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Calculation of reaction probabilities and rate coefficients for collinear three-body exchange reactions using time-dependent wave packet methods[a]

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Wave packet methods are described that permit rate coefficients for the collinear A + BC exchange reaction to be obtained directly without the necessity of computing the reaction probabilities out of all statistically significant initial BC vibrational states. Similar wave packet methods are given that allow reaction probabilities at essentially fixed energy for collinear A + BC systems to be computed by time-dependent methods. The explicit integration procedure of Harmuth is utilized to evolve the wave packets. The methods are appplied to reactions occurring on three different LEPS-type potential-energy surfaces using the hydrogen atom mass for each atom and also to the T + HD→TH + D reaction on a realistic potential-energy surface. In most cases, the results are shown to be in excellent accord with exact close-coupling calculations.

I. INTRODUCTION

Since the early work of Bauer and Wu[1] in 1953, there has been a growing interest in the quantum theoretical study of the triatomic exchange reaction A + BC → AB + C.[2,3] This problem may be examined in either a time-independent or time-dependent framework. There are advantages and disadvantages to each method, and the procedure of choice usually depends upon the quantities desired. Cross sections or reaction probabilities at a fixed energy are more conveniently obtained with a close-coupling procedure. On the other hand, it may be more efficient to compute rate coefficients using a wave packet calculation.[4-7] This is particularly true if it is necessary to include the contribution of several initial internal states.

The time-independent studies are generally carried out by solving the close-coupling equations provided the number of open channels is sufficiently small to bring the problem within range of available computational facilities. If the number of channels is too large, the problem may be simplified by the use of some type of decoupling approximation. In either case, the result is a scattering matrix whose elements yield the desired cross sections or reaction probabilities at a fixed energy.

In contrast, time-dependent wave packet calculations yield the average reaction probability for a distribution of energy. Mazur and Rubin[4] reported the first such calculations. In their investigations they employed an initial wave function representing a momentum distribution corresponding to a Maxwell–Boltzmann-like distribution of energies at a fixed temperature. McCullough and Wyatt[5] carried out similar computations using a minimum uncertainty Gaussian wave packet as well as the wave packet employed by Mazur and Rubin.[4] Kellerhals, Sathyamurthy, and Raff[6] also used Gaussian wave packets in a comparison of quasiclassical tra-

jectory results with time-dependent quantum calculations.

Attempts have been made to compare the results obtained by close-coupling methods[3] at energy E to the results of time-dependent calculations using wave functions corresponding to an average energy E.[8] Such comparisons generally show good agreement between the methods if the reaction probability is a slowly varying function at energy E, but not otherwise. The large differences frequently noted in such comparisons are due almost entirely to the distribution of momenta present in the wave packet description of the system wave function. In principle, better agreement may be obtained by employing a wave packet whose momentum space distribution approaches a delta function. In practice, however, such a procedure is not feasible since the resulting wave packet will be very diffuse in coordinate space. As a consequence, the integration of the time-dependent Schrödinger equation will have to be carried out over an extensive configuration space grid requiring an unacceptably large quantity of computer time. This limitation makes it difficult to obtain reaction probabilities and cross sections at a fixed energy using time-dependent methods.

In the next section of this paper, we discuss wave packet procedures that permit reaction probabilities to be computed at an almost precise value of the energy using time-dependent methods. By comparison, we show that the values so computed are in good accord with converged close-coupling results.[8] We also illustrate time-dependent methods that permit reaction rate coefficients to be computed in a single calculation without the necessity of first computing the reaction probabilities as a function of translational energy for each vibrational state that is statistically important in the reaction. In all calculations, integration of the time-dependent Schrödinger equation has been carried out using a simple explicit method.[7] The results of the application of the methods to a study of the H + H₂ → H₂ + H and T + HD → TH + D collinear reactions are given and discussed in the final section.

