220	1.243	1.705	1.708	0.503	0.627

I : applied to $k \leq 0.1$, optimized at $k = 0.0$

II : applied to $k > 0.1$, optimized at $k = 0.2$

do differ somewhat.

5.2 S Wave Phase Shifts

After obtaining the non-linear parameters, we applied them up to N=84 terms for the final calculation. The convergence behavior for each model is shown in tables 5.2a - d with the subscripts a, b, c and d denoting the different models HY1, HY2, HF1 and HF2 respectively. It is clear from the results that the bound theorem applies. The final results were taken at N=84 terms and they are shown in figure 5.1.

In order to make a direct comparison with other calculations we compare our results with others for a given helium model, namely HY2. In table 5.3 we list other calculations for this one-parameter Hylleraas type wave function with the correct polarizability ($\alpha = 1.376$). Column 2 is the present calculation; column 3 is from Drachman's (1968) variational method; column 4 is by Houston and Drachman (1971) and column 5 is by Humberston (1973). For the zero energy calculation without the so-called long range dipole terms, Houston and Drachman (1971) gave a lower estimate than the present calculation and hence their scattering length is better for this model. This may be due to the fact that they optimized at N=84 terms compared with the N=10 terms in the present

Table 5.2a Convergence behavior of phase shifts from model HY1

k \ N	4	10	20	35	56	84
0.0	-.1906	-.2627	-.3185	-.3399	-.3509	-.3604
0.05	.006353	.01271	.01525	.01616	.01657	.01686
0.10	.01155	.02303	.02694	.02811	.02843	.02859
0.15	.01461	.02971	.03324	.03469	.03488	.03495
0.20	.01483	.03251	.03560	.03662	.03681	.03691
0.25	.01187	.03111	.03376	.03466	.03511	.03527
0.30	.005708	.02596	.02869	.02974	.03038	.03048
0.40	-.01523	.007076	.01181	.01303	.01338	.01367
0.50	-.04488	-.01910	-.01158	-.01047	-.01023	-.009972
0.60	-.07971	-.04926	-.03978	-.03879	-.03791	-.03787
0.70	-.1168	-.08152	-.07129	-.06858	-.06801	-.06793
0.80	-.1540	-.1146	-.1040	-.09970	-.09906	-.09893
0.90	-.1899	-.1470	-.1366	-.1310	-.1300	-.1298
1.00	-.2237	-.1800	-.1681	-.1626	-.1604	-.1598

Phase shifts are in radians; the k=0 entry is the scattering length.

Table 5.2b Convergence behavior of phase shifts from model HY2

k \ N	4	10	20	35	56	84
0.0	-.2586	-.3544	-.4212	-.4485	-.4617	-.4743
0.05	.009989	.01714	.02017	.02131	.02179	.02222
0.10	.01827	.03111	.03569	.03713	.03749	.03762
0.15	.02344	.04045	.04464	.04614	.04632	.04638
0.20	.02462	.04434	.04804	.04917	.04952	.04965
0.25	.02147	.04292	.04638	.04756	.04825	.04839
0.30	.01411	.03696	.04097	.04240	.04317	.04325
0.40	-.01124	.01525	.02222	.02361	.02411	.02445
0.50	-.04650	-.01450	-.004521	-.003169	-.002511	-.002280
0.60	-.08689	-.04869	-.03696	-.03435	-.03383	-.03358
0.70	-.1289	-.08531	-.07256	-.06805	-.06750	-.06711
0.80	-.1701	-.1230	-.1092	-.1031	-.1019	-.1015
0.90	-.2092	-.1604	-.1453	-.1385	-.1361	-.1357
1.00	-.2454	-.1968	-.1807	-.1729	-.1695	-.1687

Phase shifts are in radians; the k=0 entry is the scattering length.

Table 5.2c Convergence behavior of phase shifts from model HF1

k \ N	4	10	20	35	56	84
0.0	-.2537	-.3703	-.4420	-.4701	-.4848	-.4959
0.05	.01222	.01788	.02112	.02228	.02279	.02313
0.10	.02179	.03226	.03714	.03849	.03897	.03913
0.15	.02674	.04151	.04610	.04771	.04790	.04798
0.20	.02608	.04539	.04944	.05058	.05085	.05102
0.25	.01980	.04369	.04739	.04853	.04913	.04933
0.30	.008524	.03721	.04135	.04277	.04349	.04360
0.40	-.02511	.01396	.02112	.02265	.02308	.02340
0.50	-.06718	-.01748	-.006872	-.005553	-.004939	-.004644
0.60	-.1120	-.05301	-.04024	-.03798	-.03730	-.03708
0.70	-.1561	-.09039	-.07648	-.07238	-.07179	-.07135
0.80	-.1978	-.1282	-.1134	-.1076	-.1066	-.1061
0.90	-.2360	-.1654	-.1495	-.1425	-.1407	-.1401
1.00	-.2703	-.2010	-.1839	-.1762	-.1731	-.1729

Phase shifts are in radians; the k=0 entry is the scattering length.

Table 5.2d Convergence behavior of phase shifts from model HF2

k \ N	4	10	20	35	56	84
0.0	-.2256	-.3371	-.4032	-.4295	-.4435	-.4512
0.05	.007518	.01629	.01928	.02038	.02088	.02106
0.10	.01359	.02944	.03398	.03536	.03573	.03583
0.15	.01702	.03777	.04212	.04364	.04382	.04388
0.20	.01701	.04121	.04504	.04613	.04637	.04650
0.25	.01324	.03946	.04293	.04399	.04455	.04471
0.30	.005752	.03322	.03704	.03838	.03907	.03914
0.40	-.01879	.01099	.01757	.01904	.01946	.01971
0.50	-.05244	-.01914	-.009272	-.008031	-.007454	-.007204
0.60	-.09093	-.05330	-.04129	-.03922	-.03857	-.03841
0.70	-.1310	-.08936	-.07619	-.07240	-.07183	-.07147
0.80	-.1703	-.1260	-.1119	-.1064	-.1055	-.1051
0.90	-.2077	-.1621	-.1469	-.1403	-.1385	-.1381
1.00	-.2421	-.1968	-.1804	-.1731	-.1703	-.1696

Phase shifts are in radians; the k=0 entry is the scattering length.

Table 5.3 Comparison of phase shifts with other calculations for model HY2

k	Present*	Drachman* (1968)	Houston and Drachman (1971)	Humberston (1973)
0.0†	-.4743		-.485*	
0.0††			-.524*	-.524*
0.10	.03762	.036	.035	.037
0.20	.04965	.047	.049	.051
0.30	.04325	.039	.039	.044
0.40	.02445	.020	.020	.027
0.50	-.002280	-.007	-.003	.001
0.60	-.03358	-.039	-.034	-.031
0.70	-.06711	-.073	-.069	-.066
0.80	-.1015	-.107	-.106	-.098
0.90	-.1357	-.141	-.143	-.133
1.00	-.1687	-.174	-.177	-.167

* Bound calculation within the model

† Without dipole type correlation terms

††With dipole type correlation terms

Phase shifts are in radians, the k=0 entry is the scattering length.

