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I. INTRODUCTION

Charge exchange has been demonstrated to play an important role as a pumping mechanism for population inversions in a variety of near-thermal metal vapor lasers[1]. The general process occurring is

$$R^{+} + M \longrightarrow R + M^{+*} + \Delta_f \tag{1}$$

where R is a rare gas atom and M is a metal atom. The quantity Δ_f is the energy defect of the state f for the metal ion ($\Delta_f > 0$ corresponds to an increase in kinetic energy of the infinitely separated quasi-molecule). The rate for such a process is given by

$$\text{Rate } (f) \propto v\sigma_f \tag{2}$$

where v is the relative velocity of the colliding pair and σ_f is the cross section for production of state f. One might expect that the cross section is largest for those states f with smallest energy defect Δ_f, i.e., for near resonant collisions.

Chubb and Rose[2] have suggested that the rate of charge exchange will be enhanced if the relative collision velocity v is increased over thermal velocities by using a MPD arc accelerator[3] as a high density source of rare gas ions. An important question then is whether the efficiency of the lasing system can be enhanced by assuring that the charge exchange takes place selectively to a few states f (ideally to a single state). The notion that near resonance can provide such a selection mechanism must be investigated more thoroughly.

As pointed out by Melius[4], charge transfer occurs most efficiently in the region of atom-ion separation where the potential energies of the quasi-molecular states cross (or nearly cross) one another. Therefore, even though Δ_f may be small there is no assurance that the potential curves cross in a region of strong coupling. Further there may be several final states f for which curve crossings occur in a region of strong coupling. Thus a thorough understanding of the charge exchange process requires a more detailed analysis involving the relevant potential energy curves and the coupling mechanism.

We report on a theoretical model utilizing reasonable potential energy curves and coupling matrix elements in a two state impact parameter calculation. Details are presented in the next section.

II. THEORY

We here outline the general theory appropriate to the charge exchange process discussed above.[5-7] For simplicity we discuss only the two active electrons. The two electron molecular system for fixed nuclei is described by the electronic Hamiltonian

$$H(\vec{r},\vec{R}) = \sum_{i=1}^{2}\left(T_i + V_{iR} + V_{iM}\right) + V_{12} + V_{RM} \tag{3}$$

with T_i being the kinetic energy operator for the electrons and the potentials V describe the two-body Coulomb interactions amongst the nuclei and electrons (See Fig. 1). We treat the colliding system in a quasi-classical fashion where the nuclear separation $\vec{R}$ is determined (in principle) from a classical scattering calculation. Therefore H acquires an implicit time dependence via $\vec{R}$ and we need solve a time-dependent Schrodinger equation for the wave function of the colliding system.

$$H(\vec{r},\vec{R}(t))\ \Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) \tag{4}$$

The wave function Ψ is represented as an expansion of an arbitrary orthonormal basis

$$\Psi(\vec{r},t) = \sum_{m} b_m(t)\,\phi_m(\vec{r},\vec{R})\exp\left[-\frac{i}{\hbar}\int^{t} H_{mm}(R)\,dt\right] \tag{5}$$

where $H_{mn} = \langle \phi_m | H | \phi_n \rangle$ and $b_n(t)$ are the expansion coefficients which are to be determined. Various possible choices of the bases will be described below. Insertion of Eq. 5 into Eq. 4 yields the set of coupled equations.

$$i\hbar \frac{db_n}{dt} = \sum_{m \neq n} \left[H_{mn} - i\hbar \langle \phi_n | \frac{\partial}{\partial t} | \phi_m \rangle \right] * \exp\left[-\frac{i}{\hbar} \int^t (H_{mm} - H_{nn}) dt \right] b_m \tag{6}$$

In a process where the transition probability is small it may be acceptable to truncate the sum to include only the two states of interest (we discuss an added complication below). We make this approximation calling the incident state i and the final state f. The two basis states retained, ϕ_i and ϕ_f, must have the property that as R → ∞, they represent the separated atom + ion

$$\phi_i \xrightarrow[R\to\infty]{} |R^+ M\rangle_\infty$$

$$\phi_f \xrightarrow[R\to\infty]{} |R M^{+*}\rangle_\infty$$

However this physical restriction still allows a manifold of choices for the bases ϕ. Two choices are as follows

i) Adiabatic bases.

