Electromagnetic Cascade and Chemistry of Exotic Atoms

Edited by Leopold M. Simons, Dezsö Horváth, and Gabriele Torelli

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Springer Science+Business Media, LLC

Library of Congress Cataloging-in-Publication Data

International School of Physics of Exotic Atoms (5th : 1989 : Erice, Italy)
Electromagnetic cascade and chemistry of exotic atoms / edited by Leopold M. Simons, Dezsõ Horváth, and Gabriele Torelli.
p. cm. -- (Ettore Majorana international science series. Physical sciences ; v. 52)
"Proceedings of the fifth course of the International School of Physics of Exotic Atoms ... held May 14-20, 1989, in Erice, Italy"--T.p. verso.
Includes bibliographical references and index.
ISBN 0-306-43686-8
1. Particles (Nuclear physics)--Multiplicity--Congresses. 2. Cascade shower--Congresses. 3. Electromagnetic interactions--Congresses. 4. Exotic atoms--Congresses. 5. Muons--Congresses. 6. Nuclear chemistry--Congresses. I. Simons, Leopold M. II. Horváth, Dezsõ. III. Torelli, Gabriele. IV. Title. V. Series.
QC794.6.M85I58 1989
539.7--dc20 90-48317
CIP

ISBN 978-1-4899-3703-2 ISBN 978-1-4899-3701-8 (eBook)
DOI 10.1007/978-1-4899-3701-8
Softcover reprint of the hardcover 1st edition 1990
Proceedings of the Fifth Course of the International School of Physics of Exotic Atoms on Electromagnetic Cascade and Chemistry of Exotic Atoms, held May 14–20, 1989, in Erice, Italy

Originally published by Plenum Press, New York in 1990.

PREFACE

This Workshop was organized to bring once more together the scientists of the rather heterogeneous field of exotic atoms. At present the main topic of the field seems to be the study of the atomic cascade. There are some who study it intentionally - let us call them *cascadeurs* - and others who think they investigate other features of the exotic atoms (like Coulomb capture, particle transfer, muon catalyzed fusion, chemical effects, fundamental properties, etc.) - *users* - while in fact they study some special consequences of the same atomic cascade.

We decided to get *cascadeurs* and *users* discuss the problems of exotic atoms at wonderful Erice, at the **5th Course of the International School of Physics of Exotic Atoms**. Our Workshop was quite successful, we have heard excellent talks from participants from a dozen countries and most of them have prepared written contributions for this volume.

The Organizers express their gratitude to all participants for their contributions, especially to David Measday for his concluding remarks (not printed here) and to James Cohen for jumping in for Leonid Ponomarev who had to leave unexpectedly in the middle of the meeting. We greatly appreciate the enthusiastic help of Marianne Signer in every stage of the organization work. And, of course, the Workshop could not happen at all without the incredibly efficient organization by the **Ettore Majorana Centre of Scientific Culture.**

Leopold M. Simons
Dezsö Horváth
Gabriele Torelli

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V. MUON CATALYZED FUSION

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OPENING ADDRESS

Ladies and Gentlemen!

I am very happy to open the Fifth Course of the International School of Physics of Exotic Atoms. This School was founded in the year of 1977 when Nino Zichichi convinced me that even this rather narrow field was worth covering by a special school. And indeed, the idea was accepted by the community with much enthusiasm as it successfully brought together most of the researchers working in this field.

The friendly atmosphere of the first course will certainly be remembered with pleasure by all the participants. The second course only two years later reflected the success of the quark model in that time. Hence a major topic of that exotic atoms course was the discussion of even more exotic matter as quark atoms and molecules. The renaissance of muon catalyzed fusion has affected that course quite remarkably, too.