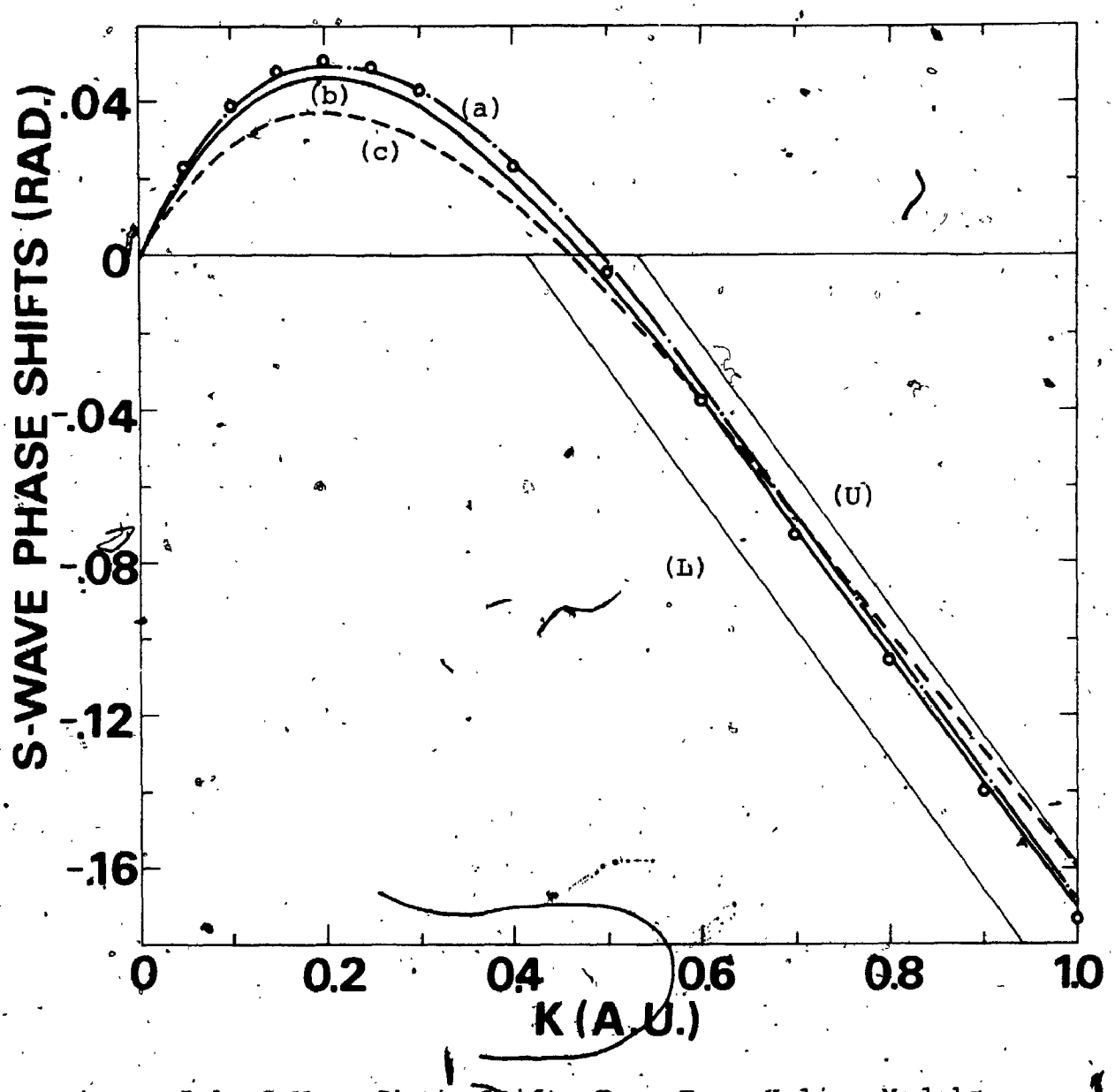

Figure 5.1 S-Wave Phase Shifts From Four Helium Models. (a) HF1; (b) HF2; (c) HY1; The circles are from model HY2; (U) and (L) represent the upper and lower correlation limits respectively of Jaduszliwer and Paul (1974).

calculation. (The scattering lengths of models HY1 and HF1 have lower values than those of Houston and Drachman (1971) for the corresponding models.) However, for non-zero energies our results give higher phase shifts than those of Drachman (1968) and Houston and Drachman (1971). We can conclude that based on the bound theorem, our results give a better estimate. On the other hand, we can not rigorously conclude that our result is better than Humberston's (1973) since he obtained higher phase shifts. However, since there is no bound theorem for his algebraic Kohn type non-zero energy calculation, and judging from the convergence behavior of our result and the conclusion by Bhatia, Temkin, Drachman and Eiserike (1971) that the correlation method is more accurate than Schwartz's (1961b) Kohn type calculation, we may conclude that our phase shifts are more reliable for this model.

The best result of this work is considered to be those of HF2, a Hartree-Fock type wave function with correct polarizability. Recently, Ho and Fraser (1975) confirmed that polarizability plays an important role in low energy scattering, especially for a method of models calculation. The result of HF2 is shown in table 5.4 and figure 5.2 together with the best results of other authors. Column 4 shows those of Houston and Drachman (1971) who based on the reason that the correct polarizability is important, considered model HY2 (their model B) gave the best result among

Table 5.4 S-wave phase shifts

k	Present† * (HF2)	Drachman† * (1968) (HY2)	Houston and Drachman† (1971) (HY2)	Humberston† (1973)
0.0	-.4512			-.472*
0.05	.02106			
0.10	.03583	.036	.035	.031
0.15	.04388			
0.20	.04650	.047	.049	.040
0.25	.04471			
0.30	.03914	.039	.039	.029
0.40	.01971	.020	.020	.007
0.50	-.007204	-.007	-.003	-.023
0.60	-.03841	-.039	-.034	-.057
0.70	-.07147	-.073	-.069	-.093
0.80	-.1051	-.107	-.106	-.128
0.90	-.1381	-.141	-.143	-.163
1.00	-.1696	-.174	-.177	-.195

Phase shifts are in radians; the k = 0 entry is the scattering length.

† "Method of models" calculation

* Bound calculation within the helium model

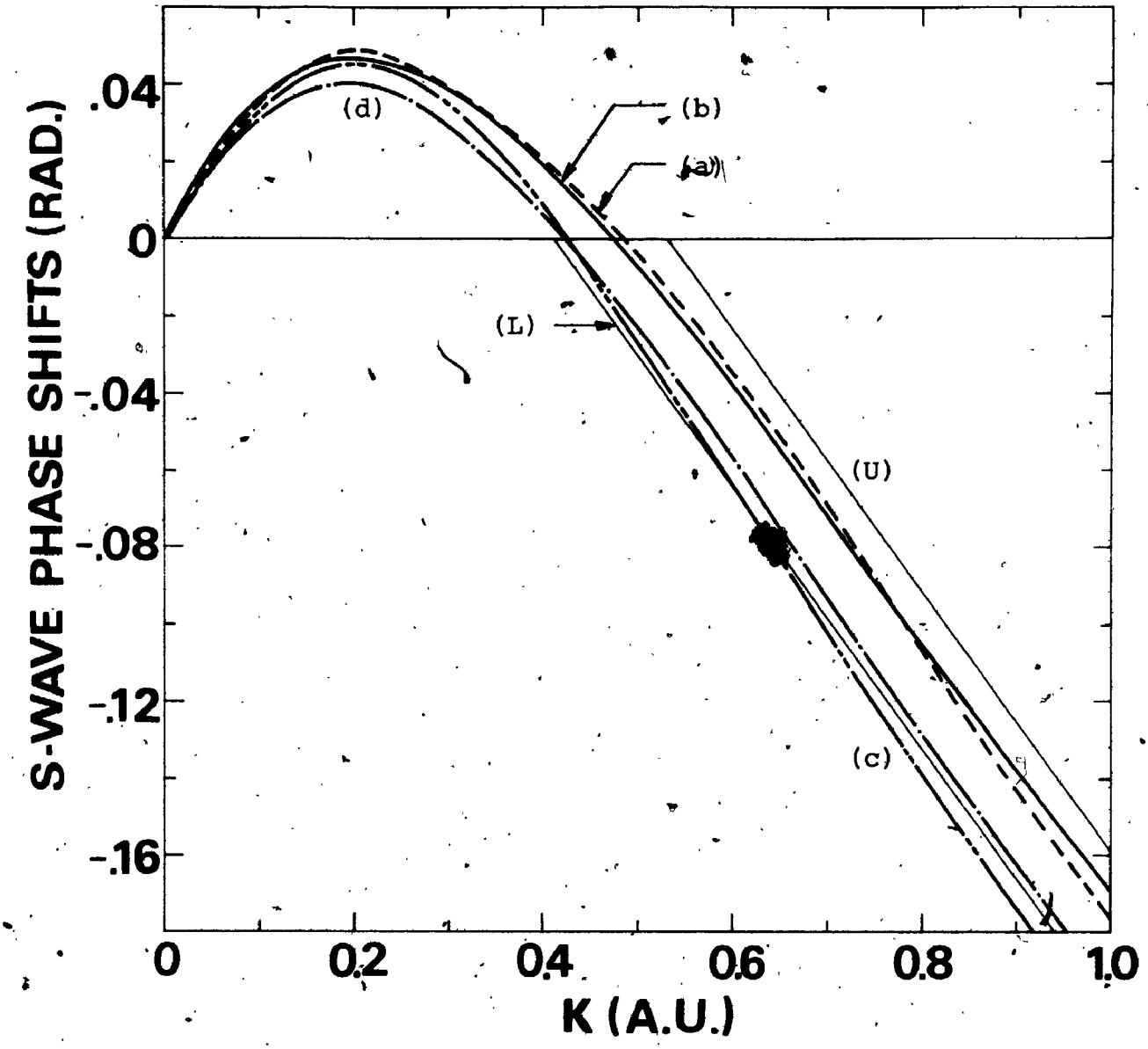

Figure 5.2 S-Wave Phase Shifts

(a) Houston and Drachman (1971); (b) Present calculation (model HF2); (c) Aulenkamp, Heiss, Wichmann (1974); (d) Humberston (1973); (U) and (L) represent the upper and lower correlation limits respectively of Jaduszliwer and Paul (1974).

the five helium models they used. The result of Humberston's (1973) model H5 is shown in column 5. This is also a method of models calculation with a five parameter Hylleraas helium function which bears essentially the correct polarizability. However, for other than zero energy, his Kohn's variational method is not a bound calculation. Also shown in figure 5.2 are the results of Aulenkamp, Heiss and Wichmann (1974) who used variant I (as termed by Peterkop and Rabik 1971) in which the true Hamiltonian and the variational energy of helium atom were employed. (Different variants of Kohn's principle will be discussed in more detail in chapter 6).

By comparing the present HF2 results with those of Humberston's (1973) H5, it is noted that they differ not insignificantly. This may suggest that for a more definitive solution a bound calculation (like the present correlation method together with the method of models) with for example Humberston's (1973) model H5 should be worth trying.

In figures 1 and 2, we also show the cross correlation limits by Jaduszliwer and Paul (1974). They are given by

$$\eta_o = \Delta - 0.34k \qquad (5.1)$$

where Δ is 0.14 and 0.18 for the lower and upper limit respectively. It is noted that the result by Aulenkamp, Heiss and Wichmann (1974) lies below this lower limit.