The functions $\phi^{(a)}$ are chosen to diagonalize the electronic Hamiltonian

$$\langle \phi_n^{(a)} | H | \phi_m^{(a)} \rangle = H_{nn}^{(a)}(R)\, \delta_{n,m} \tag{7}$$

In this expansion the first coupling term in Eq 6 is seen to vanish and transitions are caused by the non-adiabatic coupling term $\langle \phi_n^{(a)} | \frac{\partial}{\partial t} | \phi_m^{(a)} \rangle$. We mention that in such a basis set the eigenvalues $H_{nn}^{(a)}(R)$ and $H_{mm}^{(a)}(R)$ are unequal for all R unless the states have different symmetry about the molecular axis. Therefore $H_{nn}^{(a)}(R)$ can equal $H_{mm}^{(a)}(R)$ at the crossing point R_x for so-called rotational coupling but not for radial coupling. (For radial coupling $\langle \phi_n^{(a)} | \frac{\partial}{\partial t} | \phi_m^{(a)} \rangle = \frac{dR}{dt} \langle \phi_n^{(a)} | \frac{\partial}{\partial R} | \phi_m^{(a)} \rangle$ while for rotational coupling $\langle \phi_n^{(a)} | \frac{\partial}{\partial t} | \phi_m^{(a)} \rangle = \frac{d\Theta}{dt} \langle \phi_n^{(a)} | \frac{\partial}{\partial \Theta} | \phi_m^{(a)} \rangle$ where Θ describes the orientation of the molecular axis in a lab-fixed frame.)

ii) Diabatic Bases.

Here the functions $\phi^{(d)}$ are chosen such that

$$\langle \phi_n^{(d)} | \frac{\partial}{\partial t} | \phi_m^{(d)} \rangle = 0 \qquad (8)$$

Thus the second coupling term vanishes in Eq 6 and transitions are caused by the adiabatic interaction

$$\langle \phi_n^{(d)} | H | \phi_m^{(d)} \rangle = H_{nm}^{(d)}(R) \qquad (9)$$

For this basis set $H_{mm}^{(d)}$ can equal $H_{nn}^{(d)}$ even if n and m have the same symmetry. In general, if the complete expansion, Eq 5, is retained either basis set will yield the same results. However, when the basis set is truncated one can expect different results depending on the choice made. We argue that in a problem of such complexity as this, one can only hope to obtain rough estimates of the cross sections and therefore we will choose an approximate diabatic basis in which the states ϕ are represented by the non-interacting atomic wave functions for all R.

$$\phi_i = |R^+ M\rangle_\infty$$
$$\phi_f = |R\ M^{+*}\rangle_\infty \qquad (10)$$

These bases are approximate since they do not maintain the orthogonality requirement for all R. Further if the two molecular states have different symmetry about the molecular axis one is obliged to use an adiabatic representation since $H_{nm} = 0$ and transistions are caused by the rotational coupling term $\langle \phi_n^{(a)} | \frac{\partial}{\partial\Theta} | \phi_m^{(a)} \rangle$. However rotational coupling is not as important at thermal velocities due to its velocity dependence.

