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Energy-apportionment techniques based upon detailed atomic cross sections

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We briefly discuss four of the principal energy-apportionment techniques currently used in energy-deposition calculations—the Fowler equation, the Monte Carlo approach, the discrete-energy-bin method, and the Peterson-Green integral equation in the context of the continuous-slowing-down approximation (CSDA). Using a complete set of analytic inelastic cross sections for molecular hydrogen, we calculate, by each of these four methods, the energy per ion pair W associated with the degradation in H_2 of incident electrons with initial energies ranging between the ionization threshold and 1000 eV. We find that the results obtained from the first three of these methods are in very good agreement with one another, while the values of W obtained by the last method in the CSDA are consistently larger than the corresponding values obtained from any of the discrete-energy-loss approaches. Lastly, we isolate the cause of the CSDA discrepancies and propose two techniques for modifying the low-energy predictions of the CSDA so that they are in much better agreement with those of the three discrete energy-apportionment methods for all incident-electron energies.

I. INTRODUCTION

It is now generally agreed that the key to the solution of energy-deposition problems is the assembling of a complete set of cross sections which accurately describe the relevant inelastic processes that a particle traversing a medium can bring about as it transfers its energy to that medium. However, once such a set of cross sections has been assembled, a variety of methods of energy apportionment or "bookkeeping" have been used to calculate the number of excitations of a given state of a medium that are produced as the incident particle is degraded in energy. In addition to the traditional Boltzmann and Fokker-Planck equations, six other methods, each employing a detailed-atomic-cross-section (DACS) approach, may be identified. They are the Fowler equation,[1] the Spencer-Fano degradation-spectra method,[2] the Green-Barth successive-generation method,[3] the Peterson-Green integral equation,[4] the Peterson discrete-energy-bin method,[5] and the Monte Carlo collision-simulation method.[6]

A comparison of the predictions of these various apportionment methods, based on the same set of cross sections, would be of interest in assessing the relative reliability and utility of each method. One simple test consists of a comparison of the values of W, the number of eV per ion pair, obtained from each method. Molecular hydrogen is an excellent candidate as the medium or gas in such a calculation, since it has been subjected to considerable experimental study and, as the simplest molecular gas, it is the most amenable to theoretical investigation. Furthermore, it is of aeronomical interest as the principal constituent of the Jovian atmosphere and also of interest in connection with the fusion program.

We have chosen to compare four of these energy-apportionment methods. We have not explicitly considered the successive-generation approach of Green and Barth, since these generations are, in effect, summed by the Peterson-Green integral equation. However, we should note that the Green-Barth method is a practical one, since the average energy of successive generations of electrons declines very rapidly, and this technique has recently been used by Khare.[7] We have also not considered the Spencer-Fano method, since it has been recently shown,[8] using variational techniques, that the degradation spectrum obtained in that method is the universal adjoint of the state populations obtained in the Fowler method. Thus the four approaches we do examine here actually include the six principal energy-apportionment methods used in electron-energy-deposition work.

II. METHODS OF ENERGY APPORTIONMENT

The oldest discrete energy-apportionment method is that of Fowler,[9] which determines the mean total number $J_k(E)$ of excitations of the state k produced in the entire degradation process according to the equation

$$J_k(E)=p_k(E)+\sum_j p_j(E)J_k(E-E_j)+\sum_i\int_0^{(E-I_i)/2}dT\,p_i(E,T)\times[J_k(E-(I_i+T))+J_k(T)]\,, \qquad (1)$$

where $p_j(E)=\sigma_j(E)/\sigma_t(E)$ is the probability that in an inelastic collision an electron of energy E will excite the state k; $p_i(E,T)=S_i(E,T)/\sigma_t(E)$ is the probability per unit energy that in an inelastic collision an electron of energy E will produce an ion in the ith ionization continuum and a secondary electron with energy between T and $T+dT$. Here $\sigma_j(E)$ is the cross section for an electron with energy E exciting the state j in the medium through which the electron is passing, $S_i(E,T)$ is the differential ionization cross section for an electron with energy E producing a secondary electron with energy in the range T to $T+dT$ via the ith ionization continuum, and $\sigma_t(E)$ is the total inelastic cross section. The energies E_j and I_i are the thresholds of the jth discrete state and the ith ionization continuum, respectively. If we iterate the Fowler equation several times we see it records the increase in the population of the state k by following an idealized, deterministic degradation scheme.

