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Electronic excitation of H_2 by e^+ impact using adiabatic nuclear rotation model

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The adiabatic nuclear rotation (ANR) model has been employed to obtain rotational excitation cross sections for electronically elastic and electronic excitation processes in e^+-H_2 scattering. The present results are compared with the more accurate laboratory-frame rotational close-coupling approximation (LFCCA) predictions. The electronically inelastic rotational excitation results using the ANR model differ from the corresponding LFCCA results near the electronic excitation threshold energies.

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Recently, interest has been focused on e^+-atom and e^+-molecule scattering. A large number of works has been performed on e^+-atom scattering in recent years. However, few calculations have been carried out for e^+-molecule scattering with positron signature. Calculations on molecular scattering are much more complicated than the corresponding atomic calculations. In molecular scattering one has to indulge certain approximations to make the calculations tractable. The fixed nuclei (FN) approximation, in which the motion of the nuclei is considered to be freezed, enjoys the confidence of the theoretical physicists. However, laboratory-frame rotational close-coupling approximation (rotational LFCCA), in which the rotational motion of the nuclei is taken into account dynamically, has also been employed to investigate the problems. One can also predict rotational excitation cross sections by invoking the adiabatic nuclear rotation (ANR) approximation, in which the rotational motion of the nuclei is included adiabatically by employing the fixed nuclei T matrix.

In recent years, it has been noticed that near the rotational excitation threshold the rotational excitation results for electronically elastic cases obtained by using the ANR model and the rotational LFCCA approximation differ appreciably (Feldt and Morrision [1]). In the case of polar molecules similar differences have also been noticed (Ghosh *et al.* [2], Mukherjee, Basu, and Ghosh [3]). The idea of the adiabatic nuclei formalism was first given by Chase [4] and systematically developed by Temkin and Vasavada [5] and Temkin and Faisal [6]. Later on this method was employed successfully to different systems. We would like to mention that the assumptions of the ANR method reveal the shortcomings of the model in the case of polar molecules and near the rotational excitation thresholds (Lane [7]). In the present work we consider the electronic excitation of H_2 by e^+ impact using the ANR model. In this calculation we consider two states ($X\ {}^1\Sigma_g^+$ and $B\ {}^1\Sigma_u^+$) of H_2 in the expansion scheme. Positron hydrogen molecule scatterings have been studied by several workers (Armour and Humberston [8]). The calculation of Armour *et al.* [9] is the most elaborate one. To the best of our knowledge there are altogether three calculations in which the electronic excitation of the target (H_2) by e^+ impact have been studied. Mukherjee, Sur, and Ghosh [10] have employed the FN approximation to predict the total cross sections by using the same electronic basis set of H_2 as the present one, Mukherjee, Mukherjee, and Ghosh [11] have also performed the rotational LFCCA calculation by retaining the same two electronic states. They have predicted the electronically elastic, electronic excitation, and rotational excitation cross sections at different energies. In a recent calculation Lino, Germano, and Lima [12] reported the integral and differential cross sections for e^+ impact excitation of the $X\ {}^1\Sigma_g^+$-$B\ {}^1\Sigma_u^+$ transition of H_2 using the Schwinger multichannel method. There are some differences between the results of our group and those of Lino, Germano, and Lima. In their paper they discuss the differences in detail. The use of two different methods and the ansatz employed by them are expected to be responsible for this lack of agreement [13].

It is evident from the above discussions that the ANR model is not valid near the electronically elastic rotational excitation threshold. The motivation of the present work is to demonstrate the unsuitability of the ANR method for electronically inelastic rotational excitation processes by comparing them to the LFCCA cross sections of Mukherjee, Mukherjee, and Ghosh [11]. Moreover, we would like to find the energy region in which the ANR model is valid for the processes under consideration. We do not claim that our results for the cross section are of very high accuracy. This is due to the fact that the present results are not convergent with respect to the electronic eigenstates of the target. In other words, the electronic basis functions retained in the calculation include induced spherical and nonspherical polarization potential partially. One does require π orbital of H_2 in the expansion scheme to include the effect of the polarization moderately. The present study simply demonstrates the difference between the LFCCA and ANR results under identical physical conditions.