The calculation of the cross section proceeds as follows The coupled Eqs 6 reduce to

$$i\hbar \frac{db_i}{dt} = H_{if} \exp\left[-\frac{i}{\hbar}\int^t (H_{ff} - H_{ii})\,dt\right] b_f$$
$$i\hbar \frac{db_f}{dt} = H_{fi} \exp\left[-\frac{i}{\hbar}\int^t (H_{ii} - H_{ff})\,dt\right] b_i \qquad (11)$$

with the initial conditions $|b_i(t=-\infty)| = 1,\ b_f(t=-\infty) = 0$. These equations can be solved if the matrix elements H_{mn} are known for all R and if R(t) has been obtained. However, in many cases one can obtain an analytic solution to these equations. In particular, if the coupling is small then perturbation theory can be used. That the coupling is indeed small for Duffendack reactions can be seen by noting that the process involves the simultaneous exchange of one electron plus the excitation of the remaining electron in a low energy collision. To illustrate, in collisions of metal atoms with ionized helium we have $M = M(ns^2)$, $R^+ = He^+(1s)$, $M^{+*} = M^{+*}(n'\ell\sigma)$, $R = He(1s^2)$ where, in the incident molecular complex R^+M the atomic electrons have a zero component of angular momentum along the molecular symmetry axis and is therefore a Σ molerular state. Since the coupling H_{if} vanishes if the projection of the orbital angular momentum for the final state was not Σ, then the excited electron must also have a zero projection on the molecular axis. Therefore

$$H_{fi} = \langle \phi_f | H | \phi_i \rangle = \langle 1s\sigma_R(1)\, n'\ell\sigma_{M^+}(2) | H(1,2) | ns\sigma_M(1)\, ns\sigma_M(2) \rangle \tag{12}$$

where $H_{(1,2)}$ is given in Eq 3. Since ϕ_f and ϕ_i differ by two orbitals the matrix element H_{fi} vanishes identically and must be replaced by a second-order coupling determined from perturbation theory [6]

$$V_{fi} = \sum_{m \neq i,f} \frac{H_{fm} H_{mi}}{H_{mm} - H_{ii}} \tag{13}$$

the sum on m runs overall virtual intermediate states. These states ϕ_m are exactly those omitted when the coupled equations 6 were truncated to the two state equations 11. The sum over m should be dominated by a single term which represents the configuration in which the ion R^+ has excited the atom into the state $M^* = M\,(ns, n'\ell\sigma)$. Thus we take

$$
\begin{aligned}
\phi_i &= |ns\sigma_M(1)\, ns\sigma_M(2)\rangle \\
\phi_m &= |ns\sigma_M(1)\, n'\ell\sigma_M(2)\rangle \\
\phi_f &= |1s\sigma_R(1)\, n'\ell\sigma_{M^+}(2)\rangle
\end{aligned}
\tag{14}
$$

The matrix element H_{mi} is a multipole excitation of the ns_M orbital into the $n'\ell_M$ state by the charge R^+ and as such

$$H_{mi} \xrightarrow[R\to\infty]{} \frac{C_{mi}}{R^{\ell+1}} \tag{15}$$

The constant C_{mi} is the multipole moment for the transition in question

$$C_{mi} \sim \langle n'\ell\sigma_M(2)|\, r_2^{\ell}\, |ns\sigma_M(2)\rangle \tag{16}$$

The matrix element H_{fm} describes the exchange of the remaining ns_m orbital into the $1S_R$ state. For large R it is approximately equal to

$$H_{fm} \xrightarrow[R\to\infty]{} -I_m \langle ns\sigma_M(1)\,|\,1s\sigma_R(1)\rangle \tag{17}$$

where I_m is the energy needed to ionize the ns orbital in M^* and the integral is a standard overlap integral[8]. From Ref. 8 we obtain

$$H_{fm} \xrightarrow[R\to\infty]{} I_m \left(\frac{I_m}{I_H}\right)^{\frac{1}{2}} \frac{R}{a_0}\, e^{-\sqrt{\frac{I_m}{I_H}}\,\frac{R}{a_0}} \tag{18}$$

where I_H is the ionization energy of hydrogen and a_0 is the Bohr radius. (We set $a_0 = I_H = 1$ henceforth for notational simplicity.) This result is valid when $I_f \ll I_{He}$ which is the case here. When this is not the case the approximation of Olson[9] may be more appropriate. Finally we observe that at large distances the denominator in Eq 13 can be set equal to the excitation energy of M^*