The Fowler equation can be solved by first considering $E<E_{n,\min}+E_k$, where $E_{n,\min}$ is the lowest excitation energy. For such a value of E, $J_k(E)=p_k(E)$. By steadily increasing E in small increments, higher-energy solutions can be obtained from the lower-energy solutions, since the arguments of the two J_K terms in the integrand on the right-hand side of Eq. (1) are always less than E and therefore are already known from earlier calculations at lower values of E. Recently, variational techniques have been employed to solve Eq. (1).[8]

A second discrete method of energy apportionment based upon DACS, developed by Peterson[5] and others,[10,11] utilizes a deterministic, discrete-energy-bin method. In this discrete-energy-cell method, the energy range between some initial value and the threshold of the state of interest is divided into bins. The bin centered at the initial energy value is assumed to contain one electron, while the other bins are initially empty. An idealized degradation process is then assumed to commence which is very similar to the content of the Fowler equation after many iterations but which is rather different from the low-energy-to-high-energy approach used to solve the Fowler equation. In this idealized degradation scheme the initial electron is fractionally redistributed into lower-energy bins. In this idealized process the population of each state k is increased by the fraction $f_k(E)=\sigma_k(E)/\sigma_t(E)$, and that fraction of the electron is deposited in a new bin defined by its new energy $E-E_k$. The ionization continuum is divided into a group of quasidiscrete states, and the fraction of the electron producing the same fraction of a secondary with energy between $T-\frac{1}{2}\Delta T$ and $T+\frac{1}{2}\Delta T$ is $f_i(E,T)=S_i(E,T)\Delta T/\sigma_t(E)$, where ΔT is determined by the size of the energy bins. That fraction of the primary is deposited in the bin defined by $E-I_i-T$, and the same fraction of the secondary in the bin defined by T. In this manner the highest-energy bin is emptied and lower energy bins are populated with appropriate fractions of electrons. The above process is then repeated for the second-highest-energy bin, and the fraction of an electron exciting a state k and the amount by which the population of the state k is increased is now the product of $f_k(E')$ times the initial fraction of an electron in that bin, where E' is the energy at the center of the bin in question. Each energy bin is emptied in turn until all the bins above and including the bin containing the lowest threshold have been emptied. In this way the mean total number of excitations of each state which are produced in the complete degradation of an electron from a given incident energy is obtained.

In the Monte Carlo approach, the degradation process is simulated in a collision-by-collision manner. The choice of which state of the medium is excited by an electron at a particular energy is made by choosing a random number R between 0 and 1 and determining which state s *first* satisfies the inequality

$$\sum_{j=1}^{s}\frac{\sigma_j(E)}{\sigma_t(E)}>R\,, \tag{2}$$

where the summation is over possible excited states j, including ionization.

If the state s corresponds to an ionization continuum, the energy of the secondary is determined by selecting a second random number R' between 0 and 1 and solving the equation

$$\int_0^T\frac{S_s(E,T)\,dT}{\sigma_s(E)}=R' \tag{3}$$

for T. With the expression for $S_i(E,T)$ that we have used [see Eq. (9)], T can be obtained analytically.

After a given state s has been selected, the incident electron loses an energy E_s, if s corresponds to a discrete excitation, or I_s+T, if s corresponds to excitation of an ionization continuum. The population of the state s is increased by unity and the above selection process is repeated until the electron has degraded below the lowest threshold energy. Each of the secondary electrons produced in the degradation process is then allowed to degrade in exactly the same manner, as are all members of subsequent generations of electrons.