In the FN formalism the total wave function for the e^+-molecule system can be written as (excluding spin coordinates)

$$\Psi^{\mathrm{FN}}(\vec{r},\vec{x}|\vec{R})=\sum_n \Phi_n(\vec{r}|\vec{R})F_n(\vec{x}|\vec{R}), \tag{1}$$

where $\vec{r}$ collectively denotes the electronic coordinates of the molecule, $\vec{R}$ is the internuclear separation, and $\vec{x}$ is the coordinate of the positron. Φ_n is the wave function of the molecule and F_n is that of the positron. The total Hamiltonian in the FN formalism is given by

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TABLE I. FN total cross sections (a_0^2) for different symmetries with different Λ in e^+-H_2 scattering at 11.8 eV.

Symmetry	Λ	Elastic ($X\ {}^1\Sigma_g^+ \rightarrow X\ {}^1\Sigma_g^+$)	Excitation ($X\ {}^1\Sigma_g^+ \rightarrow B\ {}^1\Sigma_u^+$)
g	0	0.1907(+01)	0.1017(+00)
	1	0.3407(+00)	0.1202(+00)
	2	0.2780(−01)	0.9519(−04)
	3	0.5062(−02)	0.5673(−04)
	4	0.3659(−02)	0.1871(−04)
	5	0.6885(−03)	0.1499(−04)
	6	0.8407(−03)	0.1137(−04)
	7	0.2117(−03)	0.7718(−05)
	8	0.1928(−03)	0.3182(−05)
	9	0.9144(−04)	0.1531(−05)
u	0	0.1162(+01)	0.7554(+00)
	1	0.7276(−01)	0.5762(−02)
	2	0.2869(−01)	0.3294(−02)
	3	0.9708(−02)	0.2816(−03)
	4	0.1584(−02)	0.2437(−03)
	5	0.1636(−02)	0.1660(−03)
	6	0.3605(−03)	0.7403(−04)
	7	0.4778(−03)	0.2008(−04)
	8	0.1347(−03)	0.6169(−05)
	9	0.1896(−03)	0.3377(−06)

$$H = H_{\mathrm{mol}}(\vec{r}|\vec{R}) + T_p(\vec{x}) + V_{\text{p-mol}}(\vec{x},\vec{r}|\vec{R}), \tag{2}$$

where H_{mol} is the molecular Hamiltonian, T_p is the kinetic energy of the positron, and $V_{\text{p-mol}}$ is the interaction term for the positron-molecule system.

Using Eqs. (1) and (2) in the relevant Schrödinger equation for the present two-state process we get a set of coupled differential equations, the solutions of which give FN T-matrix elements $T_{l_n l'_{n'}}^{nn'\Lambda}$ for different values of Λ, where Λ is the projection of the projectile's orbital angular momentum along the internuclear axis, which is a good quantum number. Here n and n' indicate the electronic states, and l_n and $l'_{n'}$ are the corresponding orbital angular momenta of the projectile. The rotational excitation cross sections for electronically elastic and electronic excitation processes in the ANR formalism is calculated using the following relation:

$$\sigma^{nn'}(j'_{n'} - j_n) = \frac{\pi}{k^2(2j_n+1)} \sum_J \sum_{l_n} \sum_{l'_{n'}} \times (2J+1) \left| T^{nn'J}_{j_n l_n, j'_{n'} l'_{n'}} \right|^2, \tag{3}$$

where

$$T^{nn'J}_{j_n l_n, j'_{n'} l'_{n'}} = (-1)^{l_n + l'_{n'}} \sum_{\Lambda} (J, l_n, j_n; -\Lambda, \Lambda) \times (J, l'_{n'}, j'_{n'}; -\Lambda, \Lambda)\, T^{nn'\Lambda}_{l_n l'_{n'}}. \tag{4}$$

Here J is the total (orbital plus rotational) angular momentum of the positron molecule system.