With the commissioning of LEAR in 1982 the third course was naturally devoted to antiproton physics and helped to stimulate and develop ideas which are still being pursued. The main objective of the fourth course in 1985 had been the tests of conservation laws as, e.g., for the case μ - e conversion where exotic atoms are used to reach the initial stage of the process. At the time of the course the joint experimental and theoretical efforts in the study of muon catalyzed fusion led to such a tremendeous surge in activity that did not allow to include it in a common course any longer.

Now, in 1989 we are back to the original theme of the School. We are motivated by the fact that many of the experiments and theoretical considerations have reached a precision where effects of the formation and deexcitation mechanisms of exotic atoms can no longer be neglected but need to be studied in detail again. Thus it is time again to interchange experimental and theoretical results and to discuss different ideas. This way we should be able to assess the present and future possibilities of exotic atoms in order to exploit this beautiful field as efficiently as possible.

In this spirit I hope the Fifth Course will be a success, too.

Gabriele Torelli

I

DECELERATION AND COULOMB CAPTURE, MESIC CHEMISTRY

The White Rabbitt put on his spectacles.
"Where shall I begin, please your Majesty?", he asked.
"Begin at the beginning," the King said gravely,
"and go on till you come to the end: then stop."

Lewis Carroll: Alice in Wonderland

FORMATION OF EXOTIC HYDROGEN ATOMS

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1. INTRODUCTION

Formation of exotic hydrogen atoms has been studied theoretically for 40 years.[1] However, most of the work prior to 1980 utilized perturbative or two-state approximations that are now known to be inadequate because the slow ionizing collisions, which lead to muon capture, entail strong coupling of many intermediate states. Ironically the very first study, by Wightman[2] in 1950, has the most in common with modern treatments. His method, known as adiabatic ionization (AI), followed from the observation of Fermi and Teller[3] that there exists a critical strength of the dipole, formed by the projectile negative muon and target proton in μ^-+H collisions, for binding the electron. In collisions where the μ^- adiabatically approaches closer than this distance, the electron escapes and, if the muon is left with negative energy, the pμ^- atom is formed. The most serious failures of this simple model stem from trajectory deflection and nonadiabatic lag in the motion of the electron. The deviation from a straight-line trajectory is easily taken into account. Nonadiabatic effects have been included by a sequence of methods of increasing sophistication: diabatic states (DS),[4] classical-trajectory Monte Carlo (CTMC),[5] time-dependent Hartree Fock (TDHF),[6] and classical-quantal coupling (CQC).[7] The DS and CTMC methods have also been used to calculate the slowing-down cross sections. Consistent calculation of the slowing-down and capture cross sections is crucial for correct determination of the capture distributions in a medium.[8]

Results of all the above methods are discussed in Sec. 2 for μ^-+H collisions. Other exotic hydrogen atoms, in particular pπ^- and p$\bar{\text{p}}$, are also of interest and can be treated in a similar fashion as discussed in Sec. 3. Results for $\bar{\text{p}}$+H collisions obtained by the AI, DS, and CTMC methods are compared with the corresponding μ^-+H calculations. All exotic-atom experiments done to date actually use H_2 molecular targets. The similarities and differences of H and H_2 in the capture process are discussed. A clever new way to

Electromagnetic Cascade and Chemistry of Exotic Atoms
Edited by L. M. Simons *et al.*, Plenum Press, New York, 1990

form $p\bar{p}$ in collisions of $\bar{p}$ with the atomic hydrogen negative ion H^- has been suggested.[9] Theoretical calculations are presented that show capture by the negative ion is significantly different from capture by the neutral atom.

