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Theoretical and Experimental Positron Annihilation and Scattering Cross Sections in Helium

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A comparison is made between the experimental results and results calculated from theoretical values of annihilation and scattering (momentum-transfer) cross sections on free-positron-annihilation lifetime spectra in helium gas at temperatures of 4.2 , 77 , and 300°K. It is found the annihilation cross section calculated by Drachman using Dalgarno and Lynn's complete first-order adiabatic correlation function, incorporated with the method of variational bounds, agrees with the experimental results. It is also found that both the momentum-transfer cross section calculated by Drachman with $\alpha = 0$ and $C = 1$ and the one by Massey *et al.* fit the experimental results well, although the one by Drachman seems to be better. The limitations of this method and the results using other values of cross sections are also discussed.

I. INTRODUCTION

The values of low-energy positron-helium scattering and annihilation cross sections have always been of great interest to both the theoretician and experimentalist. At the moment, only one experimentally determined value of the scattering cross section has been reported.[1,2] A few values of annihilation cross sections at thermalized energies also have been reported and summarized in the table by Hogg *et al.*[3] For theoretical work, the early simple calculations of scattering cross sections made by Massey and Moussa,[4] and Allison *et al.*[5] were found to be in poor agreement with the one experimental value.[6] Recently, more refined calculations of scattering cross sections based upon the adiabatic approximation have been made to include the effect of polarization.[7–9] Massey *et al.*[7] made their calculation based upon the polarization potential obtained by the method of Temkin and Lamkin.[10] Drachman[9] attacked this problem by applying the exact second-order polarization potential of Dalgarno and Lynn.[11] The positron-annihilation rate in helium has also been calculated by Drachman[12,13] using a similar method.

This paper will use the method of Tao[14] to construct the positron-annihilation lifetime spectra in helium using these theoretical values of cross sections, and then compare them with the actual positron-annihilation lifetime spectra in helium obtained from experiments. Such a comparison is not very straight forward because positrons annihilate during slowing down if a radioactive element such as Na^{22} is used as a positron source. There may exist more than one combination of scattering (or momentum decrement) cross section and annihilation cross section, which may fit an actual annihilation spectrum. Therefore, this method only gives an indication of the reasonableness of the theoretical result but does not prove uniqueness. However, the ways of obtaining reasonable theoretical cross sections are limited. Besides, more restrictions will be imposed if the experiments are carried out at various temperatures. Thus, with the limitations imposed by these restrictions this will give us very important information regarding the process of positron scattering and annihilation in helium.

II. EXPERIMENTAL RESULTS

Positron annihilation in dense helium gas at temperatures of 77 and 4.2°K has been studied by Roellig and Kelly.[15,16] Their results will be used here. A series of experiments of measuring positron annihilation in helium at room temperature of 300°K has been carried out in this laboratory. A time to amplitude with resolution of full width at half-maxium (FWHM) is equal to 0.6 nsec and range of 300 nsec was used for the measurement. Special precautions were taken to keep the ultra-high purity helium gas (99.999% by spectral analysis) free from contamination.

A broad shoulder and a second peak was discovered in positron-annihilation spectra in dense helium gas at 4.2°K as reported by Roellig and Kelly.[15] This component was attributed to free positron annihilation and the appearance of the second peak was interpreted as due to liquid drop formation.[15] A spectrum of the free-positron-annihilation component at a pressure of 0.98 atm and a density of 0.0168 g cm^{-3} at 4.2°K is reproduced in Fig. 1. The average annihilation rates at the shoulder portion and the tail portion for various densities of the gas are shown in Fig. 2. This distinct peak disappears at lower densities or the higher temperature of 77 and 300°K. The annihilation rates of free positron annihilation in very dense helium gases at 77° K[16] are also shown in Fig. 2. The shoulder here is narrow and not pronounced enough to be determined accurately.

