POSITRON ANNIHILATION IN HELIUM

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Positron Annihilation in Helium

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The modified adiabatic scattering function previously used to compute

phase shifts for positron-helium scattering below the positronium threshold

is applied to the problem of annihilation in helium. A large enhancement factor

relative to the Dirac rate is found, varying with energy from 2.30 to 3.16.

The probability of finding the spectator electron in states of the He^+ ion

other than the ground state is computed and found to be small but probably

observable.

I. Positron Scattering Function

We have previously discussed the adiabatic approximation[1] and applied it to the problem of low energy positron-helium scattering.[2] Let us now consider its application to the computation of positron annihilation in helium.

The scattering wave function for a positron of momentum $\underset{\sim}{k}$ has the form:

$$\Psi_{\underset{\sim}{k}}(\underset{\sim}{r_1},\underset{\sim}{r_2},\underset{\sim}{x}) = \chi_{\underset{\sim}{k}}(\underset{\sim}{x}) \; [1 + G(\underset{\sim}{r_1},\underset{\sim}{x}) + G(\underset{\sim}{r_2},\underset{\sim}{x})] \; \phi(\underset{\sim}{r_1},\underset{\sim}{r_2}). \tag{1}$$

Here $\underset{\sim}{x}$ is the positron coordinate, and $\underset{\sim}{r_1},\underset{\sim}{r_2}$ are the coordinates of the two electrons, all measured from the helium nucleus. The function ϕ describes the ground state of the helium atom. The asymptotic form of the function Ψ will be correct if $\chi_{\underset{\sim}{k}} \to e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}$ since the correlation function G vanishes for large values of x, and the two electrons are assumed to be independently polarized.

Taking the positron interaction as perturbation

$$V = 2 \sum_{i=1,2} \left[\frac{1}{x} - \frac{1}{|\underset{\sim}{x}-\underset{\sim}{r_i}|} \right], \tag{2}$$

one can evaluate $G(\underset{\sim}{r},\underset{\sim}{x})$ correct to first order in V by the method of Dalgarno and Lewis[3]. If we make the shielding approximation employed previously[2]

$$\phi(\underset{\sim}{r_1},\underset{\sim}{r_2}) = \pi^{-1}\beta^3 \exp[-\beta(r_1+r_2)], \tag{3}$$

the equation for $G(\underset{\sim}{r},\underset{\sim}{x})$ becomes

$$\nabla_{\underset{\sim}{}}^2 G - 2\beta \frac{dG}{dr} = 2\left[\frac{1}{x} - \frac{1}{|\underset{\sim}{x}-\underset{\sim}{r}|} \right] - 2\beta e^{-2\beta x}\left[1 + \frac{1}{\beta x}\right]. \tag{4}$$

This is similar to the equation solved by Dalgarno and Lynn[4] for the case of hydrogen, and can be related to that result directly by making the change of variables $\underset{\sim}{y} = \beta\underset{\sim}{r}$, $\underset{\sim}{z} = \beta\underset{\sim}{x}$. Then one finds that $\beta G(\underset{\sim}{y},\underset{\sim}{z})$ satisfies the same equation as does the function derived by Dalgarno and Lynn[4], and can be taken over from their work. They derived an expression, in elliptical coordinates, which contains implicitly all terms in the Legendre polynomial expansion

$$G(\underset{\sim}{y},\underset{\sim}{z}) = \sum_{\ell=0}^{\infty} g_\ell(y,z)\, P_\ell(\cos\alpha), \quad [\cos\alpha = \hat{y}\cdot\hat{z}]. \tag{5}$$

Our previous experience[1] indicated that the monopole term in the expansion gives excessive short-range attraction (correlation), and in the following it will be completely suppressed. Then, in elliptical coordinates one has the modified correlation function for helium

$$G(\underset{\sim}{y},\underset{\sim}{z}) = \beta^{-1}\left[F(z,\lambda,\mu) - \tfrac{1}{2}\int_{-1}^{1} d(\cos\theta)\, F(z,\lambda,\mu)\right] \equiv \beta^{-1}[F-F_0]. \tag{6}$$

Here, $\lambda = z^{-1}[y + (y^2 + z^2 - 2yz\cos\theta)^{1/2}]$, $\quad 1 \le \lambda \le \infty$