The fourth method of energy apportionment we have considered, which was developed in the course of DACS degradation work carried out by Green and co-workers,[3,4,12,13] is the Peterson-Green integral equation,

$$J_k(E) = J_{0k}(E) + \sum_i \int_0^{(E-I_i)/2} J_k(T) n_i(E, T)\, dT\,. \qquad (4)$$

Here, $J_{0k}(E)$ is the number of excitations of the state k due directly to the incident particle as its energy is degraded from E to E_k, and $n_i(E, T)$ is the total number of secondary electrons in the ith ionization continuum with energies in the range T to $T+dT$ produced directly by an electron as its energy degrades from E to $2T+I_i$.

For exact values of J_{0k} and $n_i(E, T)$, Eq. (4) is exact. Upon iterating Eq. (4) several times, we see that this equation compiles the total number of excitations of the state k by counting the number of excitations of that state produced by each generation of electrons arising in the degradation process. We can solve Eq. (4) by the same procedure described above to solve the Fowler equation, since the argument of J_K in the integrand on the right-hand side of Eq. (4) is always less than E, the argument of J_K on the left-hand side of the equation.

The quantities $J_{0k}(E)$ and $n_i(E, T)$ are most readily calculated in the continuous-slowing-down approximation[14] (CSDA). In the form of CSDA used by Green and associates,

$$J_{0k}(E) = \int_{E_k}^{E} \frac{\sigma_k(E')}{L(E')}\, dE'\,, \qquad (5)$$

$$n_i(E, T) = \int_{2T+I_i}^{E} \frac{S_i(E', T)}{L(E')}\, dE'\,. \qquad (6)$$

The quantity $L(E)$ appearing in Eqs. (5) and (6) is the loss function or stopping power of the medium and is the fundamental quantity in the CSDA. The loss function is defined as $-n^{-1}\, dE/dx$, where x is distance into the medium, and may be evaluated in the CSDA using

$$L(E) = \sum_j \sigma_j(E) E_j + \sum_d \sigma_d(E) \bar{E}_d + \sum_i \int_0^{(E-I_i)/2} S_i(E, T)(I_i + T)\, dT\,, \qquad (7)$$

where $\sigma_d(E)$ is the total cross section for the dth dissociative excitation and $\bar{E}_d$ is the average energy loss associated with that dissociation.

Although one would expect the three discrete energy-apportionment methods described to be in close, if not exact, agreement with one another, to the best of our knowledge no rigorous proof exists linking these three approaches, and no comparison of the predictions of these three approaches using a common, realistic set of cross sections has been made to determine how closely these three discrete methods can be made to agree in practice. In addition, although Peterson[5] previously compared the predictions of his discrete-energy-bin approach with those of CSDA for He and N_2, no thorough comparison has been made using any other gas, nor has the source of the difficulties with CSDA been identified as exactly as in this present work.

III. CROSS SECTIONS FOR H_2

For the discrete excitations of H_2, we have used the cross sections obtained by Miles, Thompson, and Green (MTG),[15] with some alterations. These alterations involve a change suggested by Olivero, Bass, and Green[16] in the $C\,^1\Pi_u$ cross section and a slight change in the MTG parameters characterizing the analytic fits to the $B\,^1\Sigma_u^+$ and $E\,^1\Sigma_g^+$ cross sections which significantly improves those fits. The functional form[12] used here and in Ref. 15 to fit the discrete cross sections is

$$\sigma_k(E) = \frac{q_0 A}{W^2} \left(\frac{W}{E}\right)^{\Omega} \left[1 - \left(\frac{W}{E}\right)^{\gamma}\right]^{\nu} \qquad (8)$$

where $q_0 = 4\pi a_0^2 (\mathcal{R})^2 = 6.514\times 10^{-14}$ cm^2 eV^2 (a_0 being the Bohr radius and $\mathcal{R}$ the Rydberg constant), and where A, W, Ω, γ, and ν are parameters to be adjusted for each state. In Table I, we present only those parameters which differ from those found in MTG.[15]

