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THE STUDY OF ATOMIC TRANSITIONS BY USE OF NUMEROV TECHNIQUE IN SCHEMATIC MODEL

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The calculation of a partial cross section in atomic collision theory when the collision is inelastic and there is not a possibility of particle exchange requires the solution of a system of coupled differential equations. The Numerov technique is applied to the solution of schematic model equations, which simulate the solution of real problems but are themselves exactly solvable. We have investigated the 3^2S transition in sodium as an excellent application of a near resonance and strong coupling situation in the case of two-state approximation. The results are compared with those obtained by the Bethe and resonance distortion approximations. The difference can be ascribed to the use of the set of two-channel differential equations rather than the set of three-channel equations used in other approximations, and to the simplified treatment of the interaction potentials.

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1. *Introduction*

The study of particle collisions has a long and storied history in the annals of scientific exploration. Much of the understanding of the fundamental nature of particles and their underlying microscopic interaction has been derived from scattering experiments. Scattering plays an essential role in elastic and inelastic collisions, reactions, and rearrangements, as well as in the capture of elementary particles, nuclei, atoms, molecules, and quasi-particles.

Theoretical predictions of scattering cross sections and resonance are usually based on an underlying differential equation such as the Schrödinger equation, which can be split into a system of coupled differential equations. One of the tasks of scattering theory is to establish the mathematical tools necessary for the extraction of analytic or numerical results to show their efficacy.

Alkali-metal atoms are fertile ground for the study because they are ideally suited for the production of atomic beams, can be easily detected, and have large electron collision cross sections. The very strong coupling between the ground n^2S and the n^2P excited states in many cases simplifies the theoretical treatment of the collision problem. All these properties make them "targets of opportunity" for electron-atom collision research, both experimental and theoretical.

From the point of view of practice, we know that the D line of sodium was used in optical spectroscopy as a reference line, for example, in the determination of the refractive indices of various substances in the gaseous or liquid form, or of some alkali crystals (LiF, NaCl, KI, etc) [1]. This line plays also an essential role in theory, for example, from the experimental methods in astrophysics (observation of eclipses, study of the solar chromosphere, etc), the analysis of the absorption lines of Na leads to an accurate knowledge of the oscillation force f, which plays an important role in atomic physics [2].

Most of experimental work has thus been performed with the ground-state of the sodium atom, and includes the measurement of total [3], differential [4], direct differential [5] and exchange differential [6] elastic cross sections, as well as total [7] and differential [8] n^2S-n^2P impact-excitation cross sections. At low energies, the unifying feature of these experiments is the generally good, and sometimes excellent agreement exists between measurements and the results of few-state close coupling calculations [9].

Moreover, several measurements of differential cross sections have been carried out with excited states of Na by means of laser techniques [10].

In 1972 Moores and Norcross [11] reported four-state close-coupling calculations of cross sections for electron scattering from sodium in its ground state at energies below the ionization threshold at 5.14 eV. Their results have become the standard for comparison of experimental and theoretical determination of integral and differential cross sections for 3s $\rightarrow$ 3p excitations [7]. During the subsequent decades, however, experimental studies of electron-alkali atom scattering moved in new directions, making new demands on theory [12 – 16]. On the other hand, various theoretical calculations of the electron excitation cross section for 3s $\rightarrow$ 3p transition have differed considerably. Indeed, most calculations of the cross section have been extensions of the Bethe or first Born approximations [17]. These differ not only in magnitude but also in the shape of the cross sections as a function of energy [17]. Close-coupling calculations by Barnes et al. [18] and Karule and Peterkop [19] unfortunately disagree. However, the close-coupling calculations by Kroff [20] and Moores and Norcross [11] indicate agreement with the results of Ref. [19]. A model proposed by Vainshtein et al. [21], which attempts empirically to include the polarizations of sodium atom, gives still other cross sections. Moreover, at high energies, the first and second Born approximations describes quite accurately many collision processes [22], but in the intermediate region of energy a good theory remains to be found. In this way a number of theoretical models have been developed to cope with the complex problem and our investigation reports on the calculations of the cross sections for the 3s $\rightarrow$ 3p transition in Na by electron impact, by considering the schematic model (SM).