$\mu = z^{-1}[y - (y^2 + z^2 + 2yz\cos\theta)^{1/2}]$, $\quad -1 \le \mu \le 1$,

$\cos\theta = (1 + \lambda\mu)(\lambda + \mu)^{-1}$,

$$F(z,\lambda,\mu) = (\lambda + \mu)A + [1 + 2Az^{-1}]\,\ell n(1+\lambda) + D(z,\mu), \tag{7}$$

where $D(z,\mu) = (1 + z^{-1})[Ei(-z[1-\mu]) - \ell n(1-\mu)$

$$-e^{-2z}(Ei[z(1+\mu)] - \ell n[1+\mu])],$$

$$Ei(-x) = - \int_{x}^{\infty} e^{-t} \, t^{-1} \, dt,$$

and $\quad A = \frac{1}{2} [(1+z)e^{-2z} - 1].$

II. Annihilation Rate

The rate of annihilation of positrons in helium is given by the expression[5]

$$\lambda = \pi r_0^2 \, c \, N \, Z_k \tag{8}$$

where r_0 is the classical electron radius e^2/mc^2, N is the number density of atoms in the target gas, and Z_k is an effective electron number given by the expression

$$Z_k = \iiint d\underset{\sim}{r}_1 \, d\underset{\sim}{r}_2 \, d\underset{\sim}{x} \, | \Psi_k(\underset{\sim}{r}_1, \underset{\sim}{r}_2, \underset{\sim}{x}) |^2 \, [\delta(\underset{\sim}{r}_1 - \underset{\sim}{x}) + \delta(\underset{\sim}{r}_2 - \underset{\sim}{x})], \tag{9}$$

and provides a measure of the probability that the positron and an electron are at the same point in space. If one were to set $V = 0$, thereby reducing the distortion of the atom as well as the positron scattering to zero, then

$$\Psi_k = \phi \, e^{i\underset{\sim}{k} \cdot \underset{\sim}{x}}. \tag{10}$$

Thus the effective electron number $Z_k = 2$, and the annihilation rate goes over to the Dirac rate[5] which is the quantum electrodynamic result for free particles.

For our type of wave function,

$$\tfrac{1}{2} Z_k = \pi^{-1} \int d\underset{\sim}{z} e^{-2z} \, | \chi_k(\underset{\sim}{x}) |^2 \, [(1 + G[\underset{\sim}{z}, \underset{\sim}{z}])^2 + < G^2 >], \tag{11}$$

where $\quad < Q^2 > \equiv \iint d\underset{\sim}{r}_1 \, d\underset{\sim}{r}_2 \, \phi \, Q \, \phi.$

The energy independent parts of Z_k can be conveniently isolated by writing $\chi_{\underset{\sim}{k}}(\underset{\sim}{x})$ in a partial wave expansion

$$\chi_{\underset{\sim}{k}}(\underset{\sim}{x}) = \sum_{L=0}^{\infty} x^{-1} U_L(x) \, P_L(\cos\theta)(2L+1)i^L e^{i\delta_L}. \tag{12}$$

Using

$$e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} = \sum_{L=0}^{\infty} j_L(kx) \, P_L(\cos\theta) \, (2L+1)i^L$$

one finds

$$\int d\Omega \, | \chi_{\underset{\sim}{k}}(\underset{\sim}{x}) |^2 = \int d\Omega \, | e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}} + (\chi_{\underset{\sim}{k}}(\underset{\sim}{x}) - e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}) |^2$$

$$= 4\pi\left[1 + \sum_{L=0}^{\infty} (2L+1)(x^{-2} U_L^2 - j_L^2) \right], \tag{13}$$

and

$$\tfrac{1}{2} Z_k = 4 \int_0^{\infty} dz\, e^{-2z} \; z^2 \left[(1 + G[\underset{\sim}{z},\underset{\sim}{z}] + \langle G^2 \rangle) \right] \left\{ 1 + \sum_{L=0}^{\infty} (2L+1)\left[\beta^2 z^{-2} U_L^2\left(\tfrac{kz}{\beta}\right) - j_L^2(kz/\beta) \right] \right\}. \tag{14}$$

