THE REFINED BORN APPROXIMATION FOR ATOM-DIATOM COLLINEAR COLLISION

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The refined Born approximation introduced by Rayski is used for the description of a collinear collision of the harmonic oscillator with a structureless particle. Two models for the interaction potential are discussed. For one of them numerical results are presented. They are in good agreement with the exact ones.

1. Introduction

The modification of the well-known in collision theory Born approximation, introduced recently by Rayski, gives not only a possibility of improving the results of the original Born approximation, but also it extends considerably the domain of its applicability. The author proved this fact applying successfully his theory to some simple elastic collision models. Since this method is relatively simple in practice it seems interesting to study its utility for the description of inelastic collisions. The present work is an attempt in this direction. The refined Born approximation (RBA) is used to describe an inelastic collision of a diatomic molecule with an atom in the simplest realization of this problem, i.e., a collinear collision of the harmonic oscillator with a structureless particle.

In Sections 2 of this paper we formulate the most important elements of the quantum description of the one-dimensional diatomic molecule-atom collision in the form essentially similar to that given in [1]. Section 3 concerns the application of the refined Born approximation for this case. The more general description of the refined Born approximation and its hitherto existing applications can be found in [2] and [3]. The most important details concerning the practical realization of this task are described in Sections 4 and 5. In Section 4 we present the results of numerical tests performed for the model with the interaction potential in the form of a finite barrier, whereas in Section 5 we discuss the applicability of RBA to the model with an exponential interaction potential.

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2. Collinear collision of a particle with a diatomic molecule

The time independent Schrödinger equation for the collision model given in figure 1 has in the center-of-mass coordinates the form

$$\left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\tilde{y}^2}-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial\tilde{x}^2}+\tilde{V}_{BC}(\tilde{y})+\tilde{V}_{BC-A}(\tilde{x},\tilde{y})\right]\psi=\tilde{E}\psi, \tag{1}$$

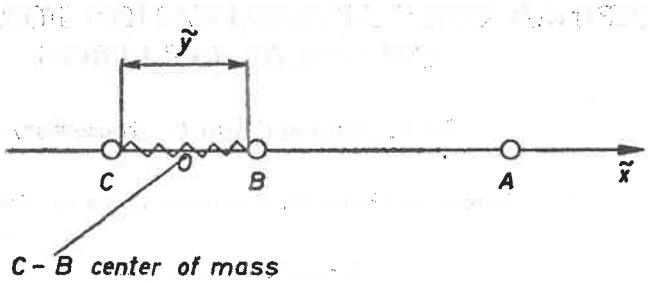

Fig. 1. Spatial arrangement of colliding objects

where M is the reduced mass of the molecule, μ is the reduced mass of the molecule--particle system and $\tilde{E}$ is the total energy. For the interaction potentials occurring in equation (1) we assume

1) $$\tilde{V}_{BC}(\tilde{y})=\tfrac{1}{2}k(\tilde{y}-\tilde{y}_{eq})^2,$$

i.e., the molecule is treated as a harmonic oscillator with $\tilde{y}_{eq}$ being the distance between the atoms B and C in the equilibrium,

2) $$\tilde{V}_{BC-A}(\tilde{x},\tilde{y})=\tilde{A}\exp\left[-\tilde{\alpha}\left(\tilde{x}-\frac{m_C}{m_B+m_C}\tilde{y}\right)\right], \tag{2}$$

or

2a) $$\tilde{V}_{BC-A}(\tilde{x},\tilde{y})=\tilde{A}\{\exp\left[-\tilde{\alpha}(|\tilde{x}|-\tfrac{1}{2}\tilde{y})\right]+\exp\left[-\tilde{\alpha}(|\tilde{x}|+\tfrac{1}{2}\tilde{y})\right]\}. \tag{3}$$