In this paper we adopt the method of close coupling in the two-state approximation to investigate quantitatively the effects of the energy separation ΔE, the magnitude of the coupling and the direct interaction potentials on the inelastic cross sections for 3s $\rightarrow$ 3p transition in Na, using the Numerov method (NM) technique [23]. The obtained results will be compared with those of other approximations.

2. Formulation of electron-atom collisions

The theory of the problem of electron-atom collision in the close-coupling approach has been widely formulated by many authors [9, 10, 20, 23 − 28] In this section, the resume of the general theory of atomic collisions will be outlined. Consider an electron with linear momentum $\hbar k_0$ colliding with an atom, which was initially in the state characterized by Ψ_0 and E_0. We shall denote the coordinates of the colliding electron by $\mathbf{r}$, those of the atomic electrons by $\mathbf{r}_1, \mathbf{r}_2, ...$ and the potential energy between the electron and the atom by $V(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, ...)$.

We also denote the angular momentum numbers of the incoming electron as $l_1 m_1$ and the initial atomic state by β, and that of the outgoing electron by $l_1' m_1'$ with all other states β' of the atom. In this paper we neglect the exchange effect between the incident electron and the atomic electrons. The total wave function [24] of the system may be written as

$$\Psi(\beta'|\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, ...) = r^{-1} \sum_{\beta} F_\beta(\beta'|r) \psi_\beta(\mathbf{r}_1, \mathbf{r}_2, ..., \widehat{r}) \,, \tag{1}$$

where $\beta = (\alpha, l, m)$ and $\psi_\beta(\mathbf{r}_1, \mathbf{r}_2, ..., \widehat{r})$ can be expressed in terms of the spherical harmonics . Substituting this equation in the Schrödinger equation, we obtain the following system of equations

$$\left[\frac{d^2}{dr^2} + k_\beta^2 - \frac{l_\beta(l_\beta + 1)}{r^2} \right] F_\beta(\beta'|r) = \sum_\gamma F_\gamma(\beta'|r) U_{\beta\gamma}(r) \,, \tag{2}$$

where

$$U_{\beta\gamma}(r) = \frac{2M}{\hbar^2} \int \psi_\beta^*(\mathbf{r}_1, \mathbf{r}_2, ...) V(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, ...\widehat{r}) \psi_\gamma(\mathbf{r}_1, \mathbf{r}_2, ...\widehat{r}) \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 ... \mathrm{d}\widehat{r} \,. \tag{3}$$

The functions F must satisfy the conditions

$$F_\beta(\beta'|0) = 0 \,, \tag{4}$$

$$F_\beta(\beta'|r) \sim \frac{1}{k_\beta^{\frac{1}{2}}} [\delta(\beta, \beta') \mathrm{e}^{-\mathrm{i}(kr - \frac{1}{2} l_\beta \pi)} - \mathbf{S}(\beta, \beta') \mathrm{e}^{\mathrm{i}(kr - \frac{1}{2} l_\beta \pi)}] \,. \tag{5}$$

The cross section for the transition $n'l'_1 \to nl_1$ can be expressed [24] in terms of the collision strength and the $\mathbf{S}$ matrix as

$$\sigma(n'l'_1 \to nl_1) = \frac{\pi\Omega(n'l'_1 nl_1)}{k^2(2l_1+1)}\,, \tag{6}$$

where the total collision strength is

$$\Omega(\alpha,\alpha') = \sum_{lm,l'm'} |\mathbf{S}(\alpha lm, \alpha' l' m')|^2\,. \tag{7}$$