Thus, a rapidly converging series of energy-dependent corrections and a single energy independent term together yield the effective electron number. The functions U_L are obtained numerically from the solutions discussed previously[2], and have the asymptotic form

$$U_L(x) \rightarrow k^{-1} \sin(kx - L\pi/2 + \delta_L).$$

The problem thus requires the evaluation of $<G^2>$ and $G(\underset{\sim}{z},\underset{\sim}{z})$ and the numerical integration of Eq. (14). In elliptical coordinates, $\underset{\sim}{y} = \underset{\sim}{z}$ is equivalent to $\lambda = \mu = 1$, since $y = z$ and $\cos\theta = 1$. For these values

$$F(z,1,1) = 2A + [1 + 2z^{-1}A]\ell n2 \qquad (15)$$

$$+(1+z^{-1})[\ell n\gamma z - e^{-2z}(Ei[2z]-\ell n2)],$$

where $\ell n\ \gamma = 0.5771....$, Euler's constant.

The integral in Eq. (6) takes the form

$$\frac{1}{2}\int_{-1}^{1}d(\cos\theta)\ F(z,\lambda,\mu)_{\lambda+\mu\ =\ 2} = A\int_{-1}^{1}d(\cos\theta)$$

$$+ [1 + 2z^{-1}A]\int_{1}^{3}d\lambda\,(\lambda-1)\ell n(1+\lambda) + \int_{-1}^{1}d\mu(1-\mu)D(z,\mu). \qquad (16)$$

Then, after performing the integrations, one obtains the result

$$G(\underset{\sim}{z},\underset{\sim}{z}) = \beta^{-1}\left\{[1+z^{-1}][\ell n\ 2\gamma z - Ei(-2z) - 1/2z + e^{-2z}(1+1/2z)] -1\right\}, \qquad (17)$$

which approaches zero as $z \to 0$, confirming the removal of the short-range parts of the correlation. Some numerical values of $(1 + G)^2$ are shown in Table I.

The remaining term required to evaluate the annihilation rate is $<G^2>$ which has been evaluated numerically from the formula

$$\langle G^2 \rangle = \beta^{-2} \left[\langle F^2 \rangle - \langle F_0^2 \rangle \right] . \qquad (18)$$

It also vanishes at $z = 0$ and decreases as z^{-4} for large z. For $\beta = 1.5992$ it is also exhibited in Table I. In Fig. 1 and Table II the values of $\frac{1}{2}Z_k$ are shown over the energy range from zero to the positronium threshold. These have been computed numerically, using one set of solutions to the scattering $[\beta=1.5992, \alpha=0]$ discussed previously[2], but including only the $L = 0$ part of the sum over partial waves. We estimate that the neglect of $L > 0$ contributes an error of less than 2% to the annihilation rate, and the error vanishes for $k \to 0$. The rates obtained are very high[6], and exhibit considerable variation with energy, which should soon be observable experimentally.[7]

III. Excitation of the Residual Ion

Suppose that an electron is annihilated when the positron is at position $\underset{\sim}{x}$. The annihilation takes place very rapidly compared with atomic times, and so the subsequent behavior of the residual He^+ ion can be treated by the sudden approximation[8]. The probability that the He^+ ion will be in the state whose wave function is ϕ_n is then given by

$$P_n = \int d\underset{\sim}{x} \, | \, a_n(\underset{\sim}{x}) \, |^2 / \sum_n \int d\underset{\sim}{x} \, | \, a_n(\underset{\sim}{x}) \, |^2 , \qquad (19)$$

where $a_n(\underset{\sim}{x}) = \int d\underset{\sim}{r} \, \phi_n^*(\underset{\sim}{r}) \, \Psi_{\underset{\sim}{k}}(\underset{\sim}{x}, \underset{\sim}{x}, \underset{\sim}{r})$.

The denominator in Eq. (19) is

$$\iiint d\underset{\sim}{r} \; d\underset{\sim}{r}' \; d\underset{\sim}{x} \; \Psi_{\underset{\sim}{k}}^*(\underset{\sim}{x},\underset{\sim}{x},\underset{\sim}{r}') \Big[\sum_n \phi_n(\underset{\sim}{r}') \; \phi_n^*(\underset{\sim}{r}) \Big] \Psi_{\underset{\sim}{k}}(\underset{\sim}{x},\underset{\sim}{x},\underset{\sim}{r}), \tag{20}$$

and since $\{\phi_n\}$ is a complete set of one-electron functions, closure can be applied to the sum in Eq. (20). Thus