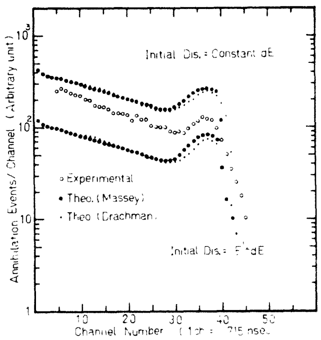

FIG. 1. Free-positron-annihilation lifetime spectrum in helium gas of density 0.0168 g cm^{-3} at 4.2°K. Experiment is the experimental result (Refs. 15 and 16). Drachman is constructed from theoretical annihilation cross section by Drachman (Ref. 13) and momentum-transfer cross section by Drachman (Ref. 9) with $\alpha = 0$, $C = 1$. Massey is constructed from theoretical annihilation cross section by Drachman (Ref. 3) and momentum-transfer cross section by Massey *et al.* (Ref. 7.)

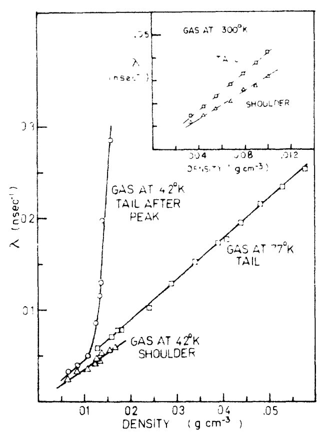

FIG. 2. Free-positron-annihilation rates at shoulder and tail parts in helium gas of various densities and temperatures of 4.2, 77, and 300° K.

The positron-annihilation spectra in helium at a density between 0.003 and 0.0109 g cm^{-3} and at room temperature, in general, show a vague shoulder part. The shoulder broadness is very difficult to determine exactly. This arises from the fact that the average free-positron-annihilation rate changes slowly at the shoulder region and no real flat region can be found.[17] One of the annihilation spectra of the free-positron-annihilation component at a helium density of 0.0090 g cm^{-3} is reproduced in Fig. 3 as an example. However, if we treat the flatter part near the prompt peak as the shoulder and the part farthest away from the shoulder as the tail, at least we are still able to calculate the averaged annihilation rates at both the shoulder and the tail parts. These rates are plotted against the density of helium in the corner of Fig. 2.

After a glance at Fig. 2, it is very interesting to note that both the average free-positron-annihilation rate in the shoulder region and in the tail region obey faithfully a linear dependence on the density of helium gas at the various temperatures. This is just the dependence one expects based on the Dirac rate equation for positrons annihilating from a free plane-wave state;

$$\lambda = \pi r_0^2 C \, Z_k \rho, \tag{1}$$

where ρ is the density of the gas and Z_k is the effective number of electrons per helium atom which participate in the annihilation process. The rate constants are calculated to be 3.5 nsec^{-1} g cm^{-3} at a temperature of 4.2 °K and 3.2 nsec^{-1}g cm^{-3} at a temperature of 300 °K for the shoulder region; and 4.4 nsec^{-3} at 4.2 and 77 °K, and 4.2 nsec^{-1} g cm^{-3} at 300 °K for the tail part. It also should be noted that at 4.2°K when the second peak gradually disappears due to the lower density of helium, the average rate of the tail part also approaches the regular rate at a temperature of 77°K. The discrepancies between the values obtained from low temperatures and room temperatures are within experimental error, particularly in view of the fact that these two sets of data have been obtained from experiments conducted in two different places at different times.

If we take the averaged values of these two sets of rate constants, we obtain 3.4 nsec^{-1} g cm^{-3} for shoulder region and 4.3 nsec^{-1}g cm^{-3} for tail region which are equivalent to $Z_k = 3.04$ and $Z_k = 3.84$, respectively. The Dirac rate is $Z_k = 2$. The value of $Z_k = 3.84$ at tail region agrees very