2. THEORETICAL METHODS FOR MUON CAPTURE BY THE HYDROGEN ATOM

2.1. *Adiabatic Ionization (AI)*

Interaction of an electron with a fixed dipole has the peculiar property of having either an infinite number of bound states or none at all; the critical dipole strength for unit charges (e.g., p and μ^-) occurs at a distance $R_c = 0.639\ a_0$.[3] The adiabatic potential energy is shown in Fig. 1. Assuming a straight-line trajectory, Wightman[2] estimated the ionization cross section to be

$$\sigma_{AI}^{SLT} = \pi R_c^2 = 0.408\ \pi a_0^2 \tag{1}$$

independent of the collision energy as shown in Fig. 2 (chain–dashed curve). This model assumes that the electron escapes adiabatically with zero kinetic energy asymptotically, so capture occurs only if the collision energy is less than the ionization energy I_a. The

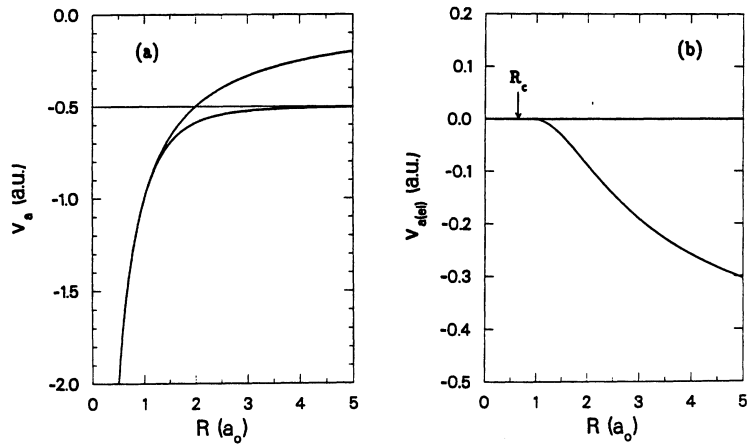

Fig. 1. Adiabatic electronic potential energy curves for μ^- + H and μ^- + H^+. In (a) the complete potential curve is shown, and in (b) the electronic energy only is shown —i.e., the -1/R Coulomb potential between the μ^- and p has been subtracted out. The potential curve is independent of the particle masses so also applies to other isotopes of hydrogen and other negative particles. The continuum is reached at R_c = 0.639 a_0.

corresponding wave function in Fig. 3 shows the electron first polarizing away from the approaching μ^-, then becoming more diffuse as the μ^- comes still closer, and finally passing into the continuum as the μ^- reaches the distance R_c.

Actually the deflection of the μ^- is quite significant at $E_{c.m.} \lesssim I_a$ and can be simply taken into account.[5] The adiabatic potential energy between μ^- and H is

$$V_a(R) = -\frac{1}{R} + V_{a(el)}(R) ; \tag{2}$$

the energy $V_{a(el)}$ of the electron for μ^- and p fixed at distance R has been exactly calculated.[10-11] The effective potential including the centrifugal repulsion can be written

$$V_{a(eff)}(R,b) = V_a(R) + \frac{b^2 E_{c.m.}}{R^2} \tag{3}$$

where $E_{c.m.}$ is the collision energy. If $V_{a(eff)}$ has no local maximum at $R > R_c$, then the

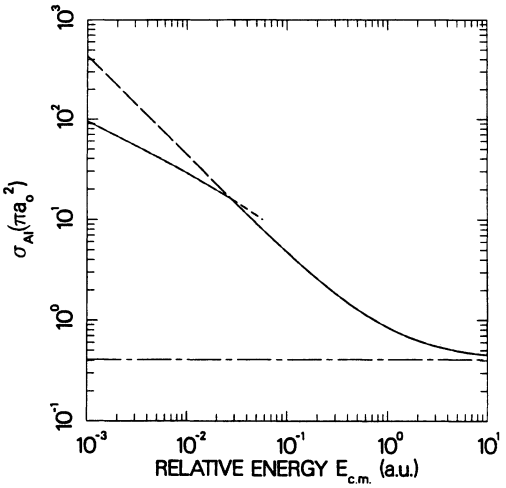

Fig. 2. Adiabatic ionization cross section with straight-line trajectory (chain-dashed curve) and curved trajectory (solid curve). In the latter case, the cross section is the lesser of Eq. (4) (long-dashed curve) and the cross section for orbiting collisions (short-dashed curve).