5.3 Cross Sections and the Real Part of the Forward Scattering Amplitude

After obtaining the S-wave phase shifts, total cross sections can be calculated from equation (2.12) where higher partial wave phase shifts are taken from other calculations. We used two sets of higher partial waves. The first set is from Drachman's (1966a) lowest P and D waves using the adiabatic method with full monopole suppression. (In S-wave scattering, such an approach led to the lowest phase shifts which was in better accord with other calculations: e.g. Houston and Drachman (1971), Humberston (1973) and the present work). The second set is from the experimental results of Jaduszliwer and Paul (1973). We used the following analytic fit for their P wave results (Hara, private discussion)

$$\eta_1 = \pi\alpha k^2/15 - 0.18\ k^3 \qquad (5.2)$$

where α is the polarizability of the helium atom.

For the contributions from higher partial waves, we used the result from the generalized effective range theory (O'Malley, Spruch and Rosenberg 1961)

$$\eta_\ell \approx \frac{\pi\alpha k^2}{(2\ell+3)(2\ell+1)(2\ell-1)} \qquad (5.3)$$

We applied this formula to the first set for $\ell \geq 3$ and for the second set for $\ell \geq 2$. The total cross sections with the S wave from model HF2 are shown in figure 5.3, where experimental results of Jaduszliwer and Paul (1973) and Canter, Coleman, Griffith and Heyland (1973) are included. We also compare with other theoretical calculations, e.g. those by Humberston (1974) and Aulenkamp, Heiss and Wichmann (1974). Humberston's (1974) total cross sections are obtained from his S-wave (model H5) with Drachman's (1966a) lowest P and D waves. This result, as we note, is very different from that given by Drachman's (1971) higher partial waves with the same (Humberston 1973) S wave phase shift.

Recently, from the phase shift analysis by Bransden and Hutt (1975), we are able to compare calculated phase shifts with experiments through Re $f_k(0)$, the real part of forward scattering amplitude by use of equation (2.11a). In figure 5.4 we show the results from Bransden and Hutt (1975) and the present calculation (model HF2) together with some theoretical results. Again, we use two sets of higher partial waves as described before, and also used equation (5.3) to include higher partial wave contributions. It appears that Re $f_k(0)$ is very sensitive to the P and D waves. For example, curves a and c which used the same S wave (Humberston's (1973) model H5) but different P and D waves (Drachman (1971)) for curve a and the lowest P and D phase shifts of Drachman

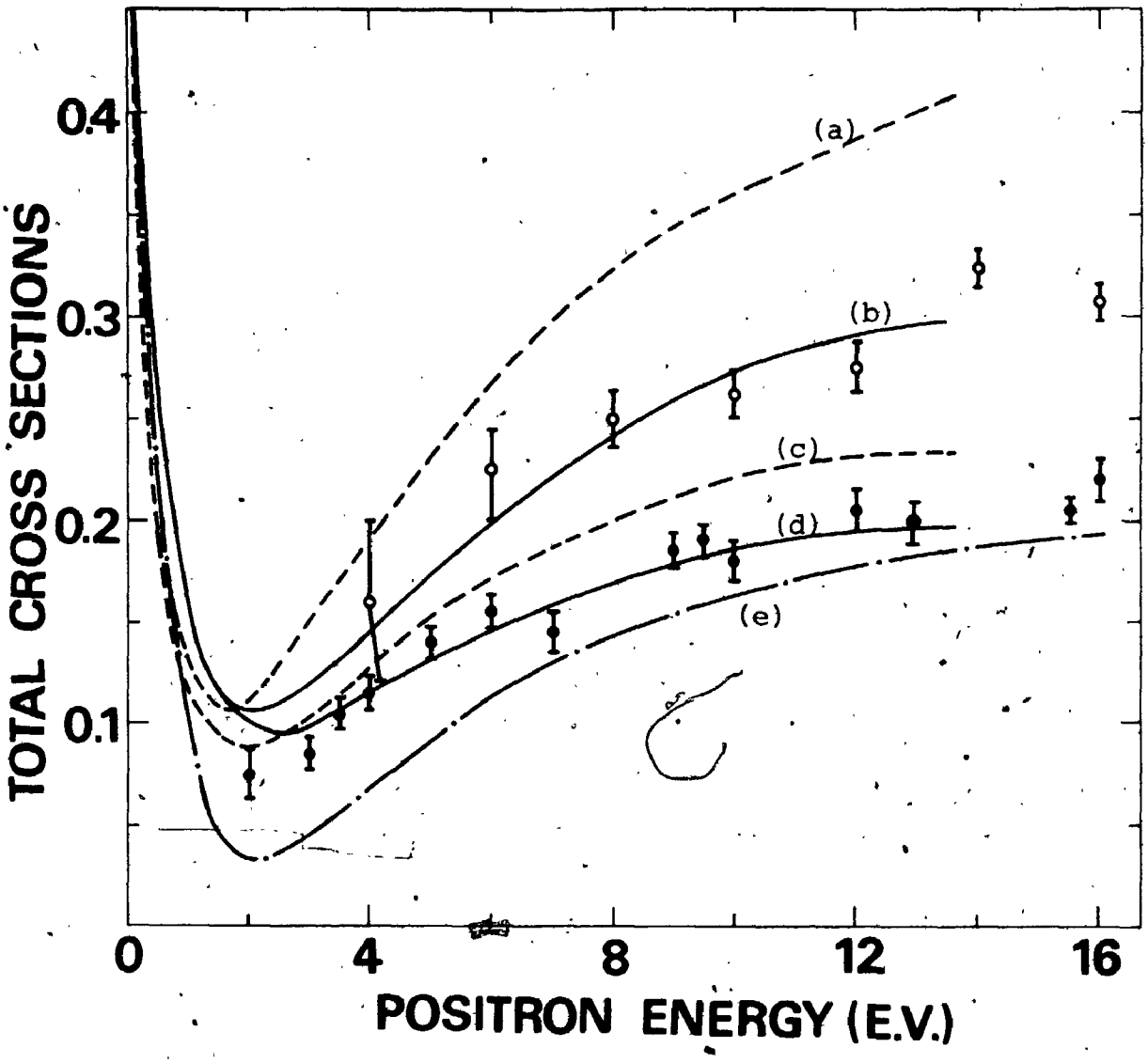

Figure 5.3 Total Elastic Cross Section (πa_o^2)
(a) Humberston's (1973) S-wave, Drachman's (1971) P- and D-waves; (b) Present (HF2) S-wave, Jaduszliwer and Paul's (1973) P-wave; (c) Humberston's (1973) S-wave, Drachman's (1966a) P- and D-waves; (d) Present (HF2) S-wave, Drachman's (1966a) P- and D-waves; (e) Aulenkamp et al (1974). Allowance is made for higher order phase shifts (eq. 5.3) for all the curves. Open circles are measured by Jaduszliwer and Paul (1973); Closed circles are from Coleman et al (1974).

(1966a) for curve d) gave very different results. It seems more accurate P and D phase shifts are certainly needed.

The results of Re $f_k(0)$ for the present four helium models are shown in table 5.5 for two sets of higher partial waves. It is clear that they are very sensitive to the P and D wave phase shifts.

The consistency of the experimental cross sections σ can be checked by verifying the sum rule based on a forward dispersion relation (Bransden and McDowell 1969)

$$a + f_B = - \frac{1}{2\pi} \int_0^\infty \sigma(k)\,dk, \qquad (5.4)$$

where a is the scattering length and f_B is the Born approximation for the direct elastic amplitude in the forward direction and k is the momentum of the incident positron. Pekeris (1959) calculated f_B as 0.791 for the electron-helium system. For the positron case, the direct Born amplitude has the same magnitude but is of opposite sign, hence we have $f_B = -0.791$. To compare with the experiment, the LHS of equation (5.4) gives -1.242 where a = -0.451 of model HF2 is employed. It is noted that the LHS has a value of -1.263 where Humberston's (1973) scattering length (model H5) is used.

A value of the RHS of equation (5.4) is -1.30 which has

Table 5.5 Re $f_k(0)$ for four helium models

	HY1		HY2		HF1		HF2	
k	(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2)
0.0	.360	.360	.474	.474	.496	.496	.451	.451
0.1	.423	.422	.513	.513	.528	.528	.496	.495
0.2	.448	.451	.512	.515	.519	.522	.495	.499
0.3	.481	.481	.524	.524	.525	.525	.510	.510
0.4	.519	.509	.545	.536	.543	.533	.534	.524
0.5	.558	.529	.574	.544	.569	.540	.564	.535
0.6	.598	.548	.605	.555	.599	.550	.597	.547
0.7	.636	.562	.638	.563	.632	.557	.631	.557
0.8	.671	.570	.668	.566	.663	.561	.664	.562
0.9	.702	.574	.696	.568	.691	.563	.693	.566
1.0	.728	.579	.719	.571	.715	.567	.718	.570

(1) P wave phase shifts from Jadusliwer and Paul (1973).
(2) P and D wave phase shifts from Drachman (1966a).

Contributions from higher partial wave phase shifts (equation 5.3) are included.