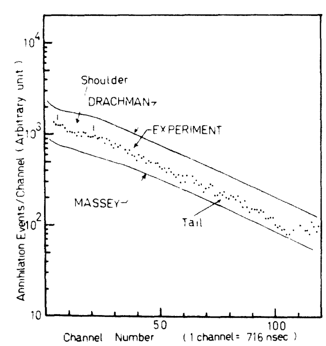

FIG. 3. Free-positron-annihilation lifetime spectrum in helium gas of density 0.0090 g cm^{-3} at 300° K. Experiment is the experimental result. Drachman is constructed from theoretical annihilation cross section by Drachman (Ref. 13) and momentum-transfer cross section by Drachman (Ref. 9) with $\alpha = 0$, $C = 1$. Massey is constructed from theoretical annihilation cross section by Drachman (Ref. 13) and momentum-transfer cross section by Massey *et al.* (Ref. 7.)

well with other experimental results.[3,18,19]

The second peak observed in the free-positron-annihilation spectrum in dense helium gas at 4.2°K deserves special attention. This is certainly a resonance phenomenon since it is highly pressure- (or density) and temperature-dependent. Since this is attributed to a special phenomena, liquid drop formation,[15] we can superimpose the effect due to this phenomenon onto the ordinary scattering process. Fortunately, because of the existence of such a high resonance annihilation at such a temperature 4.2 °K it provides a very good guide for the range of the average value of the possible scattering cross section. The sharpness of the peak at the higher densities also provides a certain limit to the pattern and the value of the scattering cross section.

III. CONSTRUCTION OF THEORETICAL ANNIHILATION SPECTRA

If the values of annihilation cross section and scattering (momentum-transfer) cross section are known, we can construct the annihilation spectra provided the initial energy distribution of positrons is known.[6] We have the annihilation events at a certain time t_i

$$R(t_i) = \sum_E \lambda(E) N(E, t_i)\,\Delta E, \tag{2}$$

where $\lambda(E) = N\sigma_a(E)\,v$ is the annihilation rate for positrons at an energy E, $N(E, t_i)$ is the energy distribution of positron at a time t_i, $\sigma_a(E)$ is the annihilation cross section, and N is the density of the medium particles. If all the electrons in the medium are considered free, the annihilation rate is given by the Dirac equation (1).

Note that the Dirac rate is not energy-dependent. Sometimes it is convenient to write

$$\lambda(E) = NZ_k(E)\,\pi r_0^{\,2} c, \tag{3}$$

where $Z_k(E)$ is called the effective number of electrons per particle.

The averaged annihilation rate at a time t_i is

$$\lambda(t_i) = R(t_i)/N(t_i), \tag{4}$$

and

$$N(t_i) = \sum_E N(E, t_i)\Delta E. \tag{5}$$

Obviously, $\lambda(t_i)$ will be a constant if either $N(E, t_i)$ is not time-dependent or $\lambda(E)$ is not energy-dependent. The experimental evidence of time varying annihilation rate indicates the $N(E, t_i)$ is time-dependent and $\lambda(E)$ is energy-dependent.

We have a recurrence relationship for the positron energy distribution at a time t_i

$$\begin{aligned} N(E, t_i) = {} & N(E, t_{i-1}) \\ & + \textstyle\sum_{E'} \lambda_s(E', E) N(E', t_{i-1})\Delta E' \\ & - \lambda(E, t_{i-1}) N(E, t_{i-1}) \\ & - \textstyle\sum_{E''} \lambda_s(E, E'') N(E, t_{i-1})\Delta E'', \end{aligned} \tag{6}$$

where $\lambda_s(E_1, E_2)$ are partial scattering rates for positron from an initial energy of E_1 to a final energy E_2.