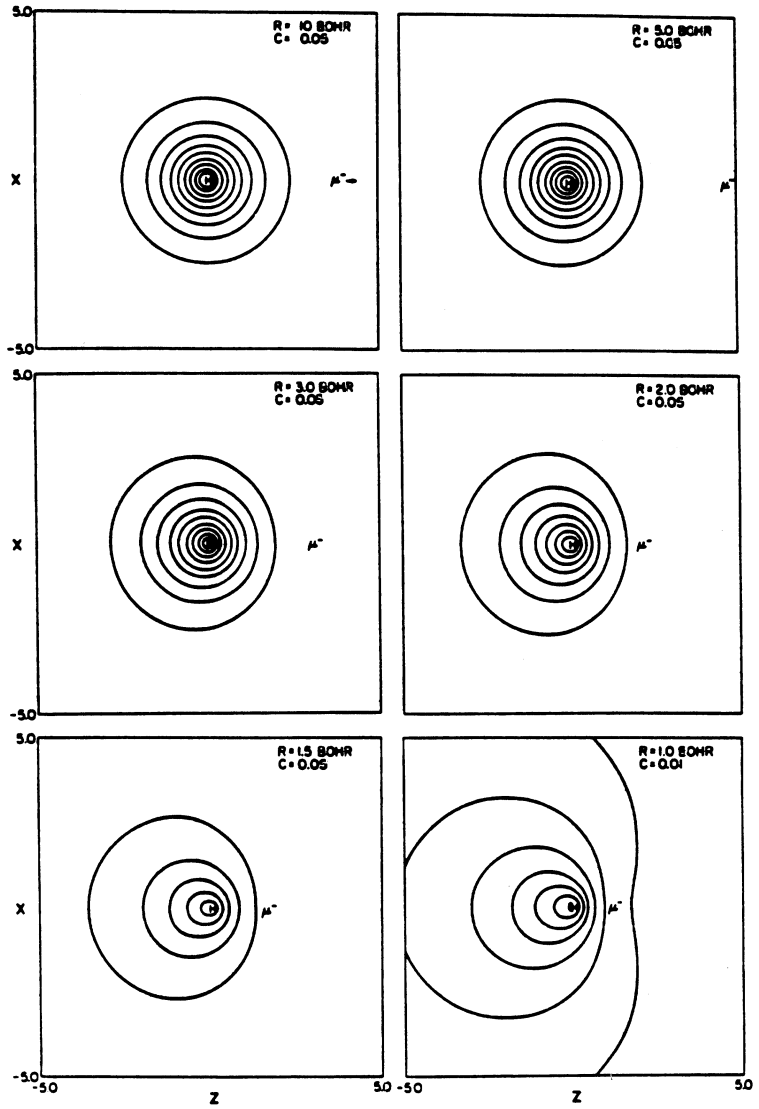

Fig. 3. Contours of the normalized adiabatic electronic wave function for various separations R between the μ^- and p. Contour values are C, 2C, 3C,... .

cross section at energy $E_{c.m.}$ is just

$$\sigma_{AI(c)}(E_{c.m.}) = \pi b_c^2 = \frac{\pi R_c^2}{E_{c.m.}} \left[E_{c.m.} + \frac{1}{R_c} - 0.5 \right] \tag{4}$$