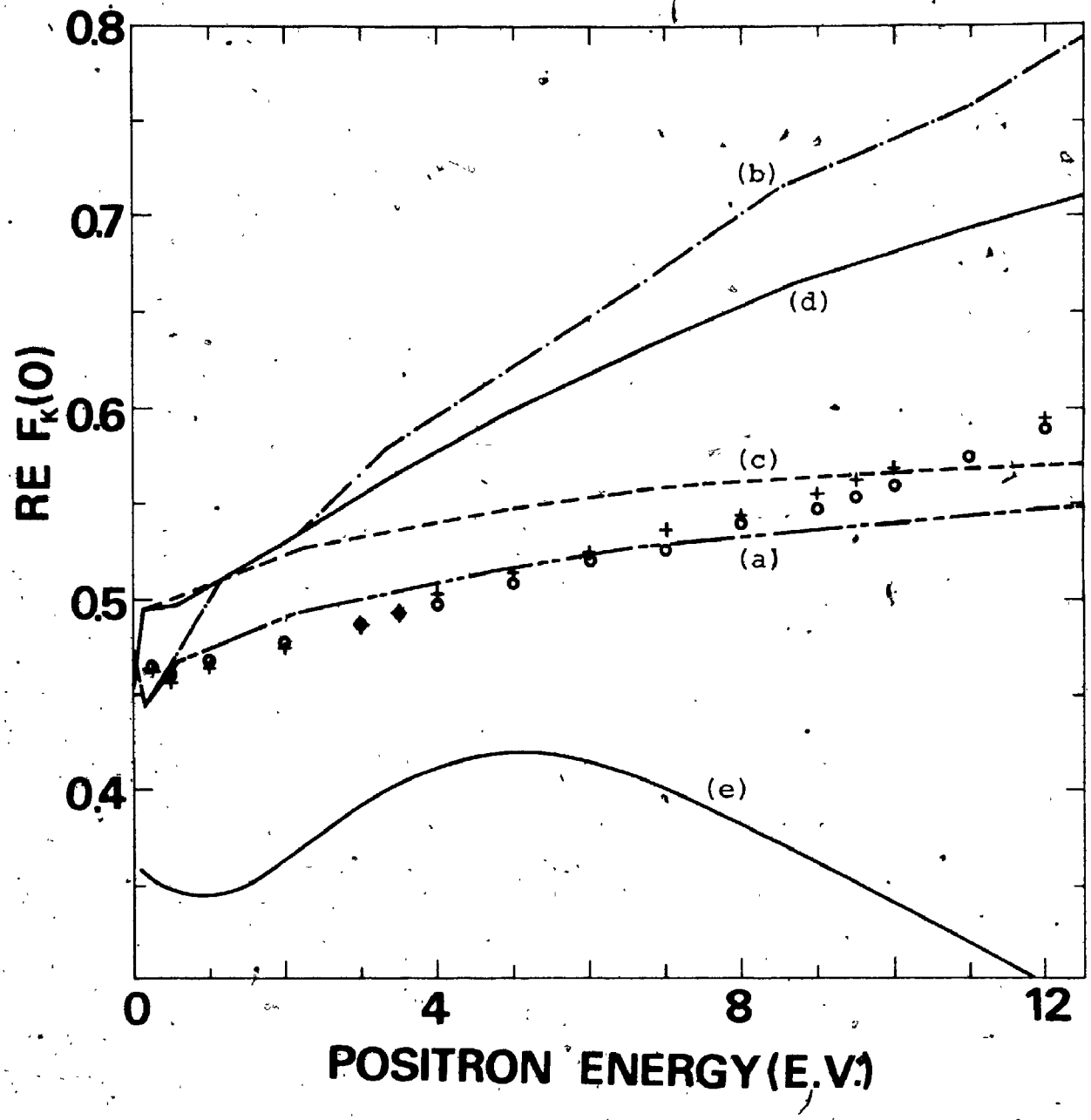

Figure 5.4 The Real Part of the Elastic Forward Scattering Amplitude

(a) Humberston's (1973) S-wave, Drachman's (1966a) P- and D-waves; (b) Humberston's (1973) S-wave, Drachman's (1971) P- and D-waves; (c) Present (HF2) S-wave, Drachman's (1966a) P- and D-waves; (d) Present (HF2) S-wave, Jaduszliwer and Paul's (1973) P-wave; (e) Aulenkamp et al (1974). Allowance is made for higher order phase shifts (eq. 5.3) for all the curves. Crosses and circles are from Bransden and Hutt (1975) in which experimental data of Jaduszliwer and Paul (1973) and Coleman et al (1974) respectively are used.

been calculated by Bransden, Hutt and Winters (1974) who employed the cross sections of Canter, Coleman, Griffith and Heyland (1973) for $k < 2.0$ and the theoretical adjustment for $k > 2.0$ such that the cross sections join smoothly to the region where the Born approximation is valid. After Coleman, Griffith, Heyland and Killeen (1974) presented the corrected cross sections and Jaduszliwer, Nakashima and Paul (1975) measured the total cross sections up to 270 eV, Bransden and Hutt (1975) obtained the RHS of equation (5.4) a value of -1.24 ± 0.05 and -1.39 respectively for these two sets of data. However, according to Jaduszliwer, Nakashima and Paul (1975), the value of the RHS is -1.015. Moreover these authors also obtained values of -1.235 and -1.315 when different extrapolations to the high energy region are used.

5.4 Effective Charge and Cusp Value

The S wave contribution to the effective charge has been calculated by using equations (4.7). The energy dependent effective charge is shown in figure 5.6 together with some other theoretical calculations, e.g. Humberston's (1974) (models H5 and HY2) and Drachman's (1968) model HY2. Some experimental results are also shown in figure 5.6; for example: the measurements at 77°K by Roellig and Kelly (1967) and by Leung and Paul (1969); at room temperature by Lee, Orth and Jones (1969) and by Coleman, Griffith, Heyland and

Killeen (1974).

The typical convergence behavior of Z_{eff} is shown in table 5.6. The fact that there is no bound theorem for Z_{eff} is demonstrated at low energies. It is noted that a similar observation has been made by Bhatia, Drachman and Temkin (1974) in a positron-hydrogen annihilation calculation.

The final result (N=84) of the energy dependent S-wave Z_{eff} for the four helium models is shown in figure 5.5 and table 5.7. In the first entry of each model in table 5.7, we show the energy dependent Z_{eff} in which the contributions from undistorted higher partial waves (equation 4.8) are included. It is noted that such contribution is less than 30% for the highest energy we considered. In particular, the result of model HF2 is shown in figure 5.5.

The S-wave positron electron cusp values at N=84 are also shown in table 5.7. The final cusp values are quite close to the exact value -0.5. However, cusp values near zero energy and near the formation threshold are relatively poor. This may indicate that for zero energy, dipole type correlation terms may improve the performance, and for energies near threshold the explicit use of a positronium wave function may give a better cusp value. The typical convergence of the cusp values is shown at table 5.8. Again, like Z_{eff}, the lack of bound principle is shown at low energies.