In this work we confine ourselves to the singly excited configuration, and since the core electron extends only over a small region near nucleus, we ignore the structure of the core. Therefore, the problem can be reduced to the one-electron atom. On making multipole expansions of the potentials we have (in atomic units),

$$U_{\beta\gamma}(r) = \sum_{\lambda} U_\lambda(\beta,\gamma|r)\,, \tag{8}$$

with

$$U_0(nl_1l_2L, n'l'_1l'_2L|r) = 2\delta(l_1l_2, l'_1l'_2)\left[-\frac{\delta(n,n')}{r} + y_0(nl_1, n'l'_1|r)\right], \tag{9}$$

$$U_\lambda(nl_1l_2L, n'l'_1l'_2L|r) = 2f_\lambda(l_1l_2l'_1l'_2, L)y_\lambda(nl_1, n'l_1|r)\,, \tag{10}$$

for $\lambda > 0$, where

$$\begin{aligned} y_\lambda(nl_1, n'l_1|r) \quad &= \quad \frac{1}{r^{\lambda+1}}\int_0^r \phi_{nl_1}(r')r'^\lambda \phi_{n'l'_1}(r')\mathrm{d}r' + \\ &\quad + r^\lambda \int_r^\infty \phi_{nl_1}(r')\frac{1}{r'^{\lambda+1}}\phi_{n'l'_1}(r')\mathrm{d}r', \end{aligned} \tag{11}$$

where ϕ_{nl} is an atomic radial function and f_λ are a generalization of similar coefficients employed in atomic structure problem and their expressions are given in Ref. [29]. For large value of r

$$y_\lambda \sim \frac{1}{r^{\lambda+1}} S_\lambda(nl_1, n'l'_1) + O(r^{-\lambda-2})\,, \tag{12}$$

where

$$S_\lambda(nl_1, n'l_1) = \int_0^\infty \phi_{nl_1}(r)r^\lambda \phi_{n'l'_1}(r)\mathrm{d}r\,, \tag{13}$$

then the dominant interactions are those for the dipole term $\lambda = 1$. It can be seen from the parity conservation conditions on the angular momentum numbers that these occur only for $l_1' = l_1 \pm 1$ which is the condition for the transitions to be optically allowed.

3. Numerov technique (NM)

Solving the coupled linear differential equations (2) is a problem encountered in the theory of atomic collisions, and extensive literature exists on the subject. A general method for separation is still not available at the moment [30] and obviously constitutes an interesting test for further investigations from the mathematical point of view. In most cases one must resort to numerical iteration procedure to solve these equations. Many different numerical techniques have been developed over the years and can be generally split into two groups, explicit (propagators) and implicit techniques. Both techniques divide the interval of the independent variable into grids. Explicit methods require the solution of the dependent variable at the preceding grid point to compute its value at the next adjacent point.These techniques are easy to code, fast, convergent, and do not require a considerable amount of computational work. The Numerov [31], Gordon [32], and log derivative propagator [33] methods are examples commonly used in atomic collision problems. A performance review of these algorithms is given in Ref. [34]. In this work, the Numerov numerical method will be used to solve the coupled-channel Schrödinger equations in a two state approximation. This technique does not require a considerable amount of computational work and converges rapidly even though the strong coupling interactions are involved. It is used also by many authors [9, 18, 23, 25, 34] to solve special cases in electron-atom collisions.

In this section, the outline of the Numerov numerical method will be presented. Indeed, in a compact matrix notation, the coupled differential equations (2) may be written as,

$$\left[\frac{d^2}{dr^2}\mathbf{I} + \mathbf{Z}(r)\right]\mathbf{F}(r) = 0\,, \tag{14}$$

where $\mathbf{I}$ is the unit matrix, the solution matrix $\mathbf{F}$ has elements $F_{\beta\beta'}$; the first index specifies a channel and the second one referes to a set of boundary conditions, and the functions $Z_{\beta\beta'}(r)$ are given by

$$Z_{\beta\beta'}(r) = \left[k_\beta^2 - \frac{l_\beta(l_\beta+1)}{r^2}\right]\delta_{\beta\beta'} - U_{\beta\beta'}\,. \tag{15}$$