(long–dashed curve in Fig. 2) where b_c satisfies

$$V_{a(eff)}(R_c, b_c) = E_{c.m.} \tag{5}$$

For $E_{c.m.} < 0.06$ a.u.,* Eq. (3) does have a maximum at some $R_0 > R_c$ satisfying $V_{a(eff)}(R_0, b_0) = E_{c.m.}$ so there are three classical turning points. The value πb_0^2 is also shown in Fig. 2 (short–dashed curve). However, for $0.03 < E_{c.m.} < 0.06$ a.u. even the innermost classical turning point is outside R_c so it is only at $E_{c.m.} < 0.03$ a.u. that the "hump" in the effective potential actually limits the cross section. Tunneling through the barrier is not expected to be important. Note that Figs. 1 and 2 are independent of the mass of the negative particle so they apply to $\bar{p}$ as well as μ^-. Only at extremely low energies ($\sim 10^{-6}$ a.u. for μ^-) where the scattering is dominated by s–waves would adiabatic ionization depend on the mass other than through the energy in the c.m. system (at 10^{-3} a.u., 6 partial waves still contribute to μ^- capture). Of course, the adiabatic ionization model itself is more valid for the heavy antiproton and breaks down completely for electron collisions.

2.2. *Diabatic States (DS)*

A conspicuous feature of Fig. 1 is that the electronic energy is extremely close to the continuum at $R \approx 1$ a_o even though it doesn't actually reach the continuum until $R_c = 0.639$ a_o. The diabatic–states treatment[4] takes into account the nonadiabatic behavior that allows the electron to be ionized at distances larger than R_c and also to carry off some kinetic energy. The nonadiabatic behavior is strengthened by the Coulomb attraction between the p and μ^- at distances $R \lesssim 1$ a_o; here the relative velocity is high enough that the electron no longer has time to adjust adiabatically.

In the DS method the μ^-–H interaction is described in the Born–Oppenheimer framework (i.e., the μ^- is treated as a heavy particle), but diabatic rather than adiabatic electronic states are used. The diabatic potential curve $V_d(R)$, unlike the adiabatic potential curve $V_a(R)$, crosses into the electronic continuum (this is true even for cases like $\mu^- + He$ or $\mu^- + H_2$ where adiabatic ionization cannot occur). In the extreme diabatic case, i.e. with the electronic orbital frozen as the 1s orbital of the H atom, this crossing

*In atomic units, $\hbar = e = m_e = 1$, so 1 a.u.(energy) = 27.21 eV, 1 a.u.(velocity) = 2.19×10^8 cm/s, 1 a.u.(time) = 2.42×10^{-17} s, and 1 a_0(distance) = 0.529 Å.

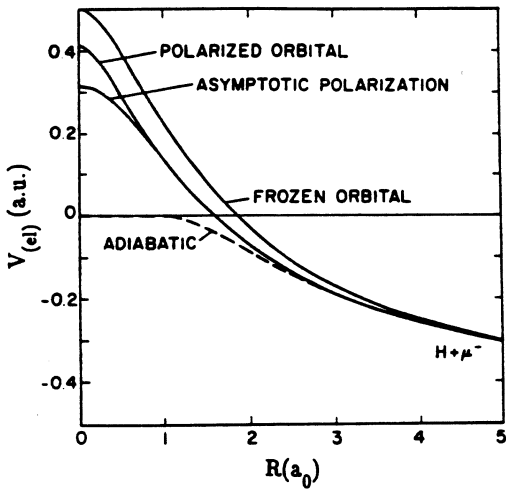

Fig. 4. Electronic potential energy curves for μ^- + H. The μ^--p Coulomb potential has been subtracted out. The dashed curve is the adiabatic energy and the solid curves are three different diabatic approximations. The DS cross sections in later figures are calculated with the polarized-orbital (po) potential.

occurs at a distance $R_x = 1.86\ a_0$ as shown in Fig. 4. This effect has been taken into account by introducing a polarizing orbital of p character. The energy is relatively insensitive to how this orbital is chosen; Fig. 4 shows the different results of optimizing the orbital (by minimizing the energy) at large distances and at the distance R_x. For definiteness the latter will be used henceforth. The effect of polarization moves the continuum crossing point in to $R_x' = 1.59\ a_0$. At $R > 2.5\ a_0$ the potential including polarization essentially coincides with the adiabatic potential.† At distances smaller than the crossing into the continuum, the diabatic state is embedded in the electronic continuum and hence has a finite autoionization width, which is calculated by "Fermi's golden rule". We avoid direct evaluation of continuum integrals by discretizing the continuum and utilizing Stieltjes moment theory; the width Γ is shown in Fig. 5.‡

†At the time Ref. 4 was published it was thought that the difference between the frozen and polarized orbital treatments was within the uncertainty of the model so cross sections were presented only with the frozen orbital. Now there seems to be empirical evidence that the method may be more accurate than expected. Where necessary, the two will be distinguished by DS–fo and DS–po.