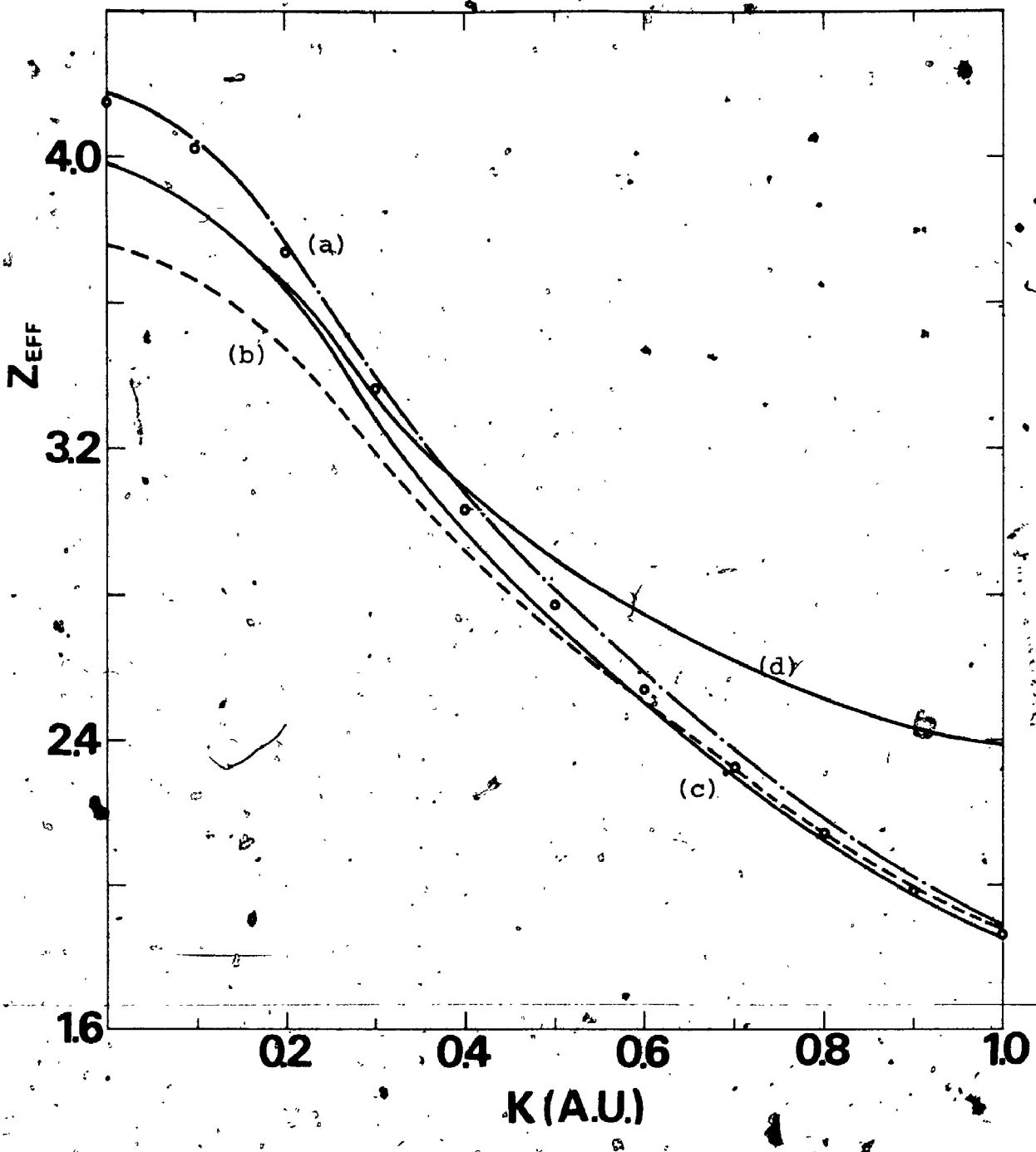

Figure 5.5 Effective Charge for Four Helium Models (a) HY2; (b) HY1; (c) HF2; The circles are from model HF1. The S-wave contribution is shown in (a)-(c) and the circles. Curve (d) is from HF2 in which the contributions from undistorted higher partial waves (eq. 4.8) are also included.

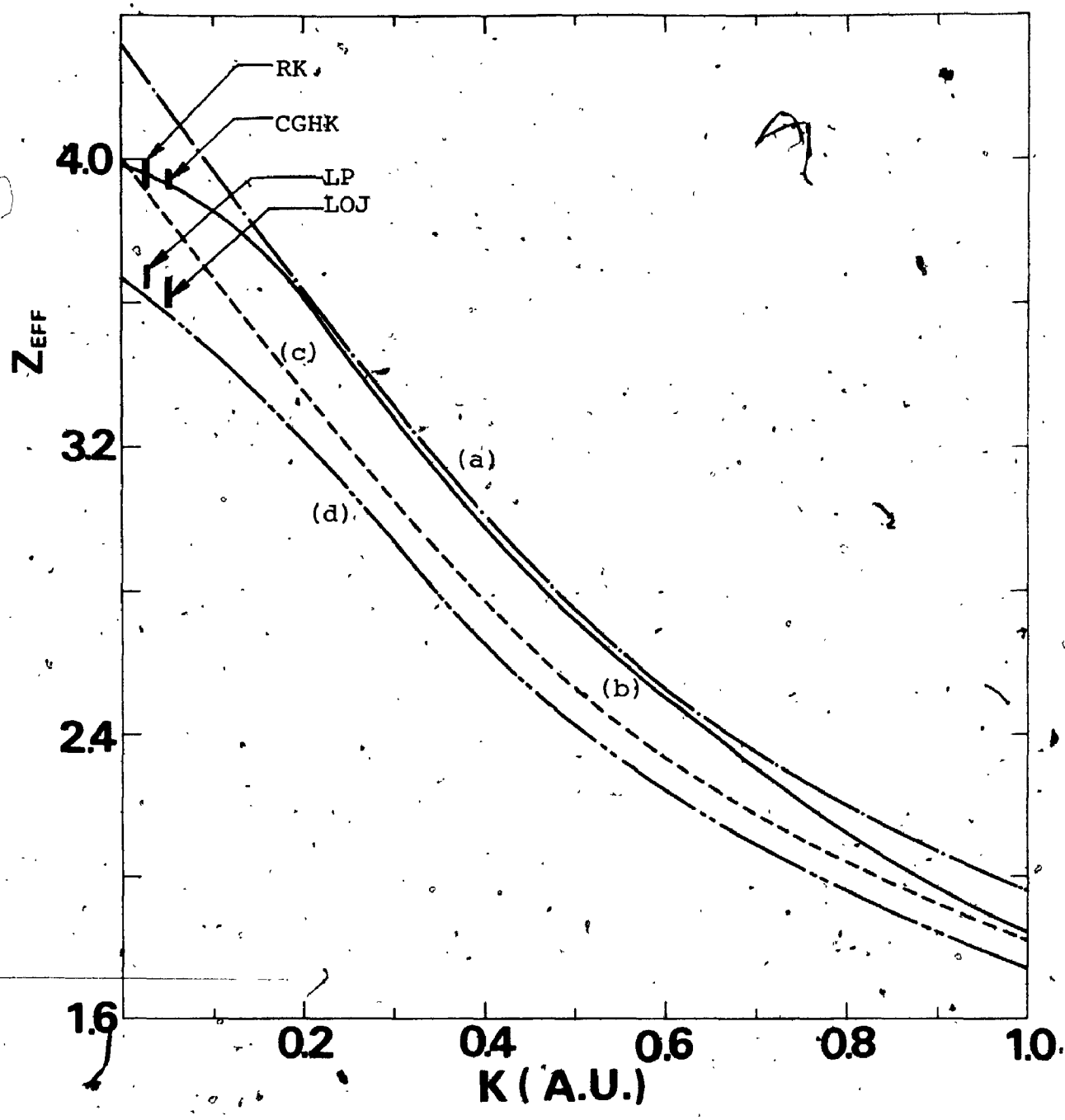

Figure 5.6 Effective Charge

The curves are from theoretical calculations in which only the S-wave contribution is included. (a) Humberston's (1974) model HY2; (b) Present work (model HF2); (c) Humberston's (1974) model H5; (d) Drachman (1968) (see Humberston 1974). The rectangles are from experimental results. LP: Leung and Paul (1969); LOJ: Lee, Orth, and Jones (1969); RK: Roellig and Kelly (1967); CGHK: Coleman, Griffith, Heyland and Killeen (1974).

Table 5.6 Convergence behavior of Z_{eff} for model HF2

k \ N	4	10	20	35	56	84
0.0	2.541	2.909	3.775	3.800	4.108	3.983
0.1	2.437	2.855	3.569	3.693	3.874	3.853
0.2	2.443	2.916	3.767	3.528	3.577	3.631
0.3	2.178	2.722	3.022	3.222	3.253	3.281
0.4	1.922	2.530	2.744	2.908	2.972	2.973
0.5	1.701	2.342	2.525	2.632	2.712	2.723
0.6	1.521	2.158	2.345	2.410	2.473	2.504
0.7	1.377	1.983	2.187	2.233	2.269	2.304
0.8	1.263	1.821	2.043	2.088	2.102	2.126
0.9	1.172	1.677	1.911	1.963	1.967	1.974
1.0	1.099	1.550	1.787	1.853	1.852	1.848

Table 5.7 Effective charge and cusp value for four helium models

k	HY1			HY2			HF1			HF2		
	Z_{eff} (a)	Z_{eff} (b)	ν_{1p} (c)	Z_{eff} (a)	Z_{eff} (b)	ν_{1p} (c)	Z_{eff} (a)	Z_{eff} (b)	ν_{1p} (c)	Z_{eff} (a)	Z_{eff} (b)	ν_{1p} (c)
0.0	3.761	3.761	-.446	4.181	4.181	-.442	4.158	4.158	-.444	3.983	3.983	-.435
0.1	3.679	3.672	-.459	4.060	4.052	-.457	4.020	4.012	-.456	3.861	3.853	-.446
0.2	3.504	3.476	-.485	3.803	3.772	-.482	3.778	3.747	-.482	3.661	3.631	-.478
0.3	3.250	3.189	-.480	3.470	3.402	-.475	3.433	3.365	-.476	3.347	3.281	-.472
0.4	3.025	2.919	-.475	3.201	3.083	-.474	3.153	3.035	-.474	3.087	2.973	-.469
0.5	2.861	2.700	-.478	3.000	2.822	-.480	2.947	2.769	-.479	2.895	2.723	-.474
0.6	2.727	2.503	-.481	2.836	2.589	-.482	2.783	2.537	-.482	2.742	2.504	-.478
0.7	2.613	2.319	-.478	2.697	2.375	-.478	2.645	2.326	-.478	2.614	2.304	-.474
0.8	2.517	2.150	-.469	2.587	2.187	-.470	2.537	2.141	-.470	2.511	2.126	-.467
0.9	2.449	2.006	-.466	2.508	2.027	-.465	2.458	1.984	-.465	2.436	1.974	-.461
1.0	2.409	1.889	-.464	2.456	1.894	-.465	2.420	1.867	-.467	2.387	1.848	-.458

(a) Contributions from undistorted higher partial waves are included
(b) S-wave contribution
(c) S-wave positron-electron cusp value in a_o^{-1}

Table 5.8 Convergence behavior of cusp value ν_{lp} for model HF2

k \ N	4	10	20	35	56	84
0.0	-.190	-.268	-.375	-.397	-.454	-.435
0.1	-.188	-.272	-.370	-.405	-.445	-.446
0.2	-.212	-.309	-.397	-.438	-.457	-.478
0.3	-.206	-.318	-.389	-.442	-.458	-.472
0.4	-.198	-.325	-.387	-.437	-.464	-.469
0.5	-.190	-.329	-.391	-.431	-.464	-.474
0.6	-.183	-.330	-.397	-.429	-.458	-.478
0.7	-.175	-.328	-.403	-.431	-.432	-.474
0.8	-.168	-.323	-.406	-.436	-.449	-.467
0.9	-.163	-.317	-.407	-.442	-.452	-.461
1.0	-.158	-.310	-.405	-.447	-.456	-.458

Cusp value is in a_o^{-1}.