$$H_{mm} - H_{ii} \equiv \epsilon_m \tag{19}$$

Therefore

$$V_{if} = V_{fi} \underset{R\to\infty}{\Longrightarrow} \frac{C_{mi}}{\epsilon_m}\, I_m^{3/2}\, R^{-\ell}\, e^{-\sqrt{I_m}\,R} \tag{20}$$

and the coupled equations for the amplitudes become

$$\begin{aligned} i\hbar \frac{db_i}{dt} &= V_{if} \exp\left[-\frac{i}{\hbar}\int^t (H_{ff}-H_{ii})\,dt\right] b_f \\ i\hbar \frac{db_f}{dt} &= V_{fi} \exp\left[-\frac{i}{\hbar}\int^t (H_{ii}-H_{ff})\,dt\right] b_i \end{aligned} \tag{11'}$$

The probability for a transition is obtained by setting

$$\mathcal{P}_f = |b_f(+\infty)|^2 \tag{21}$$

where the calculation for $\mathcal{P}$ must be performed over a range of impact parameters ρ yielding the cross section

$$\sigma_f = 2\pi \int_0^\infty \mathcal{P}_f(\rho)\,\rho\,d\rho \tag{22}$$

Under certain circumstances the coupled equations 11' can be integrated analytically. Consider the argument of the exponential, which we rewrite as

$$\int^{R(t)} \frac{(H_{ff} - H_{ii})}{dR/dt}\,dR \tag{23}$$

At low velocities the denominator of this expression is quite small and the integral will rapidly change as the system proceeds along its trajectory. The exponential function will therefore oscillate rapidly and effectively give no net coupling. However, if the trajectory takes the system through a radius R_x where $H_{ff}(R_x) = H_{ii}(R_x)$ [Fig 2] there will be a small interval where the integral changes slowly allowing for the coupling V_{fi} to be effective. This is the basis of the standard Landau-Zener method[6]. However, for very low collision energies an additional complication arises. The classical turning point, R_o, is very close to the crossing point R_x (see Fig. 2) therefore, the radial velocity $\dot{R}$ cannot be taken to have a constant value as is done in L-Z theory. In fact $\dot{R}$ will be changing signs in the vicinity of R_x. This complication has been taken into account by several authors however[5-7]. Since the potential curves H_{ff} and H_{ii} will cross at large values of R_x for Duffendack reactions and since V_{if} is exponentially small then, one can use perturbation theory[6] to solve the coupled equations 11' . The results[5-7] are

$$P_f = 4\pi^2 V_{if}^2 \left(\frac{2\mu}{\hbar^2 \bar{F} \Delta F}\right)^{2/3} Ai^2\left[-(E-U)\left(\frac{2\mu}{\hbar^2}\,\frac{\Delta F^2}{\bar{F}^4}\right)^{\frac{1}{3}}\right] \qquad (24)$$

Ai is the Airy function as defined in Ref 10 and

$\mu = \frac{m_R m_M}{m_R + m_M}$ = the reduced mass of the system

$E = \frac{1}{2}\mu v_\infty^2$ = energy of the colliding pair

$$\Delta F = \left|\frac{d\,(H_{ff} - H_{ii})}{dR}\right| \qquad (25)$$

$\bar{F}$ = effective radial force for the classical trajectory

U = effective potential energy for the classical trajectory

$= H_{ii} + E\frac{\rho^2}{R_x^2}$

and all quantities are evaluated at $R = R_x$. The fact that these results are consistent with a wave equation analysis if we choose

$$\bar{F} = \left[\left(-\frac{dH_{ii}}{dR} + 2E\frac{\rho^2}{R^3}\right)\left(-\frac{dH_{ff}}{dR} + 2E\frac{\rho^2}{R^3}\right)\right]^{\frac{1}{2}}_{R_x} \qquad (26)$$

is discussed in Refs 6 and 7.