In this calculation we have taken two states of $H_2(X\ {}^1\Sigma_g^+$ and $B\ {}^1\Sigma_u^+)$. The basis functions used in this calculation have been taken from Fraga and Ransil [14]. As our basis functions contain two eigenstates of H_2 there are three coupling potentials given by V_{11} ($\langle \psi_1 | V_{\text{p-mol}} | \psi_1 \rangle$), V_{12} ($\langle \psi_1 | V_{\text{p-mol}} | \psi_2 \rangle$), and V_{22} ($\langle \psi_2 | V_{\text{p-mol}} | \psi_2 \rangle$), where ψ_1 and ψ_2 are the ground- and excited-state electronic wave functions of H_2, respectively. The asymptotic form of the quadrupole potential for V_{11} and V_{22} behaves as Q_1/r^3 and Q_3/r^3, respectively, whereas the asymptotic form of the dipole potential for V_{12} behaves as Q_2/r^2. In the present calculation the values of Q_1, Q_2, and Q_3 are 0.48, 1.42, and 0.401 a.u., respectively. The coupled differential equations have been solved using the variable step-size Numerov method. We have developed our own computer code to solve the problem. We reproduce the results for the FN T-matrix elements obtained by Mukherjee, Sur, and Ghosh [10] by using the integral formalism. The K matrix has been evaluated up to $80a_0$.

Convergence of the scattering parameters is a key factor in molecular scattering due to the presence of several degrees of freedom. In our earlier paper [10] we have noticed that retaining moments (λ) up to 7 in the expansion scheme provides convergent results. Therefore, in the present calculation we have retained moments up to 7 (for the gereade state $\lambda = 0,2,4,6$ and for the ungereade state $\lambda = 1,3,5,7$). For the good quantum number Λ, we have found that the convergence of the results is obtained by retaining up to $\Lambda = 9$. This will be clear from Table I, where we have tabulated the results of FN total cross sections for different gereade (l is

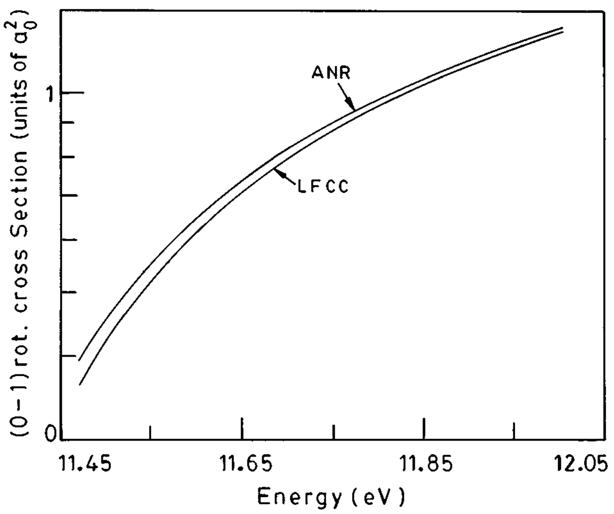

FIG. 1. Rotational $j=0$-$j'=1$ excitation cross section for electronic excitation ($X\ ^1\Sigma_g^+$-$B\ ^1\Sigma_u^+$) process in e^+-H_2 scattering.

even) and ungereade (l is odd) symmetries at the incident energy 11.8 eV. Depending on the Λ values and the g and u symmetries the maximum number of partial waves retained is 17.

In the present work, we have calculated the rotational excitation cross sections for electronically elastic as well as electronically inelastic processes in e^+-H_2 scattering using ANR formalism in the energy range 11.47 to 14.0 eV. It may be noted that the threshold energies for the $j=0$-$j'=1$ and $j=0$-$j'=3$ processes are 11.38 and 11.46 eV, respectively. Figures 1 and 2 represent the $j=0$-$j'=1$ and $j=0$-$j'=3$ rotational excitation cross sections for the electronic excited processes using the present ANR method and the LFCCA formalism of Mukherjee, Mukherjee, and Ghosh [11]. For future reference and completeness of the paper we have also tabulated in Table II the rotational $j=0$-$j'=1$ and $j=0$-$j'=3$ excitation cross sections for electronically inelastic processes along with $j=0$-$j'=0$ and $j=0$-$j'=2$ rotational excitation results for electronically elastic processes. The difference between the ANR and LFCCA predictions for the electronically elastic rotational cross section is marginal in the energy range considered, as it is far away from the rotational excitation threshold. It may be noted that the rota-