5.5 Excitation of Residual He^+ Ion

The probability P_n that the residual He^+ ion will be in a state n after annihilation has been calculated using equation (4.13). The typical convergence of different probabilities is shown at table 5.9 for model HF2 at zero energy. It is found that except for small N, the result changes little as N increases, and also the lack of bound principle is once again demonstrated. In tables 5.10a and b, we show the energy dependent probabilities for models HY2 and HF2 respectively at 84 correlation terms. It is found that they are nearly energy independent and more than 98% of the He^+ ions are in the 1S state for model HF2.

There is a favorable transition 2P-1S ultraviolet line at 304 Å for the radiative de-excitation of the residual He ion. In table 5.11, we show the results for model HY2, the fraction of each state which eventually reaches the 2P state is shown in column 3 in which cascade processes like 5S-4P-3S-2P are included. For model HY2, we found that the total probability for a 2P-1S transition after annihilation is about 0.48% compared with 1.2% found by Drachman (1966b) using the same helium model. By comparing the results of HY2 and HF2 which are shown in tables 10a and b respectively, we expect the probability is even smaller for model HF2.

Table 5.9 Convergence behavior for different probabilities for model HF2 at k = 0.0

N / states	4	10	20	35	56	84
P_{1s}	97.73	98.10	98.00	98.06	98.05	98.06
P_{2s}	.75	.92	.91	.90	.91	.91
P_{2p}	.55	.18	.19	.19	.17	.18
P_{3s}	.15	.12	.13	.14	.13	.13
P_{3p}	.055	.033	.032	.027	.027	.027
P_{3d}	.0009	.0034	.0021	.0018	.0020	.0019

Probabilities are in percentage.

Table 5.10a Energy dependent probability (in %) for model HY2 at N = 84

k states	P_{1s}	P_{2s}	P_{2p}	P_{3s}	P_{3p}	P_{3d}	P_{4s}	P_{5s}	P_{6s}
0.0	96.89	1.35	.19	.22	.032	.002	.077	.037	.020
0.1	96.89	1.35	.19	.22	.032	.002	.077	.037	.020
0.2	96.90	1.34	.19	.22	.032	.002	.077	.037	.020
0.3	96.91	1.33	.19	.22	.032	.002	.077	.036	.020
0.4	96.93	1.31	.20	.22	.033	.002	.076	.036	.020
0.5	96.96	1.28	.20	.21	.033	.002	.075	.035	.020
0.6	97.00	1.26	.20	.21	.034	.002	.073	.035	.019
0.7	97.04	1.22	.20	.20	.035	.002	.072	.034	.019
0.8	97.09	1.17	.21	.20	.037	.002	.070	.033	.018
0.9	97.16	1.12	.22	.19	.038	.002	.068	.032	.018
1.0	97.23	1.06	.22	.18	.039	.002	.065	.031	.017

Table 5.10b Energy dependent probability (in %) for model HF2 at N = 84

k (States)	P_{1s}	P_{2s}	P_{2p}	P_{3s}	P_{3p}	P_{3d}
0.0	98.06	.91	.18	.13	.027	.0019
0.1	98.06	.90	.18	.13	.027	.0019
0.2	98.07	.90	.18	.13	.027	.0019
0.3	98.08	.89	.18	.13	.027	.0019
0.4	98.10	.87	.19	.13	.028	.0019
0.5	98.12	.85	.19	.13	.029	.0018
0.6	98.15	.82	.19	.12	.030	.0018
0.7	98.19	.79	.19	.12	.031	.0017
0.8	98.23	.75	.20	.11	.032	.0017
0.9	98.29	.70	.20	.11	.033	.0016
1.0	98.35	.65	.21	.10	.034	.0015

Table 5.11 Population (in %) and branching ratio of the 2P state after annihilation.

model HY2, k = 0.0, N = 84

States	Population	Branching ratio to 2P*	Contribution to 2P state Present	Drachman (1966b)
2P	.19	1	.19	.82
3S	.22	1	.22	.32
4S	.077	.58	.045	.058
5S	.037	.45	.017	.022
6S	.020	.43	.0086	.012
Total			.48%	1.12%

* Cascades like 5S - 4P - 3S - 2P are included in this column; see Drachman(1966b) and Bethe and Salpeter (1957).

CHAPTER 6

PROBLEMS RELATED TO THE PRESENT CALCULATION

6.1 Introduction

During the course of the present work, some related calculations have also been carried out. For example, Peterkop and Rabik (1971) used different variants to test Kohn's variational method when an inexact target wave function is employed. Judging from the similarity and differences between the method of models and these variants, it is possible to carry out such calculations without much change of the existing program subroutines. Consequently we performed such calculations and the results are presented in section 2.

During the calculation of these variants, the true Hamiltonian of the e^+-He system has to be used in evaluating certain matrix elements H_{ij}. In examining the eigenvalues of the true Hamiltonian, one eigenvalue seems to be stable. The results are shown in section 3 in which a possible resonance in e^+-He scattering is discussed.

6.2 Different Variants of Peterkop and Rabik

Peterkop and Rabik (1971) investigated the effect of

inexact target wave functions in scattering length calculations using different variants of Kohn's variational method. It may be of interest to apply these variants to the e^+-He scattering problem. If we write the operator (H-E) as

$$H-E = -\nabla_p^2 - \frac{2}{r_{1p}} - \frac{2}{r_{2p}} + \frac{4}{r_p} + C(-\nabla_1^2-\nabla_2^2 + \frac{2}{r_{12}} - \frac{4}{r_1} - \frac{4}{r_2} - E_o) - k^2 \quad (6.1)$$

and characterize equation (2.16) as

$$\langle\psi_o|H-E|\psi_o F\rangle + \langle\psi_o|H-E|\Sigma C_i\chi_i\rangle \equiv (\text{open-open}) + (\text{open-closed}) = 0; \quad (6.2)$$

$$\langle\chi_j|H-E|\psi_o F\rangle + \langle\chi_j|H-E|\Sigma C_i\chi_i\rangle \equiv (\text{open-closed}) + (\text{closed-closed}) = 0, \quad (6.3)$$

we may describe the different variants as follows

Variant I $C=1, E_o=E_{av}$ in (open-closed) and (closed-closed)

Variant II $C=0, E_o=E_{av}$ in (open-closed), $C=1, E_o=E_{av}$ in (closed-closed)

Variant III $C=1, E_o=E_{ex}$ in (open-closed) and (closed-closed)

Variant IV $C=0, E_o=E_{ex}$ in (open-closed), $C=1, E_o=E_{ex}$ in (closed-closed)

For the (open-open) terms, $C=1$ and $E_o=E_{av}$ is applied to all variants so that the integral exists, and E_{av} and E_{ex} are the variational average energy and the exact energy (Pekeris

1959) of the helium atom respectively.

It should be mentioned that the bound theorem does not apply to these variants, hence it may not be useful to optimize the non-linear parameters. Consequently, we used the same set of non-linear parameters as those which gave optimized values in the method of models calculation.

We show the results of variants II and IV for models HY2 and HF2 in tables 6.1 to 6.4. The results of variant IV seem generally to behave better than those of variant II. From the result in table 5.3, it seems that the bound theorem is violated. Moreover, it is noted that phase shifts from variants II and IV are lower than those from the corresponding model in the method of models calculation.

The results of variant I are shown in table 6.5. Except for the HF models, the scattering length changes sign as N increases. This indicates that singularities exist. Furthermore, from the results of Spruch and co-workers, that the scattering length of the positron helium system must be bounded below by -0.7 (Hahn and Spruch 1974) and above by 0.796 (Blau, Rosenberg and Spruch 1975), it is clear that variant I will give unrealistic scattering lengths if the target wave function is relatively poor. The results for model HF1 are rather interesting (table 6.6). It is noted that except for low energies (i.e. for $k < 0.5$), the convergence

Table 6.1 Convergence behavior of phase shifts from model HY2 in a variant II calculation

k \ N	4	10	20	35	56	84
0.0	-.2822	-.3359	-.3942	-.4159	-.4299	-.4406
0.05	.01364	.01626	.01884	.01973	.02024	.02056
0.10	.02465	.02960	.03314	.03418	.03461	.03476
0.15	.03100	.03813	.04088	.04183	.04227	.04238
0.20	.03169	.04137	.04265	.04387	.04464	.04482
0.25	.02663	.03980	.03997	.04159	.04255	.04279
0.30	.01639	.03426	.03403	.03569	.03663	.03713
0.40	-.01579	.01424	.01463	.01545	.01661	.01754
0.50	-.05728	-.01493	-.01254	-.01201	-.01075	-.009733
0.60	-.1022	-.04924	-.04436	-.04399	-.04223	-.04136
0.70	-.1470	-.08704	-.07714	-.07838	-.06891	-.07519
0.80	-.1897	-.1245	-.09539	-.1166	-.1125	-.1095
0.90	-.2290	-.1535	-.1769	-.1521	-.1471	-.1434
1.00	-.2640	-.3551	-.2016	-.1868	-.1803	-.1770

Phase shifts are in radians; the k=0 entry is the scattering length.