To proceed further we are required to obtain expressions for H_{ii} and H_{ff} which asymptotically take on the values $\varepsilon_i \equiv 0$ and $\varepsilon_f = -\Delta_f$ (See Fig 2). Following Nikitin[7] we take for large R

$$H_{ii} = A_i R^{m_i} e^{-\alpha_i R}$$

where

$$\alpha_i = 2\sqrt{I_i}$$

$$m_i = 2\left(\frac{2}{\alpha_i} - 1\right) \tag{27}$$

and I_i is equal to the ionization energy for the ground state atom M (again we have scaled the ionization energies to I_H and the radius to a_o). In a similar fashion we have

$$H_{ff} = A_f R^{m_f} e^{-\alpha_f R} - \Delta_f \tag{28}$$

with I_f equal to the ionization energy of the ion M^{+*} (n'ℓ). That H_{ii} and H_{ff} should be exponentially decreasing for large R results from the exclusion principle and the observation that the nsσ orbitals for the incident metal atom are filled as are the 1sσ orbitals for the outgoing rare gas atom. That H_{ii} should decay more rapidly than H_{ff} results from the more diffuse nature of the M^{+*} (n'ℓσ) orbital. In both cases the attractive polarization contributions should be negligible at the large R considered. The crossing radius R_x is then determined by setting $H_{ii}(R_x) = H_{ff}(R_x)$. Since $\alpha_i >> \alpha_f$ we have

$$\Delta_f \sim A_f R_x^{m_f} e^{-\alpha_f R_x} \tag{29}$$

As discussed above, all of the parameters of the model problem can be calculated readily excepting the constants A_i, A_f [or equivalently R_X and $H_X \equiv H_{ii}(R_X)$]. The functions ΔF, $\bar{F}$ and V are then given by

$$\Delta F = \alpha_f \Delta_f$$

$$\bar{F} = \left[\left(\alpha_i H_x + 2E\frac{\rho^2}{R_x^3}\right)\left(\alpha_f \Delta_f + 2E\frac{\rho^2}{R_x^3}\right)\right]^{\frac{1}{2}} \qquad (25')$$

$$\approx \left[\alpha_f \Delta_f \left(\alpha_i H_x + 2E\,\rho^2/R_x^3\right)\right]^{1/2}$$

$$\mathcal{V} = H_x + E\frac{\rho^2}{R_x^2}$$

where we have assumed $\alpha R_X >> m$. Inserting these expressions into the transition probability we can determine its dependence on the impact parameter, ρ, from Eq 24. The ρ dependence occurs in two places $U(\rho)$ and $\bar{F}(\rho)$. Typically the ρ dependence in $\bar{F}$ is dropped which permits a considerable simplification. However we retain it for consistency.

III. PRELIMINARY RESULTS

Numerical calculations will be performed shortly. However we can qualitatively anticipate the results in two extreme cases. If the argument of the Airy function in Eq 24 has a large magnitude we can replace the Airy function by its asymptotic value.

$$Ai^2(-x) \xrightarrow[x \to +\infty]{} \frac{1}{\pi\sqrt{x}} \sin^2\left(\frac{2}{3}x^{3/2} + \pi/4\right)$$

$$Ai^2(-x) \xrightarrow[x \to -\infty]{} \frac{1}{4\pi\sqrt{x}} \exp\left(-\frac{4}{3}x^{3/2}\right) \tag{30}$$

The transition probability $\mathcal{P}_f$ can be written as

$$\mathcal{P}_f = \left(\frac{2\pi V_{if}}{\epsilon^*}\frac{\bar{F}}{\Delta F}\right)^2 Ai^2\left(-\frac{E-U}{\epsilon^*}\right) \tag{31}$$

where

$$\epsilon^* = \left(\frac{\hbar^2 \bar{F}^4}{2\mu \Delta F^2}\right)^{1/3} \tag{32}$$