The assumptions 1) and 2) correspond to the model solved exactly by Secrest and Johnson [1], whereas 2a) leads to another model in which the exponentially growing (for $\tilde{x}\to-\infty$) interaction potential (2) is replaced by the finite potential barrier (3). Under these assumptions we may transform equation (1) into the form

$$\left[-\frac{1}{m}\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+y^2+V(x,y)\right]\psi=E\psi, \tag{4}$$

where

$$m=\frac{\mu}{M},$$

$$V(x,y)=V^{S-J},$$

or

$$V(x, y) = V^m$$

for the assumptions 2) or 2a), respectively, where

$$V^{S-J} = A \exp\left[-\alpha\left(\frac{m_B+m_C}{m_C}x-y\right)\right]$$

and

$$V^m = A \exp(-2\alpha|x|)\,[\exp(\alpha y)+\exp(-2\alpha y_{eq})\exp(-\alpha y)].$$

The transformation used here is given by

$$\tilde{x} = \delta x, \quad \tilde{y} = \delta y+\tilde{y}_{eq},$$

$$\tilde{E} = \varepsilon E, \quad \tilde{V}_{BC-A}(\tilde{x}, \tilde{y}) = \varepsilon V(x, y),$$

$$\tilde{\alpha} = \frac{m_B+m_C}{m_C}\frac{\alpha}{\delta}, \quad \tilde{A} = \varepsilon A \exp\left[-\frac{m_C}{m_B+m_C}\tilde{\alpha}\tilde{y}_{eq}\right],$$

where $\delta = (\hbar/M^{1/2}k^{1/2})^{1/2}$ is the unit of length and $\varepsilon = \hbar k^{1/2}/2M^{1/2}$ is the unit of energy which is equal to the ground state energy of the molecule BC. The formal solution of equation (2) satisfying the outgoing wave condition may be written as the sum

$$\psi^I(x, y) = \phi^I(x, y)+\chi^I(x, y),$$

in which the function $\phi^I(x, y)$ is the initial incoming wave whereas $\chi^I(x, y)$ denotes the scattered wave given by

$$\chi^I(x, y) = -\int dx' \int dy' G(x, y; x', y')V(x', y')\psi^I(x', y'), \tag{5}$$

where $G(x, y; x', y')$ is the appropriate Green's function. Choosing the initial wave in the form

$$\phi^I(x, y) = H_I(y)\exp(-ik_I x),$$

where $H_I(y)$ is a normalized harmonic oscillator eigenfunction and k_I the wave number defined by the formula

$$k_I = [m(E-2I-1)]^{1/2}, \tag{6}$$

we assume that the particle approaches the molecule BC, which is in a state I, from the positive direction of the x axis. The effect of the collision is reflected in the asymptotic behaviour of the wave function $\psi^I(x, y)$. This behaviour is described by the formulae

$$\lim_{x\to\infty} \psi^I(x, y) = H_I(y)\exp(-ik_I x)+\sum_{n=0}^{\infty} R_n^I \exp(ik_n x)H_n(y),$$

$$\lim_{x\to-\infty} \psi^I(x, y) = H_I(y)\exp(-ik_I x)+\sum_{n=0}^{\infty} T_n^I \exp(-ik_n x)H_n(y),$$

where

$$R_n^I = \int dx \int dy \frac{m}{2ik_n} \exp(-ik_n x) H_n(y) V(x, y) \psi^I(x, y), \tag{7}$$

$$T_n^I = \int dx \int dy \frac{m}{2ik_n} \exp(ik_n x) H_n(y) V(x, y) \psi^I(x, y), \tag{8}$$

which are easy to obtain after inserting into (5) the explicit form of Green's function [1]

$$G(x, y; x', y') = -\sum_{n=0}^{\infty} \frac{m}{2ik_n} H_n(y) H_n(y') \exp(ik_n|x-x'|).$$

The probabilities of transitions of the molecule from the state I to n, with a simultaneous reflection or transmission of the incoming particle through the potential barrier are given in terms of the reflection, R_n^I, and transmission, T_n^I, coefficients as

$$P_{I-n}^R = \frac{k_n}{k_I} |R_n^I|^2, \tag{9}$$

$$P_{I-n}^T = \frac{k_n}{k_I} |T_n^I + \delta_{In}|^2. \tag{10}$$

They satisfy the equation

$$\sum_{n=0}^{N_0} (P_{I-n}^R + P_{I-n}^T) = 1 \quad \text{for } I = 0, 1, \ldots, N_0; \tag{11}$$

where N_0 is the index of the highest open channel[1]. The sum occurring in (11) will be further denoted by Σ^I.