$$
\begin{aligned}
P_n &= \int d\underset{\sim}{x} \; | a_n(\underset{\sim}{x}) \; |^2 / \iint d\underset{\sim}{x} d\underset{\sim}{r} \; | \Psi_{\underset{\sim}{k}}(\underset{\sim}{x},\underset{\sim}{x},\underset{\sim}{r}) \; |^2 \\
&= \int d\underset{\sim}{x} \; | a_n(\underset{\sim}{x}) \; |^2 / \tfrac{1}{2} \; Z_k,
\end{aligned}
\tag{21}
$$

and
$$\sum_n P_n = 1.$$

If the probability for exciting 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. A favorable transition might be the $2p \to 1s$ ultraviolet line at $304 \; \overset{o}{A}$, and we now proceed to compute its intensity, using the modified adiabatic wave function.

From Eqs. (1) and (19) one obtains

$$P_n = 2(\pi Z_k)^{-1} \int d\underset{\sim}{z} \; e^{-2z} \; | \chi_{\underset{\sim}{k}} \; |^2 \Big[(1 + G[\underset{\sim}{z},\underset{\sim}{z}]) Q_n + W_n(z) \Big]^2$$

where
$$Q_n = (\beta^3/\pi)^{1/2} \int d\underset{\sim}{r} \; e^{-\beta r} \; \phi_n(\underset{\sim}{r}) \tag{22}$$

$$W_n(z) = (\beta^3/\pi)^{1/2} \int d\underset{\sim}{r} \; G(\underset{\sim}{y},\underset{\sim}{z}) \; \phi_n(\underset{\sim}{r}).$$

For excitation to the 2p state of the ion $Q_n = 0$ and only the dipole part of G contributes to $W_n(z)$. This is obtained by inserting Eq. (5) into Eq. (4) and yields

$$g_1(y,z) = \beta^{-1}\left\{z^{-2}\left[y + y^2/2\right] + C_1\left[e^{-2y}/2y^2 + (1 + y^{-1} + \tfrac{1}{2}y^{-2})\right]\right\}$$

for $y < z$

$$= \beta^{-1}\left\{z + C_2\left[1 + y^{-1} + \tfrac{1}{2}y^{-2}\right]\right\}$$

(23)

for $y > z$

where $\qquad C_1 = \tfrac{3}{2}\,e^{-2z}(1 + z^{-1})^2,$

$$C_2 = C_1 - z + \tfrac{3}{2}(1 - z^{-2}),$$

and then

$$W_{2p}(z) = \tfrac{4}{3}\beta^{-5/2}\int_0^\infty dy\ y^3\ e^{-(1+\beta^{-1})y}\ g_1(y,z).$$

(24)

The probability P_{2p} has been computed for the same parameters as before and is found to be essentially independent of positron energy, (for $L = 0$ scattering) and equal to 0.82%. Thus at least 0.82% of all annihilations should be followed by the $2p \rightarrow 1s$ transition. In addition, however, the experimentally observable radiation should include the effect of cascades from other states which pass through the 2p state. S-states should dominate the cascade process.

For S-states, $W_n = 0$ since no monopole term is contained in G. The S-state probabilities are

$$P_{ns} = \left[1 + R\right]^{-1} Q_{ns}^2,$$

(25)

where $\qquad R = \int d\underset{\sim}{z}\ e^{-2z}\,|\chi_{\underset{\sim}{k}}|^2\ \langle G^2\rangle/\int d\underset{\sim}{z}\ e^{-2z}\,|\chi_{\underset{\sim}{k}}|^2\ [1 + G]^2.$

Invoking closure over S-states, one finds that P(all S) = $[1+R]^{-1}$ = 99% where R has been numerically evaluated, and proves to be essentially energy-independent. Thus 99% of all annihilations give S-states of the ion, and 0.82% go to the 2p state, leaving a negligible fraction in the higher p or L > 1 states. The partition among the various discrete S-states is then given by Q_n^2. A general formula due to Mittleman[9] is

$$Q_n^2 = (8\beta/n)^3 (2-\beta)^2 (\beta-2/n)^{2n-4} (\beta+2/n)^{-(2n+4)},\eqno(26)$$

which was used to prepare Table III, which also shows the branching ratios[10] to the 2p state. One finally finds that 1.2% of all annihilations should be followed by the 2p → 1s transition. In addition, if a sufficiently strong electric field is applied to the target gas, the metastable 2s level will mix with the 2p level[11], and an increase in the 2p → 1s transition rate to 3.2% of the annihilation rate will occur, and should be observable.