Therefore

$$\mathcal{P}_f \xrightarrow[\frac{E-U}{\epsilon^*} \gg 1]{} \frac{8\pi V_{if}^2}{\hbar \Delta F \sqrt{\frac{2}{\mu}(E-U)}} \sin^2\left[\frac{2}{3}\left(\frac{E-U}{\epsilon^*}\right)^{3/2} + \frac{\pi}{4}\right] \tag{33a}$$

$$\mathcal{P}_f \xrightarrow[\frac{E-U}{\epsilon^*} \ll -1]{} \frac{2\pi V_{if}^2}{\hbar \Delta F \sqrt{\frac{2}{\mu}(E-U)}} \exp\left[-\frac{4}{3}\left|\frac{E-U}{\epsilon^*}\right|^{3/2}\right] \tag{33b}$$

To investigate the circumstances under which the asymptotic forms can be used we refer to Eqs 25' which yield

$$E - V = E\left(1 - \rho^2/R_x^2\right) - H_x$$
$$\epsilon^* = \left[\frac{\hbar^2}{2\mu}\left(\alpha_i H_x + 2E\frac{\rho^2}{R_x^2}\right)^2\right]^{1/3} \tag{34}$$

Case A) $E >> H_x$

From Fig 2 we see that this corresponds to a small energy defect Δ_f and corresponding large crossing radius R_x. The classical distance of closest approach R_o can be less than R_x and the trajectory will pass through R_x if $\rho \lesssim R_x$. Under such circumstances we can neglect the contributions to Φ_f from $\rho > R_x$. If we further replace the rapidly oscillating $\sin^2$ term by its average value of 1/2 we obtain from Eqs 22 and 33a

$$\sigma_f^{(A)} = \frac{8\pi V_{if}^2}{\hbar \alpha_f \Delta_f v_\infty} \pi R_x^2 \tag{35}$$

This is the same result as obtained from perturbation theory when the proximity of the crossing point to the turning point is neglected.[6] Substituting the expressions for V_{if} and Δ_f from Eqs 20 and 29 we see that as $\Delta_f \to 0$ $(R_x \to \infty)$, the cross section is dominated by the exponential terms

$$\sigma_f^{(A)} \xrightarrow[\substack{\Delta_f \to 0 \\ R_x \to \infty}]{} \sim \exp\left[-2\left(\sqrt{I_m} - \sqrt{I_f}\right)R\right] \tag{36}$$

where I_m is the energy needed to ionize the ns orbital in M^* (ns n'ℓ) and I_f is the energy needed to ionize the n'ℓ orbital in M^{+*}(n'ℓ). Therefore $I_m > I_f$ and the cross section decreases as $\Delta_f \to 0$.

Case B) $E \ll H_x$

From Fig 2 we see that under such circumstances the crossing point can never be reached. Therefore $\mathcal{P}_f$ can be approximated by Eq 33b for all ρ. A qualitative interpretation can be made. Replacing the phase interference term by the average value of 1/2 in Eq 33a we formally have

$$\mathcal{P}_f^{(B)}(\text{Eq. } 33b) = \mathcal{P}_f^{(A)}(\text{Eq. } 33a) \times \frac{\exp\left[-\frac{4}{3}\left|\frac{E-U}{\epsilon^*}\right|^{3/2}\right]}{2} \qquad (37)$$

Therefore the transition probability when the crossing point cannot be reached classically, $\mathcal{P}_f^{(B)}$, equals the transition probability when the crossing point is reached, $\mathcal{P}_f^{(A)}$, multiplied by a quasi-classical transmission coefficient[6] describing the probability that the system can tunnel through the potential barrier and reach R_x. An order of magnitude estimate of the cross section is then

$$\sigma_f^{(B)} \xrightarrow[\substack{\Delta_f \to \infty \\ R_x \to 0}]{} \frac{8\pi V_{if}^2}{\hbar \alpha_f \Delta_f} \cdot \frac{\pi R_x^2}{\sqrt{2H_x/\mu}} \exp\left[-\frac{4}{3}\left(\frac{\hbar^2 \alpha_i^2}{2\mu} H_x\right)^{\frac{1}{2}}\right] \qquad (38)$$