‡This calculation was performed with the frozen–orbital wave function—the result with the polarized–orbital wave function is not expected to be too different. The nonzero value of Γ at $R > R_x$ reflects coupling to Rydberg states but since such coupling does not generally result in μ^- capture it is set to zero in the subsequent calculations.

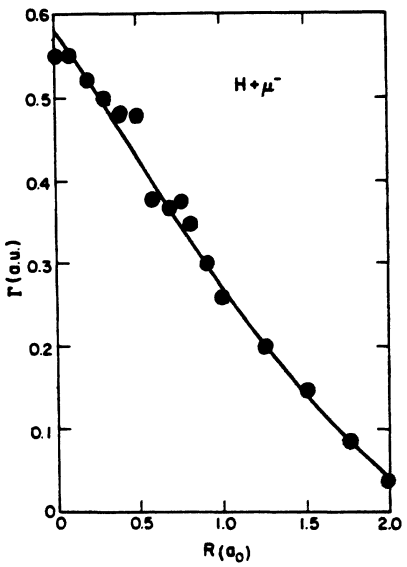

Fig. 5. Diabatic ionization width for μ^- + H. Calculations were done at the points shown.

The interaction is then formulated by the complex potential

$$W(R) = V_d(R) - i\Gamma(R)/2\,, \tag{6}$$

and the scattering in this potential is treated by the impact-parameter method with quasiclassical trajectories. The energy carried off by the electron is just the difference between the neutral and ionic potential curves, which is just $V_d(R) + 1/R$ for μ^-+H since the final state is devoid of electrons.†* For very slow collisions ($v \lesssim 0.1$ a.u.) most ionization occurs soon after crossing into the continuum so the electrons carry away little kinetic energy, but for faster collisions ($v \gtrsim 1.0$ a.u.) greater penetration is achieved and more energetic electrons are ejected (up to ~ 0.9 a.u.). Hence the two major objections to the AI model are eliminated in the DS model: (1) ionization can occur at a distance R_x' about 2.5 times larger than R_c so the cross section can be up to $(R_x'/R_c)^2 \approx 6.2$ times as big and (2) the electrons carry away kinetic energy so the stopping power is greater and the initial state of the resulting muonic hydrogen atom is determined.

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†*In Ref. 4 it was speculated that the electron energy distribution might be *broadened* according to the width Γ by dynamic effects missing in the DS model. Subsequent CTMC calculations (see next section) indicate that such broadening is unimportant and this complication can be dispensed with.