II. THEORY AND METHOD

A. Integration method

The explicit integration method given by Harmuth[7(a)] for one dimension and expanded by Askar and Cakmak[7(b)] to two dimensions has been employed in the solution of the time-dependent Schrödinger equation. For the convenience of the reader and to facilitate the description of the numerical procedures employed in the present work, we first review the essential features of the method.[7]

The wave function ψ^n at time $t = n\Delta t$ evolves as

$$\psi^{n+1} = e^{\mp i \Delta t H/\hbar} \psi^n \ . \tag{1}$$

Here Δt represents the time increment used in the evolution of the wave packet. The Hamiltonian Operator H in one dimension can be written as

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \ , \tag{2}$$

where V is the potential energy operator.

Expanding $\exp(-i\Delta t H/\hbar)$ into a Taylor series and keeping only the leading terms, one can obtain the value of ψ^{n+1} in terms of ψ^n and ψ^{n-1} on a discrete equally spaced mesh of spacing Δx:

$$\psi_j^{n+1} - \psi_j^{n-1} = -2i[(2\alpha + V_j \Delta t/\hbar)\psi_j^n - \alpha(\psi_{j+1}^n + \psi_{j-1}^n)] \ , \tag{3}$$

where

$$\alpha = \hbar \Delta t / 2m(\Delta x)^2 \ , \tag{4}$$

and j refers to the value of the wave function at the location x_j, i.e.,

$$\psi_j^n \equiv \psi(x_j, t_n) \ . \tag{5}$$

For two-dimensional space Eq. (3) becomes[7(b)]

$$\psi_{j,k}^{n+1} = \psi_{j,k}^{n-1} - 2i\{[2(\alpha_1 + \alpha_2) + V_{j,k}\Delta t/\hbar]\psi_{j,k}^n$$
$$- \alpha_1(\psi_{j+1,k}^n + \psi_{j-1,k}^n) - \alpha_2(\psi_{j,k+1}^n + \psi_{j,k-1}^n)\} \ . \tag{6}$$

If the error $\epsilon_j^n = \epsilon^n \exp(iqx_j)$ in ψ_j^n is magnified by g times in the next time step, i.e., $\epsilon_j^{n+1} = g\epsilon_j^n$, then for the method to be stable[7] $|g|$ must not exceed unity.

Substituting $\psi_j^n + \epsilon_j^n$ and $\psi_j^{n\pm1} + (g)^{\pm1}\epsilon_j^n$ for ψ_j^n and $\psi_j^{n\pm1}$ in Eq. (3), respectively, one gets[7]

$$g^2 + 2i\{2\alpha[1 - \cos(q\Delta x)] + V_j \Delta t/\hbar\}g - 1 \doteq 0 \ . \tag{7}$$

The magnitude of each of the two roots of this equation will be equal to 1 if the following condition is satisfied[7(a),7(c)]:

$$1 \geq |2\alpha[1 - \cos(q\Delta x)] + V_j \Delta t/\hbar| \ . \tag{8}$$

As q may have any value, Eq. (8) leads to the following conditions for the stability of the integration:

$$1 \geq 4\alpha \ , \quad \Delta t \leq (1 - 4\alpha)\hbar/|V_j|_{max} \ . \tag{9}$$

Similarly, for the two-dimensional case the following conditions can be obtained:

$$1 \geq 4(\alpha_1 + \alpha_2) \ , \quad \Delta t \leq [1 - 4(\alpha_1 + \alpha_2)]\hbar/|V_{j,k}|_{max} \ .$$

B. Wave packet methods

Within the Born–Oppenheimer approximation, the Schrödinger equation in the center-of-mass frame for the collinear system of three atoms A, B, and C, having coordinates x_a, x_b, and x_c and masses m_a, m_b, and m_c, respectively, can be written[5]

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2}\right) + V(q_1, q_2)\right]\psi = i\hbar\frac{\partial\psi}{\partial t} \ , \tag{10}$$

where

$$q_1 = x_a - (m_b x_b + m_c x_c)/(m_b + m_c) \ , \tag{11}$$

$$q_2 = (x_b - x_c)\{m_b m_c(m_a + m_b + m_c)/[(m_b + m_c)^2 m_a]\}^{1/2} \ , \tag{12}$$

$$\mu = m_a(m_b + m_c)/(m_a + m_b + m_c) \ , \tag{13}$$

and V represents the potential energy of the system.