For positrons in inert gases, formula (6) may be simplified

$$\begin{aligned} N(E, t_i) = {} & N(E, t_{i-1}) + \lambda_s(E') N(E', t_{i-1}) \\ & - \lambda_s(E) N(E, t_{i-1}) - \lambda(E, t_{i-1}) N(E, t_{i-1}), \end{aligned} \tag{7}$$

where $\lambda_s(E')$ is the elastic scattering rate for positrons in energy group ($E' = E + \Delta E$ to E) to energy group (E to $E - \Delta E$), $\lambda_s(E)$, energy group (E to $E - \Delta E$) to energy group ($E - \Delta E$, $E - 2\Delta E$). Such an approximation is good provided the difference $t_i - t_{i-1}$ is small such that the average energy decrement is less than the energy difference $E' - E$. The values of λ_s can be easily calculated from the value of momentum-transfer cross section by standard procedures.[6] Since the energy spread after a short duration of the slowing process is expected to be small compared with the average energy decrement[20] only a small correction is required to take into account such an energy spread. Certainly, a correction for thermal agitation is also required. Use formulas (1), (4), (5), and (7) we are able to calculate the theoretical annihilation spectrum $R(t_i)$ and also the energy varying annihilation rate $\lambda(t_i)$.

IV. THEORETICAL VALUES OF CROSS SECTIONS

The annihilation cross sections calculated by Drachman[12,13] will be used here. At the moment these are the only results which provide complete sets of annihilation cross section in helium for low-energy positrons. The momentum-transfer cross sections calculated by Massey *et al.*[7] and Drachman will be used. These are recent calculations based upon more advanced techniques. In addition, other artificially constructed cross sections have been tested.

In order to provide a sharp peak after shoulder for positron annihilation in dense helium gas at a temperature of 4.2 °K, a sharp resonance annihilation peak must be incorporated into the annihilation cross section at certain suitable energies as the ones shown in Fig. 4.

Exact knowledge of the initial energy distribution

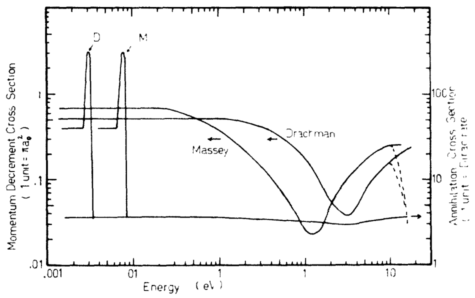

FIG. 4. Annihilation cross section and momentum-transfer cross sections used in construction of theoretical annihilation lifetime spectra such as ones shown in Figs. 1 and 3.

of positrons is not known at present. Two types of initial energy distribution from E = 17.8 to 0 eV, (i) a step function distribution constant $\times dE$ and (ii) $E^{1/2}dE$, are used in the calculation. For momentum-transfer cross sections of reasonable values the slowing down time for positrons with an initial energy of 17.8 eV to a final energy of a few electron volts is very fast, therefore, the initial energy distribution has a very small bearing on the latter energy distributions. This means that the error introduced by the assumed initial distribution is small.

V. RESULTS AND DISCUSSION

Obviously, the values Z_k calculated by the non-variational method of Drachman[12, 13] from 4.60 to 6.32 are too high for the experimental results. Theoretical free-positron-annihilation spectra constructed using this set of data and other momentum-transfer cross sections are found to disagree with any experimental spectrum. Therefore, this set of data will not be discussed again.

This leaves us only one set of data obtained by the modified method of variational treatment. However, this set of values gives good agreement when it is combined with any of the momentum-transfer cross sections of reasonable values. The results obtained based on this set of data will be discussed here.

In several sets of momentum-transfer cross sections of reasonable values two sets, (i) the one by Drachman[9] with α=0 and C=1 and (ii) the one by Massey *et al.*[7] most closely fit the experimental data and are supported by sound theoretical foundation. Both of them are shown in Fig. 4 with the annihilation cross sections used here.