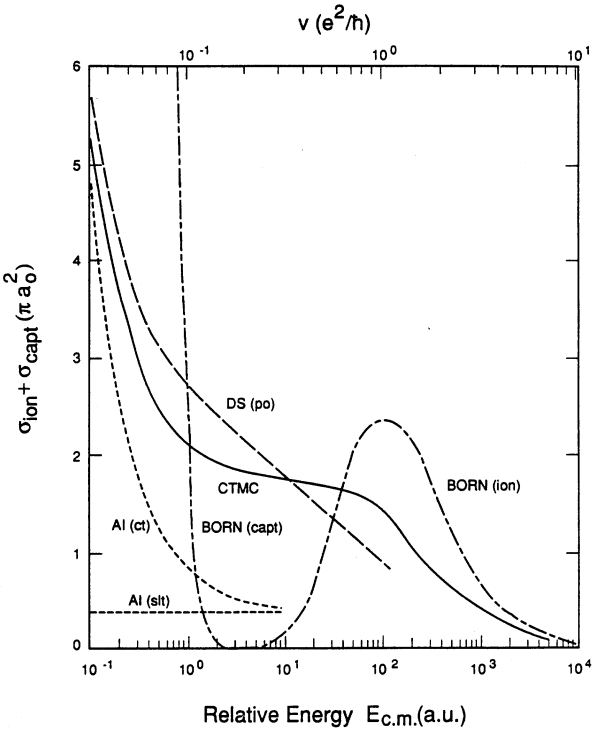

Fig. 6. Comparison of different total (ionization plus capture) cross sections for μ^- + H collisions: adiabatic ionization with straight-line trajectories and curved trajectories (short-dashed curves), diabatic states with polarized orbital (long-dashed curve), classical-trajectory Monte Carlo (solid curve), and Born approximation (chain-dashed curve—capture from Ref. 12a and ionization from Ref. 12b).

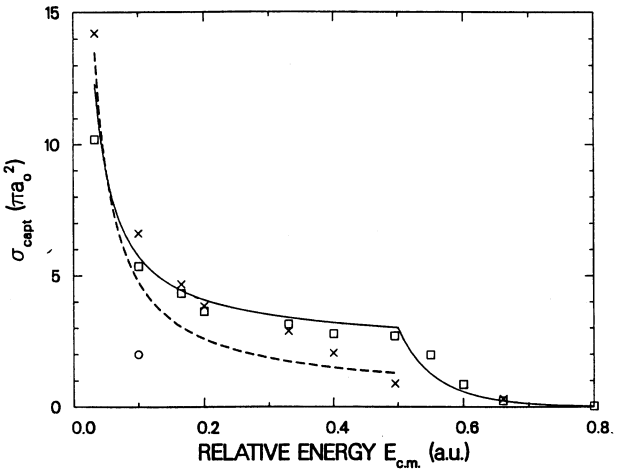

Fig. 7. Comparison of different capture cross sections for μ^- + H collisions: adiabatic ionization with curved trajectories (dashed curve), diabatic states with polarized orbital (solid curve), classical-trajectory Monte Carlo (□), time-dependent Hartree Fock (○), and classical-quantal coupling (×).

The total (ionization plus capture) cross section is shown in Fig. 6 and the capture cross section alone is shown in Fig. 7. In these two figures comparison can be made with the adiabatic ionization results as well as with the results of other methods discussed in subsequent sections. The DS cross section does not actually achieve the factor of $(R_x'/R_c)^2$ enhancement over the AI cross section but only a factor of 4.1 at $E_{c.m.} \approx 5$ a.u. At higher energies the DS cross section falls off due to the decreased interaction time and eventually behaves as $E_{c.m.}^{-\frac{1}{2}}$, whereas the AI cross section approaches a constant. However, even the DS cross section is not reliable at $v \gtrsim 1$ a.u. since it does not take into account the binary encounter mechanism of ionization shown in the next section to be dominant at high energies.

In the AI model, capture occurs only in collisions at $E_{c.m.} \leq 0.5$ a.u. In the DS model (including polarization), capture can occur at collision energies up to ~ 0.9 a.u., but the calculations show that the capture cross section decreases rapidly above 0.5 a.u. At such low energies, the width Γ is large enough to saturate the cross section; hence for $E_{c.m.} < 0.5$ a.u., the DS capture cross section could simply be calculated by Eq. (4) with R_c replaced by R_x'. The resulting formula yields a cross section larger than σ_{AI} at $E_{c.m.} > 0.05$ a.u. and slightly smaller at $E_{c.m.} < 0.05$ a.u. This crossing is visible in Fig. 7. However, σ_{DS} does not actually fall as far below σ_{AI} as indicated by Eq. (4) because at $E_{c.m.} < 0.016$ a.u. the DS and AI cross sections are limited by the same centrifugal barrier and hence become identical.