This two-dimensional time-dependent Eq. (10) is integrated over a large number of time steps by repeated application of Eq. (6), and the reaction probability $\langle P \rangle_{TD}$ is then obtained by

$$\langle P \rangle_{TD} = \int_P \psi^*(t \to \infty)\psi(t \to \infty)\,dq_1\,dq_2 \ , \tag{14}$$

where the integral is taken over the product configuration space P.[5,8] The symbol $\langle \ \rangle_{TD}$ denotes the time-dependent reaction probability averaged over the energy distribution present in the wave packet.

The initial wave function at $t = 0$ is chosen as follows:

$$\psi(t = 0) = \psi(q_1, q_2) = \phi(q_1)\sum_{n=0}^{\infty} A_n X_n(q_2) \ . \tag{15}$$

In Eq. (15), $X_n(q_2)$ is the nth state vibrational wave function for the BC Morse oscillator. If calculations for a specified vibrational state k are desired, one takes $A_n = \delta_{nk}$. The reaction probability of a thermal distribution of initial states may be computed by choosing

$$A_n = \left(Z_n \bigg/ \sum_{n=0}^{\infty} Z_n\right)^{1/2} \ , \tag{16}$$

with

$$Z_n = \exp(-E_n/k_B T) \ , \tag{17}$$

where E_n, k_B, and T are the vibrational energies of the nth state, Boltzmann's constant, and temperature, respectively.

$\phi(q_1)$ in Eq. (15) is the packet representing the relative translational motion. In this work, we have utilized four types of wave packets.

Packet I is given by

$$\phi(q_1) = (2\pi\delta^2)^{-1/4}\exp[-(q_1 - q_{10})^2/4\delta^2 - ik_0 q_1] \ . \tag{18}$$

This is the minimum uncertainty Gaussian wave packet.[5,6] Its momentum space distribution is given by its Fourier transform:

$$F(k) = (2\delta/\pi)^{1/4}\exp[-(k - k_0)^2\delta^2 + iq_{10}k] \ . \tag{19}$$

The average energy of this packet is

$$\langle E \rangle = \hbar^2 (k_0^2 + 1/4\delta^2)/2\mu \ . \tag{20}$$

Packet II is given by

$$\phi(q_1) = \exp(-ik_0 q_1)\sin\Delta k(q_1 - q_{10})/[(q_1 - q_{10})\sqrt{\pi\Delta k}] \ , \tag{21}$$

which has Fourier transform $F(k)$ and average energy $\langle E \rangle$:

$$F(k) = \begin{cases} \exp(ikq_{10})/\sqrt{2\Delta k}, & \text{for } k_0 - \Delta k < k < k_0 + \Delta k \ , \\ 0 \ , & \text{for } k > k_0 + \Delta k \text{ or } k < k_0 - \Delta k \end{cases} \tag{22}$$

$$\langle E \rangle = [k_0^2 + (\Delta k)^2/3]\ \hbar^2/2\mu \ . \tag{23}$$

This wave packet has a square distribution in momentum space.