We consider only one ionization continuum and represent the differential ionization cross section $S(E, T)$ by the Breit-Wigner form introduced by Green and Sawada.[17] We have fitted this form to the total ionization cross-section data of Rapp and Englander-Golden,[18] after subtracting the contribution to that cross section due to dissociative ionization, which we treat separately. The cross section for dissociative ionization was obtained from data of Rapp and Englander-Golden,[19] which we adjusted to take into account the fact that their data excluded ions with kinetic energies below 2.5 eV. To make this correction, we used the ion spectra for H_2 given by Crowe and McConkey.[20] In this way we obtain

$$S(E, T) = A(E) \left\{ \frac{\Gamma^2(E)}{[T - T_0(E)]^2 + \Gamma^2(E)} \right\}\,, \qquad (9)$$

with

$$A(E) = (2.871/E)\sigma_0 \ln(E/0.5114)\,, \qquad (10)$$

$$T_0(E) = 1.870 - 1000/(E + 3I)\,, \qquad (11)$$

$$\Gamma(E) = 7.070E/(E - 7.700)\,, \qquad (12)$$

$$I = 16.0 \text{ eV}\,; \qquad (13)$$

$\sigma_0 = 10^{-16}$ cm^2, and E is assumed to be given in eV.

Since there is little experimental information concerning $S(E, T)$ for dissociative ionization, we

TABLE I. New parameters to be used with Eq. (8) for the four states discussed in the text. DI stands for dissociative ionization.

State	A	W (eV)	Ω	γ	ν
$B\,^1\Sigma_u^+$	0.3674	11.370	0.7163	1.000	3.427
$E\,^1\Sigma_g^+$	0.1002	12.400	0.7134	1.000	3.410
$C\,^1\Pi_u$	1.3200	12.290	0.7500	0.300	1.000
DI	2.0704	21.026	1.4520	0.786	4.774

will treat dissociative ionization as a discrete process and will fit the corrected Rapp and Englander-Golden dissociative-ionization cross sections with the analytic form of Eq. (8) for discrete excitations. The parameters characterizing the total cross section for dissociative ionization are presented in the last row of Table I. The average energy loss $\bar{E}_d$ associated with such ionizations is given by $E_{\text{di}} + \langle \text{K.E.} \rangle$ where E_{di} is the average threshold for dissociative ionization and $\langle \text{K.E.} \rangle$ is the average kinetic energy of the ion plus atom and is equal approximately to twice that of the ion. We neglect the energy of the secondary electron.[21] The average kinetic energy of the ions can be obtained from the ion-energy spectra of Crowe and McConkey.[20] We find that $E_{\text{di}} + \langle \text{K.E.} \rangle$ is approximately $18 + 14 = 32$ eV.

With respect to dissociative excitations, the hydrogen molecule can dissociate into two neutral atoms in several ways.[22] The vast majority of excitations of any triplet state will lead by radiative transitions or by predissociation to the repulsive $b\,^3\Sigma_u^+$ state; when in that state, the molecule dissociates into two ground-state atoms. Excitations of the $D\,^1\Pi_u$ and higher Rydberg members of the $^1\Sigma_u^+$ series and the $^3\Sigma_u^+$ series can predissociate into a ground-state atom and an excited atom.[23] Two ground-state atoms can also be produced by excitation of the $B\,^1\Sigma_u^+$, $B'\,^1\Sigma_u^+$, or $a\,^3\Pi_u$ states followed by a radiative transition to the continuum of the ground state.[11] Direct excitation to the continuum of an excited singlet state can also result in dissociation, and, lastly, excitations of doubly excited states of the molecule may predissociate. With the exception of these last two mechanisms, the cross sections for all the other dissociation mechanisms are contained in the cross sections for the discrete states, since those cross sections were obtained from measurements involving energy losses of the primary electron and not by measuring final products of excitations.[24] Thus by using the cross sections for discrete excitations as they are, we implicitly include all types of dissociation except that due to the predissociation of doubly excited states and Frank-Condon-forbidden direct dissociations from singlet states. Since we are interested here only in determining W, we have not included separate cross sections for dissociation.

In calculating W we will be concerned with any electron until its energy becomes less than or equal to the ionization threshold. What happens to an electron below this energy cannot effect W. For this reason we have chosen to ignore rotational excitations, as well as the possibility for negative-ion formation, since both of these processes are significant energy-loss mechanisms only for electrons with energies well below the ionization threshold of H_2; however, we have included cross sections for excitation of the first two vibrational levels of the ground state of H_2, using the parameters of Ref. 15.