3. The refined Born approximation

In order to calculate the probabilities defined in the preceding section it is necessary to know the scattered wave $\chi^I(x, y)$. This function may be found by solving the integral equation (5). On the basis of the refined Born approximation the solution of this equation can be obtained by an iterative procedure starting with a function

$$\chi^{I(0)} = \chi^{I(0)}(x, y, \beta_1, \ldots, \beta_J),$$

which depends on a certain number of parameters $\beta_1, \ldots, \beta_J$. These parameters are then fitted in such a way that the function $\chi^{I(n)}$ obtained after performing n iterations differs little from $\chi^{I(n-1)}$(where n may be equal to 1, 2, ...), and, thereby, it approaches the exact solution of the considered equation. For practical application this main idea of the refined Born approximation must be supplied with detailed instructions for the calculation of the optimal values of the parameters inserted in $\chi^{I(0)}$. For this purpose Rayski formulat-

[1] An open channel is a channel for which the energy of the molecule in the state n, $E_n = 2n+1$, is less than the total energy E.

ed a criterion which after adopting to the investigated model may be expressed as: $\chi^{I(n)}$ differs little from $\chi^{I(n-1)}$ if the index of reliability defined by the formula

$$\Delta^{I(n)} = \int_{x_1}^{x_2} dx \int_{-\infty}^{\infty} dy |\chi^{I(n)} - \chi^{I(n-1)}|^2 \tag{12}$$

has the minimal value. Thus the optimal values of the parameters $\beta_1, \ldots, \beta_J$ are given as the solution of the set of equations

$$\frac{\partial \Delta^{I(n)}}{\partial \beta j} = 0 \quad \text{for } j = 1, 2, \ldots, J. \tag{13}$$

The scattered wave is not square integrable; therefore the finite length of the integration range is a very important element in the definition of the index of reliability. This range is defined as to give the main contribution to the integrals over x in the formulae (7) and (8). Its choice depends on the values of the potential parameters A and α. The choice of the functions $\chi^{I(0)}$ is restricted only by some general conditions: these functions should prevent us from obtaining evidently worthless solutions of the problem, and, for practical reasons, they should be also relatively simple. From many possible functions which meet these requirements this function which leads to the smalest value of the index of reliability should be regarded as the best one.

6. Calculations and results for the model with the finite barrier of interaction potential V^m

The calculations were performed with the functions $\chi^{I(0)}$ in the form

$$\chi^{I(0)} = \sum_{n=0}^{N} H_n(y) \sum_{l} \beta_{nl}^{I} \exp(i\tilde{k}_l x).$$

The set of numbers $\tilde{k}_l$ was determined for different tests according to one of the two following formulae

1) $$\tilde{k}_l = \frac{2l\pi}{x_2 - x_1} \quad \text{for } l = -l_1, -l_1+1, \ldots, l_2,$$

where the interval $x_2 - x_1$ is the same as defined in the preceding section,

2) $$\{\tilde{k}_l\} = \{sk_i\} \text{ for } s = \pm\frac{1}{M}, \pm\frac{1}{M-1}, \ldots, \pm 1, 0, \pm 2, \pm 3, \ldots, \pm M$$

$$\text{and } i = 0, 1, \ldots, N_0,$$

where k_i are given by (3) (l_1, l_2, N, M are integers, N_0 is defined in (11)). These functions linearly depend on the parameters β_{nl}^{I}. The number of these parameters is $J = (N+1)(L+1)$, where L is given by

$$L = l_1 + l_2,$$

or

$$L = (N_0+1)(4M-1) - 1$$

TABLE I

Transition probabilities obtained from the refined Born approximation, the 1-st and 2-nd order of Born approximation and from the exact method of Secrest and Johnson. The results for $m = 1.0$, $\alpha = 0.225$, $A = 0.5$, $y_{eq} = 1.0$, $x_1 = -25.0$, $x_2 = 25.0$