Packet III is given by

$$\phi(q_1) = (2\beta/\pi)^{1/2}\{\Gamma(5/4)_1F_1[5/4, 1/2, -\beta^2(q_1 - q_{10})^2]$$
$$- 2i\Gamma(7/4)\beta(q_1 - q_{10})_1F_1[7/4, 3/2, -\beta^2(q_1 - q_{10})^2]\} \tag{24}$$

Here $_1F_1$ represents the confluent hypergeometric function. The Fourier transform and average energy for this packet are

$$F(k) = (k^3/2\beta^4)^{1/2}\exp(-k^2/4\beta^2 + ikq_{10}) \tag{25}$$

and

$$\langle E \rangle = 2k_b T, \qquad T = \hbar^2\beta^2/\mu k_B \ , \tag{26}$$

where again k_b denotes the Boltzmann constant. This packet corresponds to a three-dimensional Maxwell–Boltzmann-like energy distribution at temperature T. It has previously be utilized by Mazur and Rubin[4] and by McCullough and Wyatt.[5]

Packet IV is given by

$$\phi(q_1) = \sqrt{\frac{\beta}{\pi}}\{\Gamma(3/4)_1F_1[3/4, 1/2, -\beta^2(q_1 - q_{10})^2]$$
$$- 2i\ \Gamma(5/4)(q_1 - q_{10})\beta\ _1F_1[5/4, 3/2, -\beta^2(q_1 - q_{10})^2]\}. \tag{27}$$

This packet is used to calculate the reaction rate for a system having a one-dimensional Maxwell–Boltzmann distribution of energies at temperature T. The Fourier transform $F(k)$ is

$$F(k) = \beta^{-1}k^{1/2}\exp\left(-\frac{k^2}{4\beta^2} + ikq_{10}\right) \ . \tag{28}$$

For a wave packet described by the momentum space wave function $F(k)$, the average reaction probability obtained by close-coupling methods is given by

$$\langle P \rangle_{cc} = \int_0^\infty P_{cc}(E)\,|F(k)|^2\,dk \ . \tag{29}$$

Here, $P_{cc}(E)$ denotes the reaction probability computed by close-coupling methods at relative translational energy $E(= \hbar^2 k^2/2\mu)$. Thus, $\langle P \rangle_{cc}$ of Eq. (29) and $\langle P \rangle_{TD}$ of Eq. (14) are the quantities to be compared.

Using packet II, one may obtain the reaction probability for a very sharp distribution of energy. For a packet corresponding to $k_0 = k_1$ and $\Delta k = \Delta k_1$, let the reaction probability $\langle P \rangle_{TD}$ be P_1. For a second packet with $k_0 = k_2 = k_1 + \epsilon$ and $\Delta k = \Delta k_2 = \Delta k_1 + \epsilon$, let $\langle P \rangle_{TD}$ be P_2. Since packet II is square in momentum space, it is easily seen that

$$P_{TD}(E) = (P_2\,\Delta k_2 - P_1\,\Delta k_1)/(\Delta k_2 - \Delta k_1) \ . \tag{30}$$

Here $P_{TD}(E)$ represents the reaction probability averaged over the energy values in the range $E - \Delta E$ to $E + \Delta E$ with

$$E = \hbar^2(k_1 + \Delta k_1 + \epsilon)^2/2\mu \tag{31}$$

and

$$\Delta E = \hbar^2\epsilon(k_1 + \Delta k_1 + \epsilon)/\mu \ . \tag{32}$$

In practice, ΔE can be made very small so that $P_{TD}(E)$ will approach the close-coupling result for a fixed energy. For example, for the $H + H_2$ exchange with $k_1 = 5.40$, $\Delta k = 0.90$, and $\epsilon = 0.01$ a. u.$^{-1}$, we obtain $E = 10.2$ kcal/mole and $\Delta E = 0.033$ kcal/mole, i.e., ΔE is less than the width of the points shown in Fig. 2.

Theoretically, it is possible to achieve a result equivalent to that obtained with Eqs. (30)–(32) by computing the probability at one set of values of k_0 and Δk with Δk taken to be 0.01 a. u.$^{-1}$ or less. However, as previously mentioned, this procedure gives a coordinate space wave packet so diffuse that accurate integration of the wave equation becomes prohibitively expensive.