In an exact numerical treatment, and after discretization, this system can always be cast into a series of recurrence relations [35] such as

$$\mathbf{A}_{i+1}\mathbf{F}_{i+1} = \mathbf{B}_i\mathbf{F}_i + \mathbf{C}_{i-1}\mathbf{F}_{i-1}\,, \tag{16}$$

in which, the value of the solution at any position r_{i+1} may be inferred from the knowledge of its values at previous positions r_i, r_{i-1}. We find with a Numerov's treatment that

$$\mathbf{A}_{i+1} = \mathbf{I} + \frac{h^2}{12}\mathbf{Z}(r_{i+1}), \tag{17}$$

$$\mathbf{B}_i = 2\mathbf{I} - \frac{5h^2}{6}\mathbf{Z}(r_i), \tag{18}$$

$$\mathbf{C}_{i-1} = \mathbf{I} + \frac{h^2}{12}\mathbf{Z}(r_{i-1}), \tag{19}$$

in which h stands for the increment of the variable and the error term is of order $O(h^2/240)$.

The solutions are initiated near the origin by a Frobenius-type expansion and developed out form the origin using this iterative procedure (17 - 19). The S-matrix can be found by matching the numerical solutions to (5) for two large enough values of r (e.g. r_a, r_b). These steps comprise the numerical procedure to solve the system of coupled differential equations.

4. *Application: The* 3^2s $\rightarrow$ 3^2p *transition of Na by electron impact*

In particular, we shall consider the transition 3s $\rightarrow$ 3p in Na, which is an excellent example of a near resonance and strong coupling situation and has an energy separation $\Delta E = 2.104$ eV and a rather large line strength $s^2 = 19.3$. Since this transition is optically allowed, the coupling matrix element $U_{\beta\gamma}$ becomes proportional to $1/r^2$ asymptotically, and because of this long-range interaction, it is expected that many partial waves will contribute to the total cross section.

Salmona and Seaton [26] have discussed this problem and made calculations based on the modified Bethe approximations B'I and B'II, which are found to satisfy conservation conditions. The results were found to be quite good for high energies. Cross sections for this transition have been determined experimentally and found to be large [36].

We shall calculate the partial cross sections for several values of the incident electron energy k_0^2 , and the total cross sections may then be determined by utilizing the "tail" of B'I as in Refs. [24, 27]

$$\sigma^{SM} = \sigma^{B'I} - \sum_{l=0}^{l_0} \sigma_l^{B'I} + \sum_{l=0}^{l_0} \sigma_l^{NM}, \tag{20}$$

where the Bethe approximation cross section is given in intermediate energy as [37]

$$\sigma^{B'I} = \frac{\pi}{k_0^2}\left(\frac{8s^2}{3}\right)\ln\left(\frac{k_o + k_\beta}{|k_0 - k_\beta|}\right), \tag{21}$$

and in the high energy as

$$\sigma^{B'I} = \frac{4\pi}{3}\frac{s^2}{k_0^2}\left[\ln\left(\frac{k_o+k_\beta}{|k_0-k_\beta|}\right)+\ln\left(\frac{\eta^2}{|k_0^2-k_\beta^2|}\right)\right], \tag{22}$$

where $k_0(k_\beta)$ is the wave number of the incident (scattered) electron. The adjustable parameter η introduced by Bethe is determined by fitting to the Born approximation.

5. Schematic model

We shall be concerned primarily with the special case of ns $\to$ np transition by electron impact, which involves:

(a) Strong coupling,

(b) Long range interaction potential,

(c) Near resonance.

The Numerov iteration scheme is not restricted to this type of problems. Throughout the calculations, the exchange between the incident electron and the atomic electron has been ignored, since this is justifiable for collisions with long-range interactions. However, the effect of electron exchange can be readily incorporated into the general formulation of the numerical procedure.