Table 6.2 Convergence behavior of phase shifts from model HY2 in a variant IV calculation

k \ N	4	10	20	35	56	84
0.0	-.1658	-.2800	-.3432	-.3699	-.3829	-.3944
0.05	.007931	.01349	.01638	.01751	.01797	.01835
0.10	.01381	.02416	.02863	.03012	.03048	.03076
0.15	.01605	.03017	.03490	.03638	.03674	.03705
0.20	.01378	.03102	.03566	.03741	.03809	.03853
0.25	.006892	.02717	.03225	.03443	.03531	.03584
0.30	-.004227	.01950	.02574	.02807	.02896	.02976
0.40	-.03625	-.004160	.005305	.007452	.008480	.009758
0.50	-.07620	-.03538	-.02309	-.01998	-.01907	-.01749
0.60	-.1192	-.07146	-.05668	-.05168	-.05074	-.04879
0.70	-.1622	-.1102	-.09291	-.08620	-.08439	-.08217
0.80	-.2034	-.1498	-.1300	-.1220	-.1189	-.1161
0.90	-.2418	-.1887	-.1668	-.1577	-.1535	-.1496
1.00	-.2770	-.2259	-.2024	-.1922	-.1866	-.1826

Phase shifts are in radians; the k=0 entry is the scattering length.

Table 6.3 Convergence behavior of phase shifts from model HF2 in a variant II calculation

k \ N	4	10	20	35	56	84
0.0	-.2039	-.3203	-.3868	-.4137	-.4144	-.4201
0.05	.009802	.01546	.01848	.01962	.01946	.01955
0.10	.01737	.02786	.03248	.03395	.03308	.03281
0.15	.02098	.03525	.04001	.04147	.04006	.03960
0.20	.01973	.03712	.04160	.04339	.04190	.04132
0.25	.01352	.03400	.03876	.04102	.03944	.03867
0.30	.002812	.02685	.03265	.03504	.03330	.03253
0.40	-.02888	.003897	.01273	.01470	.01308	-.01250
0.50	-.06871	-.02685	-.01527	-.01269	-.01419	-.01439
0.60	-.1115	-.06252	-.04833	-.04427	-.04521	-.04499
0.70	-.1540	-.1008	-.08376	-.07836	-.07722	-.07693
0.80	-.1943	-.1398	-.1197	-.1130	-.09842	-.1133
0.90	-.2316	-.1778	-.1548	-.1390	-.1465	-.1400
1.00	-.2652	-.2137	-.1871	-.1847	-.1836	-.1817

Phase shifts are in radians; the k=0 entry is the scattering length

Table 6.4 Convergence behavior of phase shifts from model HF2 in a variant IV calculation

k \ N	4	10	20	35	56	84
0.0	-.1737	-.2900	-.3534	-.3789	-.3922	-.4074
0.05	.008315	.01398	.01686	.01793	.01841	.01898
0.10	.01453	.02506	.02949	.03086	.03121	.03191
0.15	.01704	.03138	.03598	.03733	.03763	.03861
0.20	.01498	.03244	.03685	.03849	.03908	.04036
0.25	.008219	.02873	.03349	.03559	.03634	.03781
0.30	-.002802	.02116	.02702	.02927	.03002	.03180
0.40	-.03463	-.002286	.006702	.008684	.009607	.01190
0.50	-.07426	-.03321	-.02143	-.01860	-.01779	-.01524
0.60	-.1167	-.06883	-.05455	-.04992	-.04913	-.04640
0.70	-.1589	-.1070	-.09006	-.08379	-.08220	-.07953
0.80	-.1990	-.1457	-.1262	-.1187	-.1159	-.1130
0.90	-.2362	-.1836	-.1619	-.1532	-.1493	-.1459
1.00	-.2699	-.2195	-.1962	-.1863	-.1812	-.1781

Phase shifts are in radians; the k=0 entry is the scattering length.

Table 6.5 Scattering lengths from variant I for different models

models \ N	4	10	20	35	56	84
HY1	-1.455	-20.865	39.847	23.875	18.825	18.891
HY2	-9.085	25.909	17.291	15.737	13.763	16.572
HF1	-0.1429	-0.3323	-0.4057	-0.4653	-0.5271	-0.6425
HF2	-0.6569	-1.958	-3.985	-7.859	-14.953	-30.228

Table 6.6 Convergence behavior of phase shifts from model HF1 in a variant I calculation .

k \ N	4	10	20	35	56	84
0.0	-.1429	-.3302	-.4057	-.4653	-.5271	-.6425
0.05	.006888	.01600	.01946	.02199	.02440	.02888
0.10	.01228	.02913	.03450	.03760	.03995	.04474
0.15	.01495	.03739	.04287	.04500	.04637	.05053
0.20	.01410	.04002	.04470	.04597	.04728	.05149
0.25	.009406	.03729	.04140	.04263	.04433	.04798
0.30	.0009671	.03002	.03441	.03604	.03767	.04036
0.40	-.02547	.005871	.01293	.01470	.01559	.01749
0.50	-.06085	-.02594	-.01582	-.01434	-.01342	-.01214
0.60	-.1008	-.06160	-.04957	-.04727	-.04641	-.04552
0.70	-.1420	-.09905	-.08587	-.08196	-.08125	-.08032
0.80	-.1823	-.1369	-.1227	-.1173	-.1162	-.1155
0.90	-.2204	-.1741	-.1586	-.1522	-.1503	-.1497
1.00	-.2554	-.2097	-.1927	-.1857	-.1826	-.1802

Phase shifts are in radians; the k=0 entry is the scattering length.

behavior is not unreasonable. This suggests that for an open channel calculation which variant I is the natural choice, model HF1 may give meaningful results (Ho, Fraser and Kraidy 1975). Model HF2 also has similar behavior at $k > 0.6$, even though the scattering length is rather disappointing. For simplicity, we do not show the results of variant III, but it is the worst among these variants. The singularity in the scattering length even appears earlier as N increases.

For the final result of this thesis, we prefer the results from the method of models calculation. Since by taking the advantage of bound property, we are able to improve the results systematically. However, judging from the good convergence behavior of variant IV, we suggest that in calculations on electron-atom scattering where the method of models no longer applies, variant IV type calculations may be worth trying.

6.3 Possible Resonance in Positron Helium Scattering

In evaluating the matrix elements H_{ij} in the previous section, we have to employ the true Hamiltonian of the positron-helium system. It is interesting to examine the behavior of the eigenvalues of the true Hamiltonian. First of all, it is found that the lowest eigenvalue in the basis of the true Hamiltonian of the positron-helium system is

higher than the ground state energy of helium (Pekeris 1959). This is consistent with the conclusions by Gertler, Snodgrass and Spruch (1968) that a positron and a helium atom do not bind. Secondly, the result of one set of non-linear parameters ($\alpha=\beta=1.6875$, $\gamma=0.65$) is worth mentioning. The lowest ten eigenvalues which were calculated on increasing the basis by step of 2 are shown in figure (6.1). The fifth eigenvalue seems to be stable in the region of N=38 to 52. Furthermore, it is taken over by the sixth eigenvalue in the region N=58 to 80. In the context of stabilization, this corresponds to a resonance in the e^+-He system.

Several authors have used the stabilization method in recent years. Taylor (1970) in a review article discussed the nature of stabilization. Hazi and co-workers applied this method to model problems for elastic scattering (Hazi and Taylor 1970) and inelastic scattering (Fels and Hazi 1972). The H^- and He^- problems have been investigated by Taylor and Thomas (1972) and Elizer and Pan (1970) respectively. Bhatia (1974a, b) has applied this method to H^- and He antoionization calculations. Recently, Drachman and Houston (1975) used this method to locate a possible resonance position for the positronium hydrogen system.

If we consider the mid-point of the stabilized region to be the stabilized eigenvalue, we have $E_s=-4.3099$ and the