Test No.	E	$I-j$	P^R_{I-j}				P^T_{I-j}				$\sum^I$		
			RBA	Born I	Born II	exact	RBA	Born I	Born II	exact	RBA	Born I	Born II
1	3.5	0−0	.1495(−2)	.5351(−3)	.1868(−2)	.1503(−2)	.9978 (0)	.2358 (1)	.1577 (1)	.9984 (0)	.9994	2.359	1.580
		0−1	.2250(−4)	.5219(−5)	.6269(−4)	.2146(−4)	.5030(−4)	.1653(−3)	.7851(−3)	.4985(−4)			
2	3.5	1−0	.2150(−4)	.5219(−5)	.6269(−4)	.2146(−4)	.4960(−4)	.1653(−3)	.7851(−3)	.4985(−4)	.9973	8.200	18.44
		1−1	.7781 (0)	.6035(−1)	.9089 (0)	.7794 (0)	.2191 (0)	.8140 (1)	.1753 (2)	.2206 (0)			
3	4.0	0−0	.7242(−3)	.3117(−3)	.9538(−3)	.7349(−3)	.9975 (0)	.2132 (1)	.1400 (1)	.9991 (0)	.9984	2.132	1.402
		0−1	.1216(−4)	.1695(−5)	.1271(−4)	.1223(−4)	.1635(−3)	.1828(−3)	.5781(−3)	.1652(−3)			
4	4.0	1−0	.1201(−4)	.1695(−5)	.1271(−4)	.1223(−4)	.1639(−3)	.1828(−3)	.5781(−3)	.1652(−3)	.9969	4.578	5.091
		1−1	.9223(−1)	.8289(−2)	.6473(−1)	.9279(−1)	.9045 (0)	.4570 (1)	.5026 (1)	.9070 (0)			
5	4.9	0−0	.2070(−3)	.1430(−3)	.3672(−3)	.2743(−3)	.9994 (0)	.1871 (1)	.1236 (1)	.9995 (0)	.9998	1.871	1.237
		0−1	.4085(−6)	.4839(−6)	.2446(−5)	.1997(−5)	.1870(−3)	.2034 (−3)	.4718(−3)	.2011(−3)			
6	4.9	1−0	.1152(−5)	.4839(−6)	.2446(−5)	.1997(−5)	.1773(−3)	.2034(−3)	.4718(−3)	.2011(−3)	.9945	2.880	2.108
		1−1	.4505(−2)	.1266(−2)	.5623(−2)	.5112(−2)	.9899 (0)	.2879 (1)	.2102 (1)	.9947 (0)			
7	6.9	0−0	.5845(−4)	.4166(−4)	.8435(−4)	.6252(−4)	.9939 (0)	.1576 (1)	.1103 (1)	.9997 (0)	.9941	1.576	1.103
		0−1	.1720(−6)	.9369(−7)	.3374(−6)	.2345(−6)	.1823(−3)	.2153(−3)	.3769(−3)	.2176(−3)			
		0−2	.1280(−6)	.6167(−7)	.2430(−6)	.1698(−6)	.6000(−5)	.7809(−5)	.1734(−4)	.7211(−5)			
8	6.9	1−0	.1634(−6)	.9369(−7)	.3374(−6)	.2345(−6)	.1765(−3)	.2153(−3)	.3769(−3)	.2176(−3)	.9739	1.916	1.261
		1−1	.2108(−3)	.1503(−3)	.3958(−3)	.2933(−3)	.9732 (0)	.1915 (1)	.1259 (1)	.9991 (0)			
		1−2	.2052(−5)	.9924(−6)	.5174(−5)	.4249(−5)	.2853(−3)	.4173(−3)	.9958(−3)	.4120(−3)			
9	6.9	2−0	.1166(−6)	.6167(−7)	.2430(−6)	.1698(−6)	.5736(−5)	.7809(−5)	.1734(−4)	.7211(−5)	.9641	2.976	2.217
		2−1	.1818(−5)	.9924(−6)	.5147(−5)	.4249(−5)	.3002(−3)	.4173(−3)	.9958(−3)	.4120(−3)			
		2−2	.4097(−2)	.1330(−2)	.6089(−2)	.5586(−2)	.9597 (0)	.2974 (1)	.2210 (1)	.9940 (0)			