In the approximation where the coupling between two states is strong and with all other states is ignored, a two-channel problem results. Then the coupled equations (2) can be replaced by

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k_0^2-\frac{l_0(l_0+1)}{r^2}-U_{00}\right]F_0 = U_{0\beta}F_\beta\,, \tag{23}$$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k_\beta^2-\frac{l_\beta(l_\beta+1)}{r^2}-U_{\beta\beta}\right]F_\beta = U_{\beta0}F_0\,. \tag{24}$$

This system is solved by the Numerov procedure [12,19]. It is instructive to consider first a schematic model in which it is assumed that

$$U_{00} = U_{\beta\beta} = 0\,, \tag{25}$$

$$U_{0\beta} = U_{\beta0} = -A/r^2\,, \tag{26}$$

where

$$A = -\frac{2s}{3}\,. \tag{27}$$

With these forms of potentials, it is possible to obtain analytical solutions for F_0 and F_β in the limiting case of exact resonance ($k_0 = k_n$). Indeed, the system can be separated by introducing the following transformation [30]

$$X(a) = \begin{pmatrix} 1-a & 1+a \\ -(1+a) & 1-a \end{pmatrix} \tag{28}$$

where the quantity a is given by

$$\begin{aligned} a &= 0, \qquad \text{if} \quad l_0 = l_\beta \,, \\ &= 2\varepsilon \pm \sqrt{1+4\varepsilon^2}\,, \quad \text{if} \quad l_0 \neq l_\beta \,, \end{aligned} \tag{29}$$

where

$$\epsilon = \frac{A}{\Delta L}\,, \tag{30}$$

and

$$\Delta L = l_0(l_0+1) - l_\beta(l_\beta+1)\,. \tag{31}$$

The separated equations of this system are

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k_0^2 - \frac{\nu^{\pm 2}}{r^2}\right] Z^\pm = 0\,, \tag{32}$$

where

$$\nu^{\pm 2} = \frac{1}{2}[l_0(l_0+1) + l_\beta(l_\beta+1) \pm \sqrt{(\Delta L)^2 + 4A^2}]\,. \tag{33}$$

The solutions of equation (32) which satisfy the initial conditions (4) can be expressed in terms of the Bessel functions of the first kind of order $\mu^\pm = \sqrt{\nu^{\pm 2} + \frac{1}{4}}$ which are real constants. Then the valid solutions are given by the following condition

$$A > (l_0 + \frac{1}{2})(l_\beta + \frac{1}{2})\,. \tag{34}$$

The cross sections can not be calculated for the very small values of the angular momentum numbers in the schematic model. The functions F_0 and F_β may be recovered by the inversion transformation

$$\begin{bmatrix} F_0 \\ F_\beta \end{bmatrix} = X^{-1} \begin{bmatrix} Z^+ \\ Z^- \end{bmatrix}. \tag{35}$$

The partial inelastic cross sections can be calculated from F_β as in Ref. [30]

$$\sigma_l = \frac{\pi}{k_0^2}(2L+1)\left(\frac{1-a^2}{1+a^2}\right)^2 \sin^2(\eta_L^+ - \eta_L^-)\,, \tag{36}$$

where $\eta_L^{\pm}$ are the conventional partial phase shifts and are given by

$$\eta_L^{\pm} = \frac{1}{2}\pi\mu^{\pm} \,. \tag{37}$$

For problems involving energies near resonance, it is not possible to decouple the system, and we have recourse to the use of the numerical treatment. In carrying out the solution by Numerov method, the iterative cycle was repeated until the solutions had converged to the required accuracy. It was found satisfactory to use an integration step of $\delta r = 0.1$ and to match the asymptotic expression at $r = 249.9$ and $r_b = 250.0$.

6. *General results and conclusion*

In the previous sections, a technique was briefly discussed whereby inelastic cross sections for collisions and transitions under near resonance conditions can be determined. It is now wished to investigate the calculations on the behavior of these cross sections for different parameters of coupling and resonance and to compare them with results obtained by other methods of calculations.