Of these two sets of momentum-transfer cross sections the set (i) by Drachman is found to give the better fit to experimental data, to both positron-annihilation lifetime spectra in helium gas both at 4.2 and at 300 °K. Two sets of these constructed spectra are shown in Figs. 1 and 3 as examples. Although a different initial energy distribution gives a slightly different shape to the lifetime spectrum in helium gas at 4.2 °K, no significant variation appears to the lifetime spectrum in helium gas at 300 °K from the two initial energy distributions. The set (ii) by Massey *et al.* does not agree with the experimental data as well as the set (i) and two of the constructed spectra are also shown in Figs. 1 and 3. The set (ii) by Massey gives a broader peak in the spectrum for free positron annihilation in helium gas of density 0.0168 g cm^{-3} at 4.2°K and a not so well-defined shoulder in the spectrum for free positron annihilation in helium gas of density 0.0090 g cm^{-3} at 300°K. This can be more easily visualized in the plot of $\lambda(t)$ against time shown in Fig. 5. Here the shape of $\lambda(t)$ curve calculated from set (i) agrees with the experimental result much better than the curve calculated from set (ii). These are due to the fact that the minimum of the momentum-transfer cross section of set (ii) is situated at lower energy than the minimum of the momentum-transfer cross section of set (i). The coincidence of the minimum of the annihilation cross section and the minimum of the momentum-transfer cross section (i) gives a more well-defined shoulder although the minimum of the annihilation cross section is very shallow. The closeness of the increasing trend of momentum-transfer cross section with decrease of energy to the resonance annihilation peak introduces a broader peak.

Here, the assistance provided by the resonance annihilation peak is apparent. In order to have a resonance annihilation peak, there are two conditions that must be satisfied. First, there must exist a sudden and large increase of annihilation rate at or below certain energy such that very small amounts of positrons will be able to escape the annihilation sink. Secondly, since there exists a strong sink at or below certain energy the total averaged annihilation rate will be transport controlled, that is, the rate depends on the number of positrons transported into this sink. In order

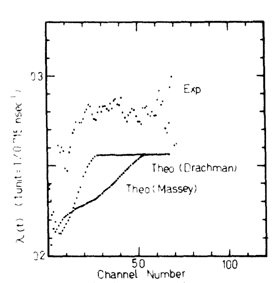

FIG. 5. $\lambda(t)$ plots for free-positron-annihilation lifetime spectrum in helium gas of density 0.0090 g cm^{-3} at 300° K. The meanings of notations are similar to Fig. 3.

to achieve a high averaged transport rate, the positron energy distribution must be narrow at the time the resonance is attained. This automatically rejects any momentum-transfer cross section which increases with decreasing energy, preceding the resonance annihilation peak or sink. In addition, the momentum-transfer cross section must also be large enough at the sink such that a high transport rate can be maintained.

Another restriction provided by the resonance annihilation peak is that imposed on the possible averaged values of momentum-transfer cross section in the energy region greater than the energy where the resonance annihilation peak is situated. Since the peak in the free-positron-annihilation lifetime spectra is sharp the energy where the resonance annihilation peak is situated must be greater than the thermal energy 4.2 °K. It is also expected this energy will not be much greater than the energy equivalent to thermal positron at 77 °K. This restricts the energy range of the resonance peak from $E = 0.002$ to 0.01 eV. From the position of the peak in free-positron-annihilation spectra, the allowable values of averaged momentum-transfer sections are from $0.2\pi a_0^2$ to $0.6\pi a_0^2$. Incidentally, both the sets (i) and (ii) satisfy the above criterion. If the momentum-transfer cross section of set (i) is used the energy of resonance annihilation is 0.003 eV and if the momentum-transfer cross section of set (ii) is used the energy of resonance annihilation is 0.008 eV.

From above criterion many types of momentum-transfer cross section have been found to be unsatisfactory. These include the one by Drachman[9] with $\alpha=1$ and $C=1$ and the one with a constant value of $0.023\pi a_0^2$.[1,2]

The values of energy-decrement cross sections of both (i) and (ii) at high energies greater than 10 eV are of the magnitude of $0.15\pi a_0^2$ or more, which is much greater than the one value of $0.023\pi a_0^2$ obtained experimentally.[1,2] However, if the cross sections at these higher energies are modified and reduced to the values as indicated by the dashed lines in Fig. 2 the change to the constructed annihilation spectra, in general, is negligible. Therefore, the exact value of the momentum-transfer cross section at such energies requires further study.