for formulae 1) or 2), respectively. In the performed computations we have determined the parameters β_{nl}^{I} as the solution of the following equation set

$$\frac{\partial \tilde{\Delta}^{I(1)}}{\partial \beta_{nl}^{I}} = 0 \quad \text{for } n = 0, 1, \ldots, N \text{ and } l = 0, 1, \ldots, L, \tag{14}$$

where

$$\tilde{\Delta}^{I(1)} = \int_{x_1}^{x_2} dx W(x) \int_{-\infty}^{\infty} dy |\chi^{I(1)} - \chi^{I(0)}|^2 \tag{15}$$

$$W(x) = \frac{\exp(-2\alpha|x|)}{\int_{x_1}^{x_2} \exp(-2\alpha|x|) dx}.$$

Inserting the weight function $W(x)$ into the definition of the index of reliability we modulate the accuracy of fitting of the function $\chi^{I(1)}(x, y)$ to $\chi^{I(0)}(x, y)$ along the interval $[x_1, x_2]$. Thus this accuracy is highest for the region of the largest values of the interaction potential. We believe that the above modification of the original Rayski's criterion results in an improvement of the evaluated probabilities P_{i-j}^{R} and P_{i-j}^{T}. For the calculation of these probabilities we substitute into (7) and (8) the functions $\chi^{I(0)}(x, y)$ instead of $\chi^{I}(x, y)$.

The results of the performed numerical tests are exhibited in Tables I—IV. The best results from the point of view of the theory presented in the foregoing section are listed in Table I (the columns marked by RBA). The numerical details of the computations are described in Table II. The comparison of these results with the exact values obtained

TABLE II

Form of the function $\chi^{I(0)}$ used in computation of the RBA probabilities listed in Table I

Test No	l_1	l_2	M	N	J
1	15	15	—	1	62
2	15	15	—	1	62
3	15	15	—	1	62
4	15	15	—	1	62
5	22	2	—	1	50
6	15	15	—	1	62
7	—	—	2	1	63
8	—	—	2	1	63
9	—	—	2	1	63

in the present work with the "amplitude density function" method and with those given by the original Born approximation leads to the following conclusions:

(*i*) by the use of the RBA one can obtain results which satisfy the relation (11) with a high accuracy;

(*ii*) the RBA predicts correctly, first of all, these probabilities which have relatively large values;

(*iii*) this approximation preserves the proper relations between small probabilities;

TABLE III

Transition probabilities from state 0 for many values of the "index of reliability". The results for $E = 3.5$, $m = 1.0$, $\alpha = 0.225$, $A = 0.5$, $y_{eq} = 1.0$, $x_1 = -25.0$, $x_2 = 25.0$