III. RESULTS AND DISCUSSION

Calculations of the reaction probability for a collinear $A + BC$ exchange reaction have been carried out on three hypothetical LEPS-type potential-energy hypersurfaces[6] where the masses employed are those for the $H + H_2$ systems. The notations surface I (asymmetric barrier in the exit channel), surface II (symmetric), and sur-

TABLE I. Comparison of back-evolution accuracy of the "explicit"[a] and "implicit"[b] methods using a Gaussian wave packet ($\delta = 0.25$) on surface I with $A_n = \delta_{n0}$.

Method	E_t (kcal/mole)	$t \times 10^{16}$ (sec)	$\Delta t \times 10^{16}$ (sec)	n	Deviations	
					Maximum $\Delta|\psi_{i,j}|^2$	Average $\Delta|\psi_{i,j}|^2$
Explicit[c]	9.50	269.375	0.269375	2000	1.5×10^{-4}	1.9×10^{-6}
Implicit[b]	3.50	35.019	1.0775	20	4.0×10^{-4}	5.5×10^{-6}
Implicit[b]	3.50	99.668	1.0775	20	7.9×10^{-5}	3.2×10^{-6}

[a]Reference 7.   [b]Reference 5.   [c]Present work.

face III (asymmetric barrier in the entrance channel) of Ref. (6) will be adopted here. For the T + HD system, the potential used by Garrett et al.[9] has been employed.

The time evolution of wave function ψ described by Eq. (10) has been carried out using Eq. (6) with $\alpha_1 = \alpha_2$, $dq_1 = dq_2 = 0.11$ a.u., and $\Delta t = 0.269\,375 \times 10^{-16}$ sec. Since the explicit integration method[7] has not been previously utilized to propagate a wave packet over thousands of time steps, we first examine the accuracy of the method by back-evolution techniques, i.e., the wave packet is first evolved from time t to $t + n\Delta t$. Then, by replacing Δt in Eqs. (4) and (6) by $-\Delta t$, the wave function is "back evolved" n steps to time t. The difference $\Delta\psi_{ij}$ between the back-evolved function $\psi_{ij}^{(b)}(t)$ and the initial value $\psi_{ij}^{(i)}(t)$ at mesh point (i, j) serves as a measure of the accuracy of the method. The results are given in Table I along with those obtained by Kellerhals et al.[6] using the implicit Gauss–Seidel method.[5] A comparison of these data shows that the accuracy of the explicit method is very good. (In this connection it should be mentioned that the present calculations have been carried
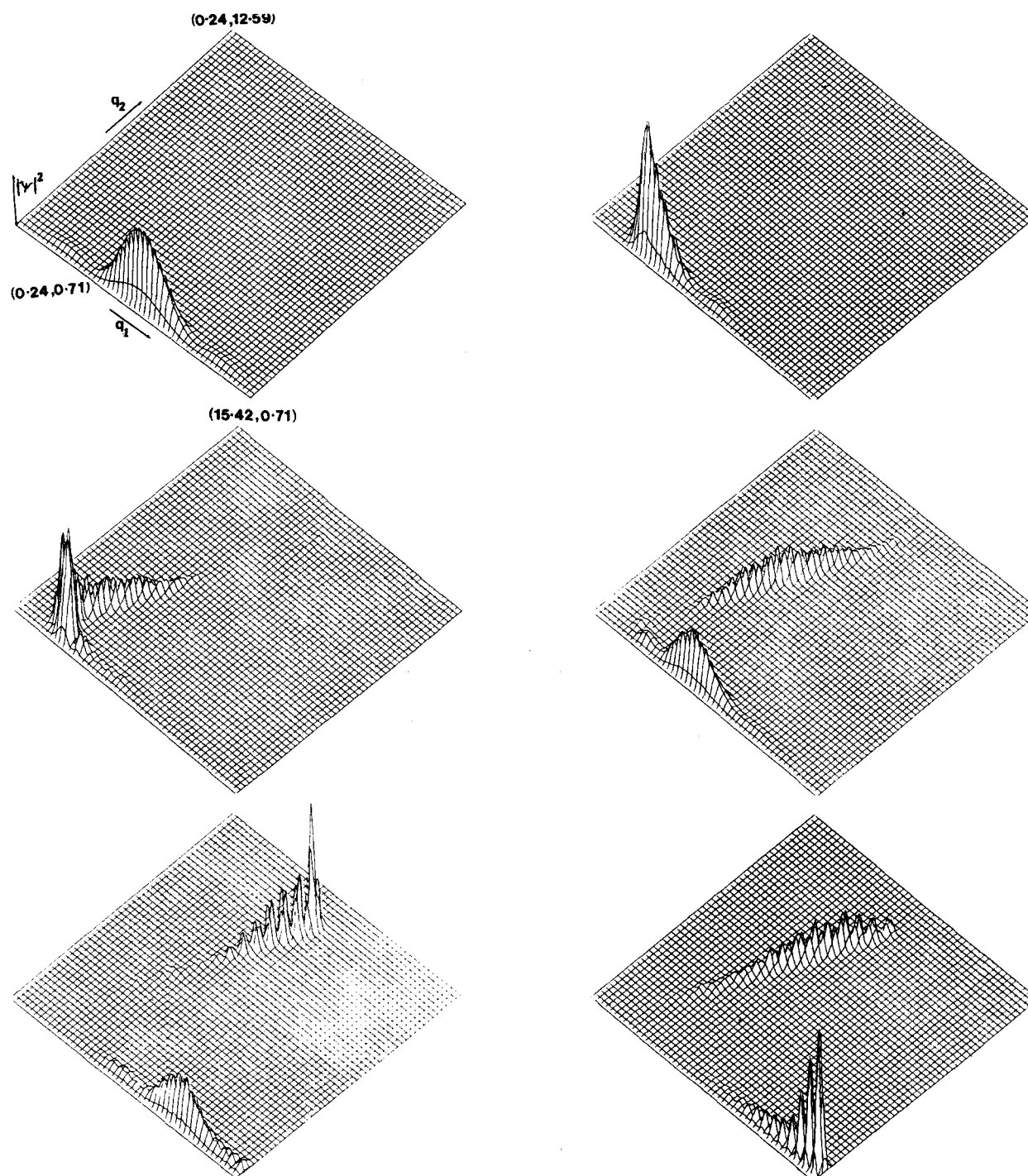