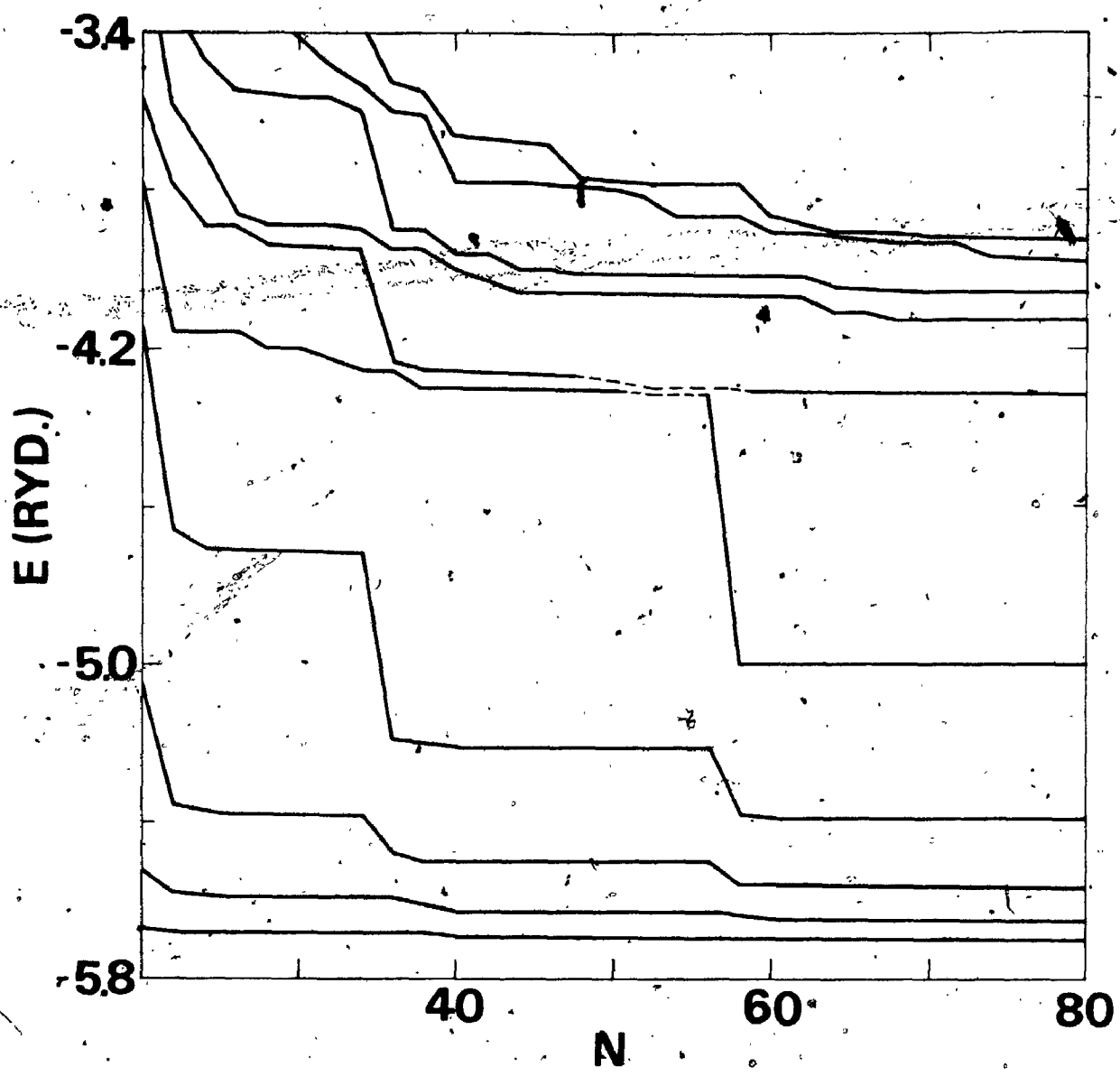

Figure 6.1 Eigenvalues of the e^+-He Hamiltonian

The lowest ten eigenvalues are plotted as a function of N in steps of N=2 ($\alpha=\beta=1.6875$, $\gamma=0.65$; see eq. 3.2)

resonance position (if a resonance does exist) would be $E_s - E_{He} \simeq 20.375$ eV, where E_{He} is the ground state energy of the helium atom (Pekeris 1959). This resonance is located in a region above the positronium formation threshold and just below the first singlet excitation of helium atom at 20.6 eV (see equation 2.4c).

There has been some interest in the positron-hydrogen resonance problem in the energy region above the positronium formation threshold and below the first hydrogen excitation threshold. Mittleman (1966) has pointed out that there could be an infinite series of resonances just below the first hydrogen excitation threshold, through the same mechanism as in the electron case. Hahn (1974) (and some references contained therein) discussed the difficulties in the theoretical calculation of such resonances and a series of tests were proposed to clarify the question. There have been some indications that such resonances must lie considerably higher than in the corresponding e^--H case (Chan and Fraser 1973, Drachman 1975) or that they are even pushed over the first excitation level of hydrogen (Chan and Fraser 1973). It is interesting that Chan and Fraser (1973) observed no stabilization of eigenvalues in the positron-hydrogen problem.

The resonance for e^+-He system at 20.375 eV is still yet to be confirmed. Nevertheless, this calculation hopefully

will provide some reference for future investigation, both experimental and theoretical.

CHAPTER 7

CONCLUSION

We have performed a bound calculation based on the method of models for positron-helium scattering below the positronium formation threshold in terms of various target helium atom models. We used the correlation method to construct an optical potential and the phase shifts are obtained from the solution for the scattering function. The integro-differential equation for the radial function was first converted into an integral equation by use of Green's function, and the numerical functional values of the radial function was then obtained by solving a system of linear equations.

In order to retain the bound properties, the method of models (Drachman 1972b) has been employed such that the phase shifts (scattering lengths) are lower (upper) bounds in terms of the helium models. Four helium wave functions have been used throughout this thesis. It has been found that the bound theorem indeed applies. Furthermore, if we compare our results with other calculations for a particular helium model, namely HY2, it has been found that our phase shifts

are higher than some other calculations (Drachman 1968, Houston and Drachman 1971) and based on the bound principle, we are able to conclude that our results are more reliable for that particular model.

The final results of this thesis are chosen to be those from model HF2, a three parameter Hartree-Fock type wave function with the correct polarizability. The importance of being correctly polarizable for target atom in low energy scattering has been confirmed by Ho and Fraser (1975) for the positron-hydrogen problem. However, the results of model HF2 differ significantly from those by Humberston (1973) who used an elaborate five parameter helium wave function and employed an algebraic Kohn type calculation which lacks a bound property for phase shifts. It may suggest that a more definitive solution, similar to the e^+-H case (Bhatia, Temkin, Drachman and Eiserike 1971), could be obtained using the present method (correlation method together with the method of models) and more elaborate helium wave functions. It is the intention that such calculation will be carried out in the near future.

The total cross sections have been calculated using S-wave phase shifts from the present results and higher partial waves from other calculations and experiments. When we combined S wave phase shifts from model HF2 and the P wave

from Jaduszliwer and Paul (1973) the total cross sections are closer to Jaduszliwer and Paul (1973) than those of Canter, Coleman, Griffith and Heyland (1973). However, a more accurate P and D wave calculation should be done in order to get a better picture.

The sensitivity to the P and D waves is more clear if we consider the real part of the forward scattering amplitude. It has been found that using the same S wave phase shifts but different P and D waves (i.e. Drachman 1971 and the lowest phase shifts of Drachman 1966a) gave very different results. A bound calculation using the present method (correlation method together with the method of models) should provide a better calculation for P and D waves.

The energy dependent Z_{eff} has also been evaluated. At thermal energy where the S wave component of Z_{eff} dominates the contribution, the result of HF2 is close to experimental measurements by Roellig and Kelly (1968) and Coleman, Griffith, Heyland and Killeen (1974). Of course, if the dipole type correlation terms are included, it is expected that Z_{eff} will increase. Cusp values which may probe the accuracy of the trial function near the point of coalescence between positron and electron have been calculated. It has been found that they are quite close to the exact value -0.5.

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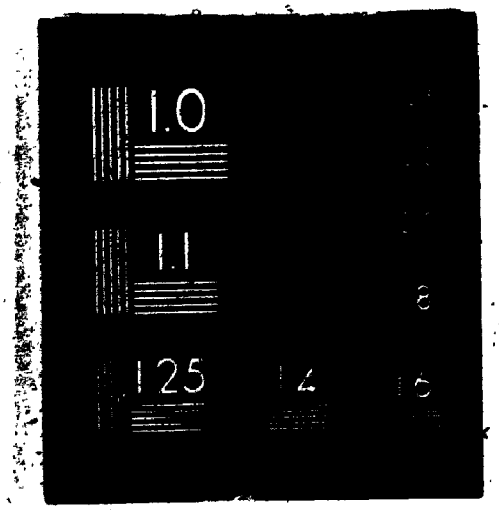

The different probabilities P_n of finding the residual He^+ ion in state n following an annihilation also have been calculated. It has been found that more than 98% of the He^+ ions are in the 1S state. The radiative de-excitation of 2P-1S transition, including the cascade process from higher S states to the 2P state, is found to be less than 0.48%. Moreover, P_n is found to be nearly independent of the energy of the incoming positron for energies considered in this work.

Besides the method of models calculation, different variants of Peterkop and Rabik (1971) also have been tried. The lack of bound principle is clear for variant I and III where violently varying results have been observed. However, the reasonable convergence behavior for energies near threshold for model HF1 in a variant I calculation suggest that an open channel calculation where variant I is the natural choice, may be meaningful to pursue. Even though the bound principle does not apply, the convergence behavior of variants II and IV are quite good and these give relatively lower phase shifts compared with the corresponding method of models calculation. The good convergence behavior of variant IV may suggest an e^--He calculation where the method of models no longer applies, is worth a try. A variant IV type calculation for e^+-He with more elaborate helium wave function is also worthwhile to try. Since the correlation terms need

not have the product form of $\psi_o\chi$ (equation 2.29) in a variant IV calculation, it requires less computation to evaluate the matrix elements H_{ij}, A_{ij} etc., compared with the method of models when an elaborate helium wave function is employed. Essentially, all the four variants and the method of models should lead to the same result as the target wave function approaches exactness.

In examining the eigenvalues of the true Hamiltonian, one eigenvalue seems to be stable. This corresponds to a possible e^+-He resonance at 20.375 eV, just below the first singlet excitation of He atom of 20.6 eV. Of course, this indicated resonance needs to be confirmed. The present calculation hopefully will provide some reference for future investigation both experimentally and theoretically.

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