P^R_{i-j}		P^T_{i-j}		$\sum^0$	$\tilde{\Delta}^{0(0)}$	$\chi^{0(0)}$				
0−0	0−1	0−0	0−1			l_1	l_2	M	N	J
.6371(−3)	.6259(−4)	.1663(1)	.1169(−3)	1.664	.3528 (0)	9	9	—	1	38
.8199(−3)	.4168(−4)	.1251(1)	.7987(−4)	1.215	.2373 (0)	10	10	—	1	42
.8851(−3)	.2687(−4)	.9483(0)	.5186(−4)	.9493	.1083 (0)	11	11	—	1	46
.1165(−2)	.2277(−4)	.9500(0)	.4802(−4)	.9513	.3070(−1)	12	12	—	1	50
.1258(−2)	.2161(−4)	.9726(0)	.4853(−4)	.9739	.1843(−1)	—	—	2	1	28
.1387(−2)	.2312(−4)	.9858(0)	.5108(−4)	.9872	.8756(−2)	—	—	3	1	44
.1433(−2)	.2255(−4)	.9925(0)	.4977(−4)	.9940	.4696(−2)	13	13	—	1	54
.1481(−2)	.2251(−4)	.9966(0)	.5014(−4)	.9982	.1188(−2)	14	14	—	1	58
.1016(−2)	.5130(−5)	.9976(0)	.4493(−4)	.9986	.9759(−3)	15	3	—	1	38
.9132(−3)	.1102(−5)	.9981(0)	.3441(−4)	.9990	.6765(−3)	19	−1	—	1	38
.9592(−3)	.1347(−5)	.9980(0)	.3524(−4)	.9990	.6727(−3)	17	1	—	1	38
.9565(−3)	.1351(−5)	.9982(0)	.3531(−4)	.9992	.5825(−3)	29	1	—	1	62
.1087(−2)	.1965(−4)	.9981(0)	.4916(−4)	.9993	.5052(−3)	25	5	—	1	62
.1495(−2)	.2250(−4)	.9978(0)	.5030(−4)	.9994	.4314(−3)	15	15	—	1	62
Exact values										
.1503(−2)	.2146(−4)	.9984(0)	.4985(−4)	1.0000						

TABLE IV

Transition probabilities from state 1 for many values of the "index of reliability". The results for $E = 3.5$, $m = 1.0$, $\alpha = 0.225$, $A = 0.5$, $y_{eq} = 1.0$, $x_1 = -25.0$, $x_2 = 25.0$

P^R_{i-j}		P^T_{i-j}		$\sum^0$	$\tilde{\Delta}^{0(1)}$	$\chi^{0(0)}$				
1−0	1−1	1−0	1−1			l_1	l_2	M	N	J
.3797(−5)	.5132(−1)	.3939(−4)	.1862(0)	.2376	.9854(−1)	19	−1	—	1	38
.3750(−5)	.5099(−1)	.3684(−4)	.2297(0)	.2807	.8004(−1)	17	1	—	1	38
.3748(−5)	.5100(−1)	.3689(−4)	.2297(0)	.2808	.8003(−1)	29	1	—	1	62
.7208(−5)	.1572 (0)	.4471(−4)	.2877(0)	.4450	.4702(−1)	15	3	—	1	38
.2064(−4)	.5889 (0)	.4786(−4)	.2188(0)	.8077	.1059(−1)	25	5	—	1	62
.1942(−4)	.7342 (0)	.4535(−4)	.1950(0)	.9293	.7423(−2)	—	—	2	1	28
.2000(−4)	.7767 (0)	.4629(−4)	.2175(0)	.9943	.6254(−3)	—	—	3	1	44
.1806(−4)	.7772 (0)	.4274(−4)	.2186(0)	.9958	.3668(−3)	9	9	—	1	38
.1774(−4)	.7775 (0)	.4183(−4)	.2188(0)	.9964	.3088(−3)	10	10	—	1	42
.1790(−4)	.7778 (0)	.4151(−4)	.2190(0)	.9968	.2677(−3)	11	11	—	1	46
.1921(−4)	.7779 (0)	.4442(−4)	.2191(0)	.9970	.2505(−3)	12	12	—	1	50
.2099(−4)	.7780 (0)	.4847(−4)	.2191(0)	.9972	.2373(−3)	13	13	—	1	54
.2140(−4)	.7780 (0)	.4935(−4)	.2191(0)	.9972	.2316(−3)	14	14	—	1	58
.2150(−4)	.7781 (0)	.4960(−4)	.2191(0)	.9973	.2266(−3)	15	15	—	1	62
Exact values										
.2146(−4)	.7794 (0)	.4985(−4)	.2206(0)	1.0000						