FIG. 1. Probability density evaluated over configuration space on surface III with packet II having $k_0 = 5.31$, $\Delta k = 0.91$, $q_{10} = 8.0$ a.u., and $A_n = \delta_{n0}$ at time steps (a) $n = 0$, (b) $n = 1000$, (c) $n = 2000$, (d) $n = 3000$, (e) $n = 4000$, and (f) $n = 5000$. (One time step $= 0.269\,375 \times 10^{-16}$ sec.)

TABLE II. Comparison of time-dependent results on surface I at an average relative translational energy of 9.5 kcal/mole for the Gaussian wave packet with different packet widths and $A_n = \delta_{n0}$.

Packet width (δ)	Probability	
	$\langle P \rangle_{TD}$	$\langle P \rangle_{cc}$
0.25	0.20	0.21
1.70	0.22	0.22
1.90	0.20	0.20
2.10	0.19	0.18
2.20	0.18	0.17
2.80	0.14	0.13

out in double precision whereas those of Kellerhals et al.[6] were done in single precision.) As a further check, previous results using wave packet I with the Gauss–Seidel method[6] were reproduced with good accuracy with the present method.

A comparison of the efficiency of the two integration methods is complicated by the use of different computers in the two studies, but it would appear that the explicit procedure[7] is faster than the Gauss–Seidel method.[5] One set of calculations using the Gauss–Seidel procedure[5] required about 4–6 h of CPU time on an IBM 360/65. Equivalent computations with the explicit method needed 10–15 min on an IBM 370/168. Askar and Cakmak[7(b)] reported that the explicit procedure is faster by a factor of 10^2 per time step. However, with the present Hamiltonian, the stability criteria given by Eq. (9) require that Δt be chosen very small. Consequently, the overall reduction in CPU time was significantly less than a factor of 10^2.