6.1. *Effect of the energy separation ΔE*

Typical curves, representing partial cross sections for $A = 3$ and different energy separations ΔE, are given in Fig. 1. It can be seen that the values of σ_l increase

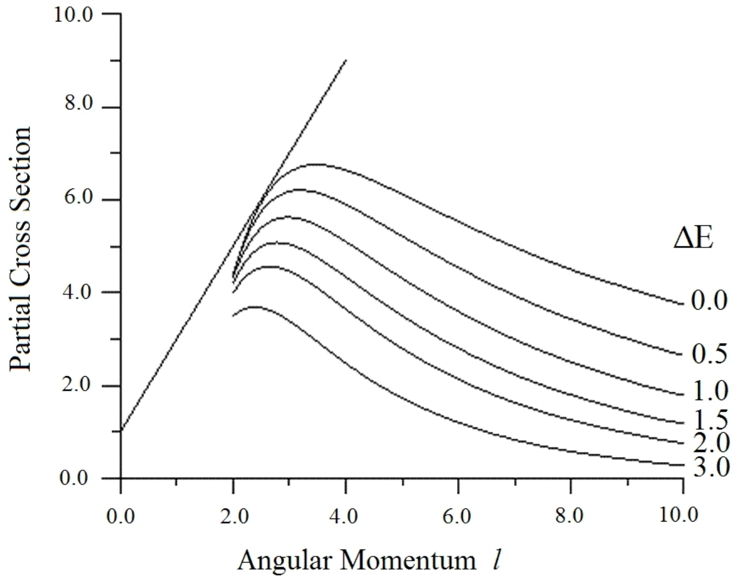

Fig. 1. Partial cross sections σ_l for different values of separation energy ΔE (eV) *and $A = 3$, with $E = 13.6$ eV, calculated by using the schematic model (SM). The straight line is calculated by Eq. (39).*

steadily with the decrease of ΔE, the maximum occurring for $\Delta E = 0$. It is important to note that these partial cross sections remain below the maximum allowed by conservation.

We further note that the main features of results obtained by this numerical procedure coincide with those obtained by the method of separation of coupled equations [39]. The partial cross sections for $l = 0$ and 1 are not shown since they cannot be calculated by this scheme.

6.2. Effect of the magnitude of coupling

In Fig. 2, the collision strength in the schematic model for $n\mathrm{s} \to n\mathrm{p}$ transition, at exact resonance, is given with the magnitude of the coupling strength A. It has been shown that for exact resonance collisions, as one increases the strength of coupling (from the weak coupling), the collision strength first increases rapidly, then reaches a certain saturation stage, and finally behaves in an oscillatory manner. The saturation effect is more pronounced at low values of l, and the collision strength for higher l requires even stronger coupling for complete saturation. These results also concur with those obtained by the method of separation of coupled equations for the case of the three-channel problem [39, 38].

For the case of near (but not exact) resonance, the qualitative behavior of the partial collision strengths with respect to the degree of coupling is similar to that of exact resonance. Figure 3 shows the variation of $\Omega_l/(2l+1)$ with respect to A for an energy separation of the initial and final states ΔE of 2.0 eV.

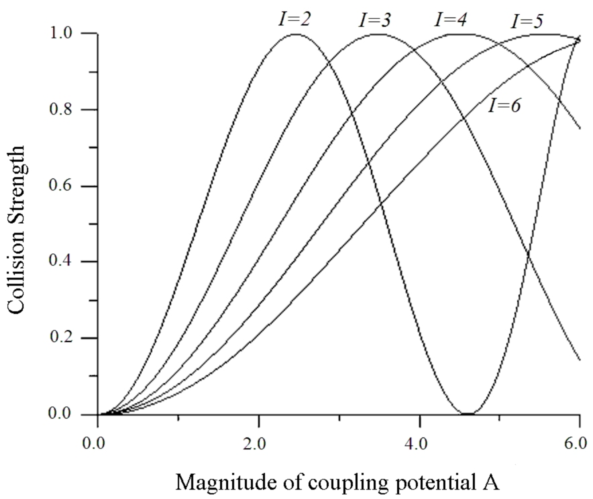

Fig. 2. Collision strength $\Omega_l/(2l+1)$ $(\Delta E = 0)$ for $n\mathrm{s} \to n\mathrm{p}$ transition in the schematic model, with exact resonance $\Delta E = 0$. in terms of the magnitude of the coupling strength A, for an incident energy of 13.6 eV.