IV. RESULTS

In a comparison of this type, care must be taken to minimize the discrepancies that arise among the various approaches from numerical differences in the various computer programs used, rather than from differences inherent in the different approaches themselves. In addition to using the same set of cross sections in all four methods, we have been careful to ensure that the size of the energy cells used in each program were small enough that their finiteness had a negligible effect on the results.

In Fig. 1 and Table II we present the values of the energy per ion pair,

$$W = E / J_i(E) , \tag{14}$$

which we obtained by each of the four energy-apportionment methods we examined. As Fig. 1 and Table II indicate, the three discrete-energy-loss approaches agree very well, as we would hope, in their prediction of W at any energy. The Fowler and discrete-energy-bin approaches yield values of W that agree to within 0.15% or less and the Monte Carlo results are usually within one standard deviation and always within two standard deviations of the result of the other two discrete methods. Several factors contribute to the numerical differences that remain. The solutions of the Fowler equation are obtained in such a way that the higher-energy results depend on lower-energy results; on the other hand, in both the discrete-energy-bin approach and the Monte Carlo method, we begin at high energies and progressively work down to lower energies. Thus numerical errors propagate differently in the Fowler equation, as it is solved here, then in the other

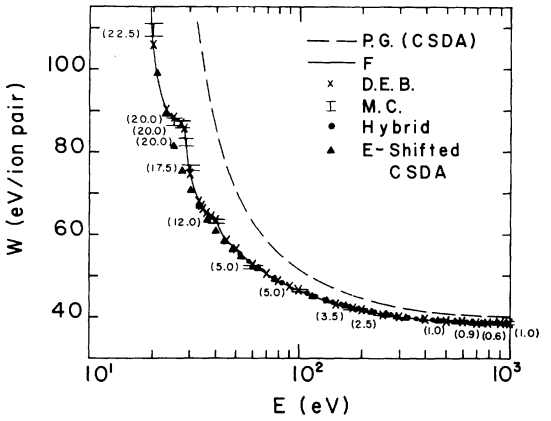

FIG. 1. Values of W in eV/(ion pair) plotted vs incident-electron energy E in eV. See the caption of Table II for an explanation of the abbreviations. The numbers in parentheses beside each Monte Carlo data point, multiplied by 1000, represent the number of simulations required to obtain that point with an uncertainty characterized by the accompanying error bars of ±(one standard deviation).

two discrete approaches. In addition, its stochastic nature dictates that there be statistical fluctuations in the Monte Carlo results which are absent from the results of the other two discrete, but deterministic, approaches. These differences, plus the fact that the computer programs employed in conjunction with each of these approaches may still have some numerical differences inherent in them, should account for the small discrepancies in W which we obtained. We feel that the close agreement we obtained is excellent numerical confirmation of the equivalence of these three discrete approaches.

Recently, there have been several calculations of W for H_2.[9,11,25] The cross sections used in Ref. 11 were adjusted to yield an asymptotic value of W which would agree with experiment,[26] so it is difficult to make any meaningful statement concerning the relationship between that work and the work here. With all singlet states grouped together as one state and all triplet states grouped together as a second state, Jones[25] obtained a value for W of 37.12 eV (per ion pair) at 1000 eV which, when extrapolated to 4 keV, is in remarkably good agreement with experiment. Gerhart,[9] using cross sections which were adjusted to satisfy certain sum rules, obtained a value of W of 40.12 eV at 1000 eV.

In each of these studies a different philosophy was employed in obtaining a set of cross sections to use in the calculations; consequently, in each study a different set of cross sections was obtained. Thus it is understandable that they should differ somewhat in their values for W at any given energy. Nevertheless, our mean value for W of 38.63 eV at 1000 eV, obtained from the three discrete-loss approaches, although below Gerhart's value, is in qualitative agreement with his finding that the asymptotic value of W obtained from a detailed-atomic-cross-section approach is somewhat larger than that obtained from experiment. Gerhart has proposed that Penning ionization may play a significant role in producing additional ions which result in a lower experimental value of W.