IV. Discussion

We have presented above a calculation of the energy-dependent annihilation rate of positrons incident on a helium target, as well as a prediction of the intensity of the He^+ ultraviolet radiation which is expected to follow the annihilation. In this work a simple model wave function describes both processes, as well as the elastic scattering. The predictions are thus not expected to be exact, but previous experience has given some cause for optimism.

Nevertheless the results derived here must be used cautiously, as a guide only, until such time as more accurate solutions of the positron-helium scattering problem become available. As an example, we may note that the value of

the parameter $\beta = 1.5992$ used throughout has been chosen to produce agreement with the long-range x^{-4} potential[12], and thus does not necessarily represent well some of the other properties of the system. In a somewhat different context, Mittleman[9] has used a five-term exponential approximation to describe the helium atom wave function, and finds that a more accurate value of the 2s excitation probability is 2.23%, rather than our 2.00%. This agreement indicates that our qualitative results should be used as preliminary estimates in designing experiments, which may eventually test the future detailed theories.

References and Footnotes

1) R. J. Drachman, Phys. Rev. 138, A1582 (1965).

2) R. J. Drachman, Phys. Rev. 144, 25 (1966).

3) A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. (London) A233, 70 (1955).

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

5) R. A. Ferrell, Revs. Mod. Phys. 28, 308 (1956).

6) The rates are about twice as large as those obtained by H.S.W. Massey, J. Lawson and D. G. Thompson [preprint, 1966] who have not attempted to include the correlations at all, and who have used an adiabatic potential with dipole parts only in their scattering equation. Their results should seriously underestimate the correct annihilation rates.

7) W. R. Falk, P. H. R. Orth and G. Jones, Phys. Rev. Letters 14, 447 (1965).

8) L. I. Schiff in Quantum Mechanics, (McGraw-Hill Book Co., Inc., New York, 1955) 2nd ed., pp. 213-220.

9) M. H. Mittleman, Phys. Rev. Letters 16, 498 (1966). See also Ref. 11, which includes a one-term calculation like ours, but with $\beta = 27/16$.

10) H. A. Bethe and E. E. Salpeter in Quantum Mechanics of One-and Two Electron Atoms, (Academic Press, Inc., New York, 1957), p. 266.

11) W. E. Lamb and M. Skinner, Phys. Rev. 78, 539 (1950). This paper contains a derivation of the dipole radiative lifetime of the metastable 2s state of helium in the presence of an electric field, $\tau = 1.6 \times 10^{-2} E^{-2}$, with E in volts/cm. If this lifetime is shorter than that for collisional deexcitation, enhancement of the 304 Å line occurs. A measurement of the latter value could in principle be made this way.

12) See Ref. 2, where another choice of β is made. As long as full monopole suppression is maintained the results should be similar. The inclusion of short-range monopole parts in G will increase the effective electron number, and will reduce the relative excitation of the 2p state of the ion.

Table I. Numerical values of correlation functions required for the calculation of the positron-helium annihilation rate, for full monopole suppression and $\beta = 1.5992$.

z	$[1 + G(z,z)]^2$	$\langle G^2 \rangle$
0	1	0
0.5	1.886	.0230
1.0	2.733	.0473
1.5	3.447	.0495
2.0	4.028	.0397
2.5	4.503	.0282
3.0	4.900	.0188
3.5	5.241	.0123
4.0	5.541	.0080
4.5	5.810	.0053
5.0	6.055	.0036

Table II. Effective electron number for annihilation at selected values of
incident positron energy. The Dirac rate corresponds to $\frac{1}{2}Z_k = 1$.

Energy (eV)	$\frac{1}{2}Z_k$
0	3.16
0.54	2.79
1.22	2.58
2.17	2.43
3.40	2.35
4.90	2.31
6.66	2.30
8.70	2.33
11.0	2.38
13.6	2.44
17.8	2.54

Table III. Population and branching ratios following annihilation. The probability for exciting the various S-states of He$^+$ listed in column 1 are shown in column 2, and the fraction of each which eventually reaches the 2p state is shown in column 3. [Cascades like 5s → 4p → 3s → 2p are included, but are very small]. Column 4 gives the observable population of the 2p state due to each S-state.