We observe then that as Δ_f increases, the crossing radius decreases and the coupling at the crossing point V_{if} increases. However since the crossing point cannot be reached classically the cross section is dominated by the transmission coefficient which decreases rapidly as H_x grows. Thus the cross section for a Duffendack reaction is seen to decrease for $\Delta_f \to 0$ and for $\Delta_f \to \infty$. In the former case the decrease is due to a decrease in the coupling V_{if} while in the latter limit the decrease is due to the inability of the classical trajectory to reach the crossing point where transitions are most likely. Such a behavior was seen in the experimental work of Turner-Smith et. al.[1]

Two remarks are made in conclusion. If the distance of closest approach R_o, is much larger than the crossing radius R_x the transition probability $\mathcal{P}_+$ given in Eq 24 is no longer correct. In such circumstances Delos and Thorson[5] have shown that the correct expression is given by

$$\mathcal{P}_+ = \pi^2 b^{4/3} \mathrm{Ai}^2(-x) \tag{3a}$$

The quantities x and b are given there and reduce to Eq 24 if the variations of V_{if}, $\bar{F}$ and ΔF are negligible in the interval R_o to R_x. Finally we point out that to more directly compare the theoretical and experimental work a thermal average of the cross sections must be performed.

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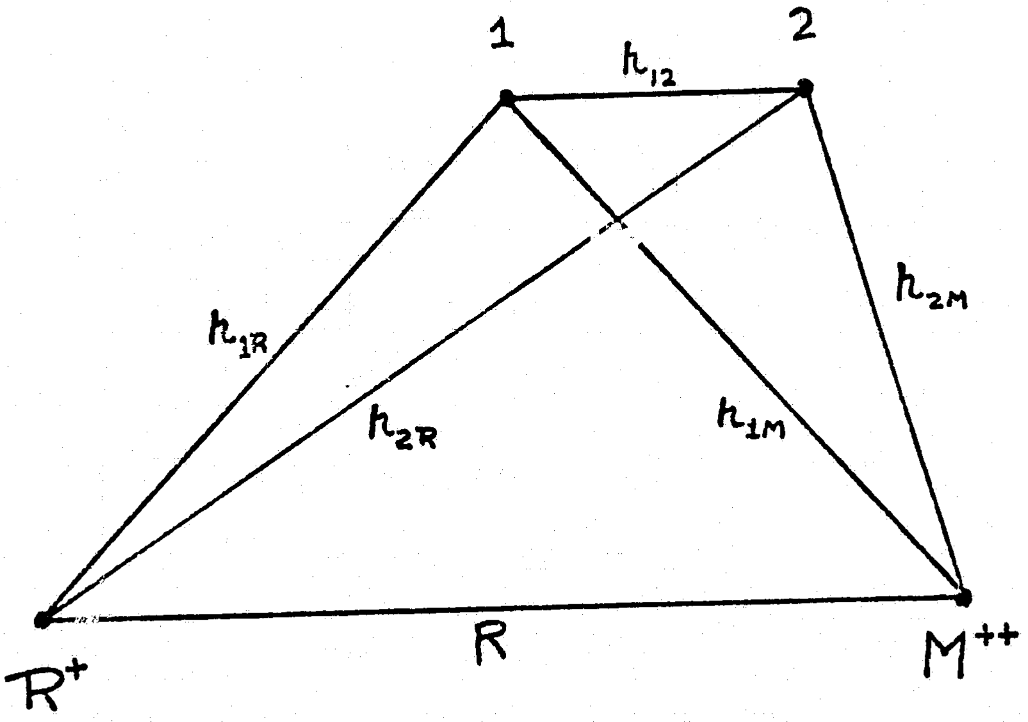