From Fig. 1 and Table II we see that the Peterson-Green integral equation yields values of W which are consistently larger than the results of the discrete-loss calculations. This is consistent with the findings of Peterson for He and N_2. This discrepancy in the prediction of the Peterson-Green equation must be due to its reliance on the CSDA to determine $J_{0k}(E)$ and $n_i(E, T)$. The CSDA is an approximation which breaks down whenever the energy lost in an inelastic collision by the exciting electron is appreciable compared to the electron's energy before the collision. Such a situation exists when the electron is a low-energy

TABLE II. Values of W in eV/(ion pair) for various values of incident energy E. In the column headings, MC stands for Monte Carlo, DEB for discrete energy bin, F for Fowler, PG for Peterson and Green, H for hybrid, and ES for energy shifted. The Monte Carlo results contain the value of W and the standard deviation associated with that value for various values of E.

E	MC	DEB	F	PG-CSDA	H	ES-CSDA
20.0	109.4 ±1.55	107.2	107.1	503.3	107.1	103.4
40.0	63.27 ± 0.53	63.50	63.50	85.06	63.50	60.77
60.0	52.26 ± 0.45	52.86	52.87	61.77	53.00	52.60
100.0	46.51 ± 0.28	46.35	46.36	51.50	46.62	46.50
250.0	40.81 ± 0.19	40.75	40.77	43.26	40.92	40.84
500.0	39.01 ± 0.19	39.07	39.10	40.88	39.13	39.06
700.0	38.70 ± 0.17	38.72	38.76	40.36	38.76	38.69
1000.0	38.44 ± 0.13	38.60	38.65	40.13	38.62	38.54

one to begin with or when a relatively high-energy secondary is produced. In the former situation, if E is the same order of magnitude as E_K, $J_{0k}(E)$ will be in error as determined by Eq. (5), and in the latter case $n_i(E, T)$ will be in error as determined by Eq. (6) for large values of T at any E and for all T when E is the same order of magnitude as I_i. Recalling that even for a high-energy electron a large number of the excitations produced in the degradation process are due to low-energy secondaries, which are not handled correctly by the CSDA, we see that the CSDA will be in error at all energies.

In addition to this physical difficulty, there is a mathematical difficulty arising from the fact that the Peterson-Green equation is solved so that the high-energy solutions depend on and are built upon the low-energy solutions. Thus any error in the low-energy solutions is propagated through the solutions at higher energies, where we should expect CSDA to be a rather good approximation. For instance, even for an incident energy of 1000 eV, we find the CSDA prediction of W to be 4% above the predictions of the three discrete methods.

V. IMPROVING THE CSDA

Recognizing the low-energy error inherent in any CSDA calculation, we have developed a hybrid energy-apportionment technique which yields results which agree with discrete-loss techniques but is more economical when a large energy range is being considered. This hybrid technique uses the Fowler equation to obtain $J_{0k}(E)$ for low energies and also uses these values in the integrand of the Peterson-Green equation to obtain $J_k(E)$ at higher energies, where the CSDA yields reasonable values for $J_{0k}(E)$ and $n_i(E, T)$. We note that for $E \leq I_i + 2E_k$ any secondary electron produced cannot have enough energy to excite state k itself, and thus $J_k(E)$ obtained from the Fowler equation is just $J_{0k}(E)$. For this reason, in the hybrid technique we use the Fowler equation for energies less than or equal to $E_{c0} = I_i + 2E_k$. Above this energy, we use the Peterson-Green equation and calculate $J_{0k}(E)$ according to

$$J_{0k}(E) = \int_{E_{c0}}^{E} \frac{\sigma(E')}{L(E')}\, dE' + J_k(E_{c0}) . \tag{15}$$

Here, E_{c0} is 48.0 eV.