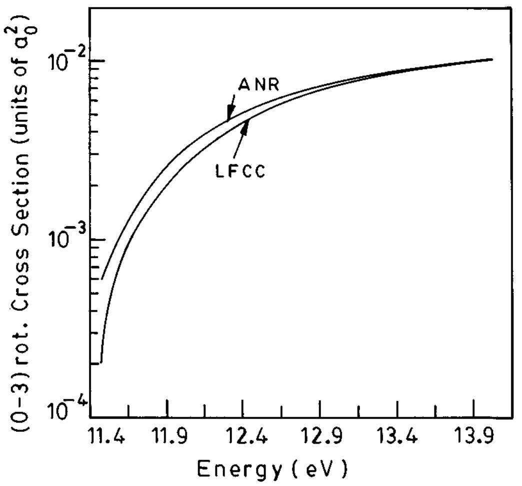

FIG. 2. Rotational $j=0$-$j'=3$ excitation cross section for electronic excitation ($X\ ^1\Sigma_g^+$-$B\ ^1\Sigma_u^+$) process in e^+-H_2 scattering.

TABLE II. Rotational cross sections (a_0^2) for electronically elastic and excitation processes in e^+-H_2 scattering.

E	Elastic ($X\ ^1\Sigma_g^+ \rightarrow X\ ^1\Sigma_g^+$)				Excitation ($X\ ^1\Sigma_g^+ \rightarrow B\ ^1\Sigma_u^+$)			
(eV)	j_1'	j_1	LFCC [a]	ANR [b]	j_2'	j_1	LFCC [a]	ANR [b]
11.47	0	0	2.5559	2.5483	1	0	0.3608	0.3951
	2	0	1.0279	1.0264	3	0	0.0002	0.0006
11.5	0	0	2.5602	2.5515	1	0	0.4245	0.4575
	2	0	1.0253	1.0243	3	0	0.0004	0.0007
11.6	0	0	2.5650	2.5558	1	0	0.6213	0.6525
	2	0	1.0208	1.0201	3	0	0.0008	0.0011
11.7	0	0	2.5670	2.2676	1	0	0.8009	0.8289
	2	0	1.0134	1.0134	3	0	0.0012	0.0015
11.8	0	0	2.5584	2.5581	1	0	0.9604	0.9851
	2	0	1.0049	1.0043	3	0	0.0016	0.0021
12.0	0	0	2.5622	2.5622	1	0	1.2333	1.2555
	2	0	0.9869	0.9859	3	0	0.0026	0.0032
12.5	0	0	2.5781	2.5779	1	0	1.8597	1.8853
	2	0	0.9651	0.9642	3	0	0.0052	0.0057
13.0	0	0	2.5808	0.9642	1	0	2.4646	2.4897
	2	0	0.9360	0.9350	3	0	0.0074	0.0077
14.0	0	0	2.5678	2.5664	1	0	3.4189	3.4442
	2	0	0.8734	0.8726	3	0	0.0102	0.0104

[a] Results of Mukherjee, Mukherjee, and Ghosh [11].

[b] Present results.

tional cross sections for electronically elastic process obtained by the LFCCA and ANR models differ just above the rotational excitation threshold (Feldt and Morrision [1]). Figures 1 and 2 demonstrate that the electronically inelastic rotational excitation cross sections for $j=0$-$j'=1$ and $j=0$-$j'=3$ using ANR formalism differ from those of LFCCA near the electronic excitation threshold energies, LFCCA results being lower. With the increase of energy the difference decreases. Above the incident energy 14.0 eV two results nearly coalesce. It should be noted that the ANR cross section for the $j=0$-$j'=1$ transition is higher than the corresponding LFCCA prediction by 9.7% at 11.47 eV and only 0.74% at 14.0 eV. As the value of the cross section for the $j=0$-$j'=3$ transition is very small, here we have not given the percentage of difference for this process.

In this paper we have performed a calculation on e^+-H_2 scattering considering electronic excitation of H_2 using the ANR method. The present scattering parameters quoted here are an ANR calculation for the e^+-H_2 scattering with positron signature. Our earlier two studies [2,3] along with the investigation of Feldt and Morrision [1] indicate that near the rotational excitation threshold, electronically elastic rotational excitation cross section using the ANR model differ from the corresponding LFCCA predictions, LFCCA results being more reliable. The present study shows that near the electronic excitation threshold, the electronically inelastic rotational excitation results also differ appreciably using the two different methods. The results predicted using the ANR method near the excitation threshold for the electronic excitation processes are less reliable than the corresponding LFCCA predictions. However, except near the electronic excitation threshold, the ANR method is found to be valid.

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