Figures 1(a)–1(e) show perspective plots of probability density in configuration space $0.24 \le q_1 \le 15.42$ and $0.71 \le q_2 \le 12.59$ a.u. for wave packet II on surface III with $A_n = \delta_{n0}$, $k_0 = 5.31$, $\delta k = 0.91$, and $q_{10} = 8.0$ in atomic units As can be seen, the wave equation has been integrated over a sufficiently large portion of configuration space so that a clear demarcation between the portion of the final wave packet in the product space and that in the reactant space is obtained. If the range of q_2 is reduced to $0.71 \le q_2 \le 6.43$ a.u., the resulting configuration space is too small to permit such a clear separation. Similar perspective plots have been previously

TABLE III. Comparison of the time-dependent and time-independent results on surface I for packet II with $A_n = \delta_{n0}$.

k_0 (a.u.)$^{-1}$	Δk (a.u.)$^{-1}$	Probability	
		$\langle P \rangle_{TD}$	$\langle P \rangle_{cc}$
3.75	2.00	0.18	0.18
4.70	1.00	0.34	0.35
5.11	1.00	0.42	0.39
5.23	0.90	0.45	0.42
5.40	0.90	0.43	0.40
5.55	0.90	0.41	0.41
5.84	0.90	0.37	0.38
6.35	1.00	0.25	0.26
7.51	0.90	0.15	0.13

TABLE IV. Comparison of the time-dependent and the time-independent results on surface II for packet III with $A_n = \delta_{n0}$.

Temperature (°K)	Probability	
	$\langle P \rangle_{TD}$	$\langle P \rangle_{cc}$
500.0	0.15	0.14
1000.0	0.45	0.45
2000.0	0.66	0.65

given for the Gaussian wave packet.[6]

Time-dependent and time-independent results are most easily compared by averaging the close-coupling probabilities over the distribution of translational energies present in the time-dependent calculations, i.e., we may compare $\langle P \rangle_{cc}$ from Eq. (29) with $\langle P \rangle_{TD}$ obtained from Eq. (14). Such a comparison has been made using wave packets I and II on surface I and wave packet III on surface II with $A_n = \delta_{n0}$. In each case the close-coupling results are those recently reported by Bergeron and Leforestier.[8] The results of these comparison studies are reported in Tables II–IV. In all cases, the agreement obtained is excellent.

Using Eqs. (30)–(32), reaction probabilities at nearly precise energies may be computed by time-dependent
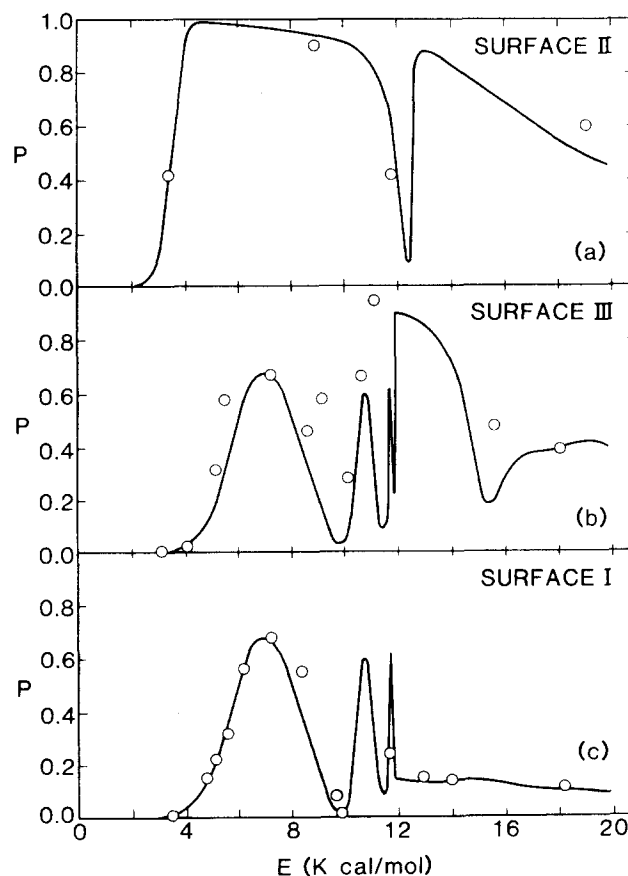