In Fig. 1 and Table II, we present the results obtained by this hybrid approach. The improvement over the CSDA results is striking. These hybrid results show that the effect of any error in the CSDA determination of $n_i(E, T)$ on state populations obtained from the Peterson-Green equation are negligible. The error arises because of the CSDA determination of $J_{0k}(E)$ is in error for very small $E \leq E_{c0}$. To further demonstrate this point we have devised a second way of improving the CSDA results. Our earlier results indicate that for $E \leq E_{c0}$ the values of $J_i(E)$ predicted by the Fowler equation are roughly equal to the CSDA predictions of J_{0i} evaluated not at E but at a higher energies near $E + \frac{1}{2}I$. We modified the Peterson-Green equation to give it the slightly altered form

$$J_i(E) = J_{0i}(E + \tfrac{1}{2}I) + \int_0^{(E-I)/2} J_i(T) n_i(E, T)\, dT . \tag{16}$$

The effect of this adjustment of the inhomogeneous term in the integral equation is also presented in Fig. 1 and Table II. The energy shift of the argument of the J_{0i} term brings the low-energy values of this term into close enough agreement with the predictions of the discrete methods that the values of J_i at all energies are now in good agreement with the predictions of the discrete approaches. This particular energy shift will not be appropriate for any other state or any other gas, but the fact that such a fairly rough correction, which includes none of the low-energy structure of the exact $J_{0i}(E)$, results in substantial improvement of the CSDA predictions is further proof that it is the errors in the low-energy values of $J_{0i}(E)$ and not errors in $n_i(E, T)$ which cause the CSDA calculations of W to be in error.

VI. CONCLUSIONS

Using a common set of cross sections, we have obtained values for the energy per ion pair of H_2 at energies between threshold and 1 keV by three different discrete-loss energy-apportionment methods, and have found the predictions of the value of W by each of these three methods to be in very good agreement with one another. The predictions of the CSDA we obtained with the Peterson-Green integral equation are always higher than those of the discrete techniques. We have demonstrated by investigations with a hybrid technique and an energy-shift method that this problem with the CSDA can be corrected by using better values for $J_{0i}(E)$ at low energies.

We summarize below the advantages and disadvantages of each of the energy-apportionment techniques we have considered. The Fowler equation, as it is solved here, besides taking the discrete nature of the energy-degradation process into account, gives accurate estimates of the population of a given state at many energies. It has the disadvantages that (a) a relatively fine energy grid must be employed to obtain these results, and this increases the cost of the calculations, (b) the high-energy solutions depend on low-energy solutions, which in turn depend on the least reliable cross-section data, and (c) no spatial information can be obtained from this method.

The discrete-energy-bin method yields estimates of the population of states at only a few selected energies, but the high-energy results do not depend so strongly on the low-energy results. In addition, it has been shown recently[11] that the degradation spectrum can be obtained from this method, but the method cannot give any spatial information.

The Monte Carlo approach also gives state populations at only a few selected energies, and is more costly than either of the other two discrete methods, but it alone is capable of describing all the pertinent spatial aspects of the degradation process.

The unaltered CSDA method is the least expensive of all the methods we considered, since it requires the least fine energy grid. However, its results are only approximate even at high energies, because the inaccurate low-energy solutions to the Peterson-Green equation effect the high-energy solutions. The CSDA can be used to predict approximate range-energy relationships and the spatial rate of energy loss. However, the CSDA does not give information concerning the locations of excitations occurring at points away from the primary track.

The hybrid approach we have presented here would be the most economical way to get accurate populations of any excited states over a large range of incident energies, since it requires a less find grid than does the Fowler equation and yields values at any intermediate energies desired. However, its high-energy results are dependent on low-energy yields and it can give only the same limited, approximate spatial information as does the CSDA.

The energy-shifted CSDA method we presented in Sec. V could be used in a predictive manner by comparing $J_k(E)$ from the Fowler equation with J_{0k} of the CSDA for $E \leq E_{c0}$ to determine the proper negative or positive energy shift needed to bring the CSDA results into good agreement with the Fowler results at low energies. Once this shift is determined for the state k, Eq. (16), with the correct energy-shifted argument in the J_{0k} term, could be used to obtain accurate, low-cost values for $J_k(E)$ for large E extending into the relativistic regime, where discrete techniques would be prohibitively costly.

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