VI. CONCLUSION

A method is developed to construct theoretical free-positron-annihilation lifetime spectra in helium by using theoretical values of annihilation cross section and momentum-transfer cross section. Then, the theoretical spectra are compared with the spectra obtained experimentally. Experimental results for positron annihilation in helium gas at temperatures of 4.2, 77, and 300 °K are used.

The choice of theoretical calculated annihilation cross section is quite limited. However, the one calculated by Drachman[13] based on an adiabatic approximation and a variational technique is found to be very close to experimental results.

The existence of a sharp resonance annihilation peak in the positron-annihilation component for positrons in dense helium gas at 4.2 °K prove to be very valuable in narrowing down the possible choices of momentum-transfer cross section. The allowable values of averaged momentum-transfer cross section in an energy range from 17.8 to 0.1 eV are from $0.2\pi a_0^2$ to $0.6\pi a_0^2$. Two sets of momentum-transfer cross sections (i) by Drachman[9] with $\alpha=0$ and $C=1$ and (ii) by Massey *et al.*,[7] are found to agree quite well with the experimental data. The set (i) by Drachman[9] with $\alpha=0$ and $C=1$ gives a better fit to experimental data than the set (ii) by Massey *et al.*

As mentioned before, this method does not give a direct proof to the correctness of the theoretical results. Therefore, one must be warned not to treat the conclusions of this work as final. However, it is very encouraging that certain combinations of theoretical calculated annihilation cross section and momentum-transfer cross section do agree well with the experimental results. This indicates at least the theoretical approaches adopted by Drachman[8,9,12,13] and Massey *et al.*[7] are proceeding in the right directions. This also means that adiabatic method is a good approximation here and in the modified adiabatic method used by Drachman[9] the parameter α, the amount of a monopole distortion retained in the scattering function should be suppressed.

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Unified Classical-Path Treatment of Stark Broadening in Plasmas

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A theoretical treatment of spectral line broadening in plasmas is developed using classical-path methods. This treatment unifies certain aspects of the familiar impact, one-electron, and relaxation theories to produce results which are valid from the line center to the far line wings where the electrons may behave quasistatically. Calculations of the Lyman-α line of hydrogen are used to illustrate the theory.

I. INTRODUCTION

A theoretical treatment of spectral line broadening in plasmas will be developed using classical-path methods[1,2] (Refs. 1 and 2 will henceforth be referred to as I and II). This treatment unifies certain aspects of the familiar impact,[2–4] one-electron,[2,3] and relaxation[5,6] theories to produce a more general theory which is correct from the line center to the far line wings.

In describing the center region of a line profile, most theories expand the time-development operator for the perturbed radiator to second order in the perturbation potential. The so-called "strong collisions," for which such a perturbation treatment breaks down, are usually treated by some type of strong collision cutoffs. This procedure works quite well, for example, in hydrogen where most of the broadening is done by the weaker interactions. For some isolated lines, however, the strong collisions may produce a large percentage of the broadening and it would be desirable to treat such interactions more accurately. This situation is also common in neutral gases (i.e., not plasmas) where essentially all of the broadening is due to strong collisions. In such cases one generally uses the impact theory which describes the collisions in terms of S matrices.

The unified classical-path approach developed in this paper is formally the same as the quantum-mechanical relaxation theory.[5,6] Since the latter is known to be valid in the line center when strong collisions are not too important (e.g., hydrogen lines), it is obvious that the unified approach will be similarly valid. For cases where strong collisions produce an appreciable percentage of the broadening, the collisions are treated by a time-development operator which is similar to the S-matrix treatment in the impact theory. In fact, the only essential difference between the impact theory and the unified theory is due to the fact that the unified theory does not make the "completed collision assumption."

The completed collision assumption assumes that any collision which occurs during the time of interest can be completed during that time.[2,7] It is this assumption which replaces the time-devel-