FIG. 2. Reaction probability as a function of incident translational energy on surfaces I, II, and III with $A_n = \delta_{n0}$. The curve represents the close-coupling results of Ref. 8. The present time-dependent results are shown as points.

TABLE V. Comparison of rate coefficients for the collinear reaction T + HD = TH + D.

| Temperature (°K) | Rate coefficients (cm/sec) | |
	Present time-dependent calculations	Close-coupling calculations[a]
1000	4.8×10^3	4.51×10^3
1500	1.26×10^4	1.38×10^4
2400	3.25×10^4	3.21×10^4

[a]Reference 9.

methods. Such calculations have been carried out on surfaces I, II, and III at several energies with $A_n = \delta_{n0}$. In all cases, the ratio $(\Delta E/E)$ is less than 0.006 so that the results, shown in Fig. 2, are essentially equivalent to close-coupling calculations at a specified energy. On surfaces I and II there is excellent agreement between the time-dependent results and the close-coupling probabilities obtained by Bergerson and Leforestier.[8] However, the extent of agreement between the two methods on surface III is not satisfactory. The lack of agreement on surface III might be due to a magnification of error introduced in Eq. (30), which involves the small difference of two large numbers. However, our studies suggest that this is not the only possibility and that the problem may be more subtle. This question is currently being investigated and will be discussed in a future publication.

Garrett et al.[9] have recently reported rate coefficients for the T + HD → TH + D collinear reaction. In their study the reaction probabilities over the range $0.0 \leq E_{tr} \leq 32$ kcal mole⁻¹ were first computed by time-independent methods for both the $v = 0$ and $v = 1$ vibrational states of HD. Rate coefficients out of each state were then obtained by averaging these probabilities over the one-dimensional distribution function of translational energies using Eqs. (28) and (29), i.e.,

$$k_i = (k_B T/2\pi\mu)^{1/2} \int_0^\infty P_{cc}^i(E) \exp(-E/k_B T) d(E/k_B T) ,$$
(34)

where k_i represents the rate coefficient and $P_{cc}^i(E)$ denotes the reaction probability at translational energy E out of initial vibration state i. The total rate coefficients were obtained from

$$k_T = \sum_{i=0}^{i=1} A_i^2 k_i ,$$
(35)

where the A_i are given by Eq. (16).

These calculations may be carried out much more directly using Eq. (15) with 1 as the upper limit on the summation and $\phi(q_1)$ given by Eq. (27). The total rate coefficient is then calculated by the following relation:

$$k_T = (k_B T/2\pi\mu)^{1/2} \langle P \rangle_{TD} .$$
(36)

Table V compares the results of such calculations with

those reported by Garrett et al.[9] As can be seen, the agreement is very good to excellent.

In the above computations, only the first two vibrational states are significant. However, at very high temperature or for systems having a low vibrational frequency, it will become necessary to include the contribution of a much larger ensemble of vibrational states. At higher temperatures or for systems with larger mass, both time-independent and time-dependent calculations will require more computation time. However, close-coupling calculations will rapidly increase in difficulty as the number of channels increases, whereas time-dependent computations are essentially independent of the number of vibrational states included in Eq. (15). Consequently, under such conditions, wave packet calculations become the optimum method for computation of rate coefficients.

ACKNOWLEDGMENTS

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