(*iv*) the above points are the most important consequences of the modification introduced by Rayski to the original Born approximation;
(*v*) all presented RBA results are in good agreement with the exact ones.

It seems that the criterion of the index of reliability is of a crucial importance for the usefulness of the refined Born approximation in the investigation of the collision problems. The results of the numerical tests collected in Tables III and IV can serve as a basis for an evaluation of its merits in the case presented here. It is easy to see from these tables that a diminishing of the index of reliability always leads to an improvement of the respective sum of probabilities Σ^I and almost in all cases it changes properly the values of the large probabilities. But the influence of the "index" on the small probabilities is not so strong. These facts result from the variational nature of Rayski's procedure. Thus, the index of reliability defined by (12) (or by (15)) can be used indeed as a measure of correctness for the global description of a given problem rather than for its particular elements.

The interval $[x_1, x_2]$ should include the greater part of the potential range. However, in order to achieve a sufficient accuracy in the fitting procedure for a large interval $[x_1, x_2]$ we must take, in principle, a function $\chi^{I(0)}$ that depends on a large number of parameters. This enlarges the computational effort needed. Thus, it would be desirable to have a more precise criterion for the choice of the optimal interval $[x_1, x_2]$.

5. *Discussion of the applicability of the RBA to the model with the exponential interaction potential* V^{S-J}

The essentially new point of this model, as compared with that described above, is the infinity of the interaction potential for $x \to -\infty$. Formally, there is no obstacle in applying the refined Born approximation to this model. In fact, also in this case it is necessary to find the scattered wave only for a finite range of the x variable. As before, this is connected with the possibility of reduction of the infinite integration range over x in (4) and (5) to the finite interval $[x_1, x_2]$. However, in this case such a possibility results not only from decaying of the interaction potential (for $x \to +\infty$), but also from vanishing of the wave function $\psi^I(x, y)$ (for $x \to -\infty$). This is a source of some practical difficulties. Namely, we have not enough information even for a rough determination of the point x_1 because the function $\psi^I(x, y)$ is unknown. In consequence of this difficulty it is unlikely that one could obtain a reasonable result by applying the RBA in this case. For the correctness of the calculated coefficients R_n^I and T_n^I it is necessary to achieve the best fit of the functions $\chi^{I(n)}$ and $\chi^{I(n-1)}$ just near to the point x_1, where the potential $V^{S-J}(x, y)$ has large values.

6. *Summary*

The numerical results presented in Section 4 indicate that the refined Born approximation is well-adopted for the description of the inelastic processes. Our calculations were performed for the one-dimensional model with the low barrier of the interaction

potential V^m only. We believe that the RBA may also be successfully applied to the high potential barriers in this model as well as to other models. The most serious difficulty which could appear in further applications of this approximation concerns a proper estimation of the integration interval occurring in Rayski's criterion. Fortunately, for many models existing in the theory of inelastic collisions such an estimation could be easily obtained from knowledge of the shape of interaction potential. As we have shown in Section 5, it would be, however, extremely difficult for the case of the exponentially growing (for $x \to -\infty$) interaction potential. Therefore, the RBA is rather inadequate for the description of the model given by Secrest and Johnson. A rough determination of the above mentioned interval can prove to be sufficient. Our numerical results can serve as an example. However, in order to make the refined Born approximation an efficient procedure for solving collision problems one should, in our opinion, supply it with a precise criterion for the choice of the optimal integration range in the formula for the index of reliability.

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