Figure 1. Coordinates of the $(RM)^+$ molecule

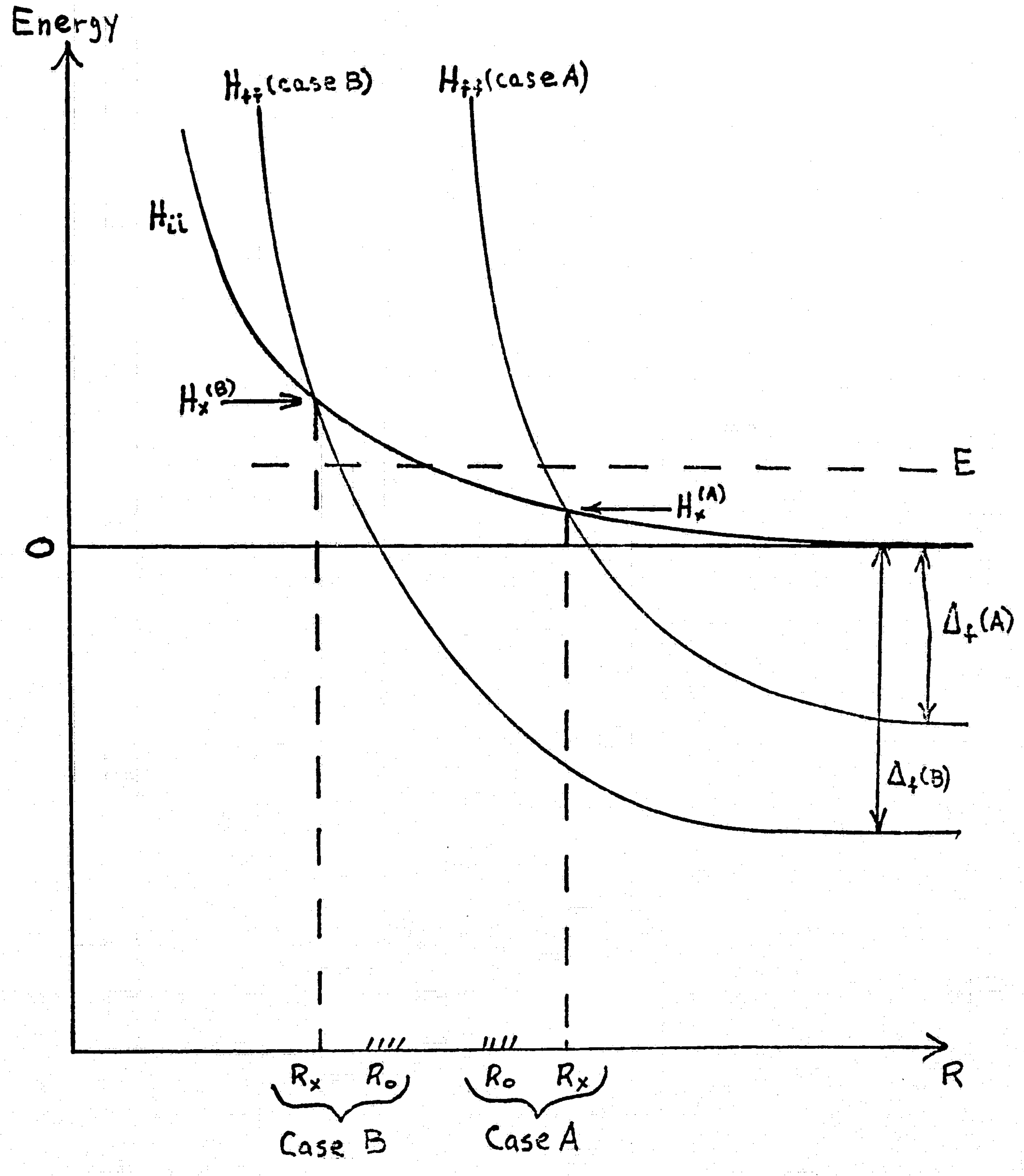

Figure 2. Molecular Potential Energies.
Case A. R_x in classically allowed region.
Case B. R_x in classically forbidden region.

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