State	Population	Branching Ratio to 2p	Contribution to 2p Population
1s	95.34%	0	0
2s	2.00%	0	0
3s	0.30%	1	.30%
4s	0.10%	0.58	.058%
5s	0.049%	0.45	.022%
6s	0.027%	0.43	.012%
			Total = .39%

Figure Captions

Fig. 1. Effective electron number for annihilation versus incident positron

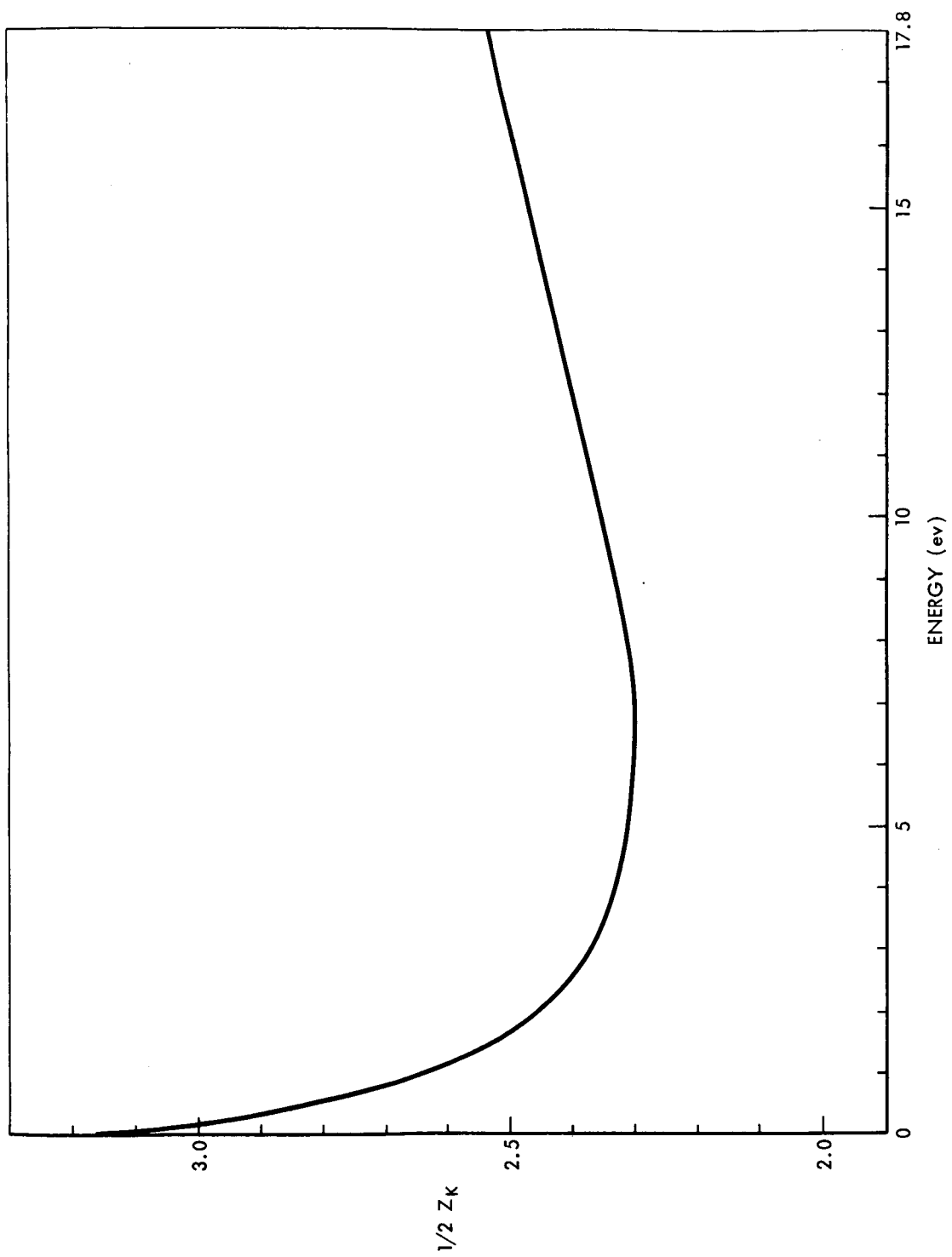energy in eV. The Dirac rate corresponds to $^1/_2 \, Z_k = 1$.

ENERGY (ev)

Figure 1

1/2 z_K