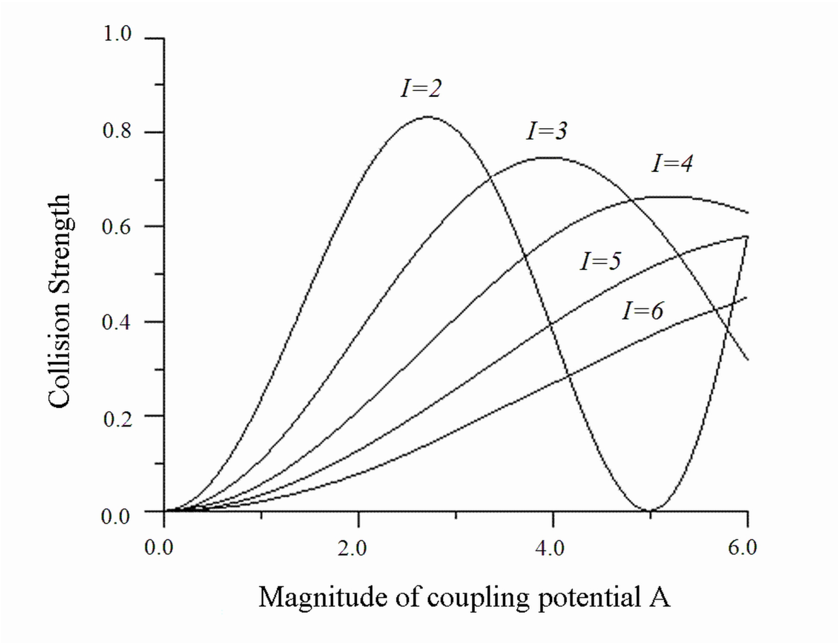

Fig. 3. Values of collision strength $\Omega_l/(2l+1)$ *for different* l *and* $\Delta E = 2.0$ eV, *in terms of the magnitude of the coupling strength* A *for the incident energy of* 13.6 eV.

6.3. Effect of direct interaction potentials

For electron-atom collisions, the direct potentials U_{00} and $U_{\beta\beta}$ behave like e^{-ar}/r near the origin and decay rapidly on account of the exponential factor. The radial part of the coupling potential $U_{0\beta}$ is proportional to r^{-2} at large distances (for the ns $\to$ np transition) but attains a maximum and eventually passes through the origin as r decreases to zero. Numerical values of σ_l^{SM} with and without the direct potentials are given in Table 1 for two values of the incident energy. For different values of energy, the partial cross-sections in the two cases agree quite well with each other. This is understandable because for a particular value of l, the classical distance of closest approach is

$$r_l^2 = l(l+1)/k^2 \,, \tag{38}$$

which increases with the decrease of energy, thereby causing the region close to the atom to be less important to the scattering of the partial wave, and hence for such energies the cross section is quite insensitive to the detailed behavior of the elements $U_{ij}(r)$ near the origin.

TABLE 1. Partial cross sections $\sigma_l(\pi a_0^2)$, where the indices 'w' and 'o' represent the case with and without direct potential, respectively, for two values of the incident energy, line strength $s^2 = 19.0$ and $\Delta E = 2.104$ eV.

	$E = 13.676$ eV		$E = 33.66$ eV	
l	σ_l^w	σ_l^o	σ_l^w	σ_l^o
2	4.068	3.992	1.819	1.816
3	4.251	4.194	2.322	2.279
4	3.365	3.350	2.090	1.759
5	2.544	2.540	1.770	1.479
6	1.915	1.917	1.483	1.244
7	1.451	1.448	1.246	1.054
8	1.103	1.103	1.055	0.898
9	0.849	0.849	0.898	0.770
10	0.657	0.657	0.771	0.665

6.4. Comparison with other methods

For the purpose of comparison, calculations of collision strength for $3^2\mathrm{S} \to 3^2\mathrm{P}$ transition in Na, which has an energy separation $\Delta E = 2.104$ eV, and rather large line strength $s^2 = 19.3$, have been made by the use of the Bethe approximation and the resonance-distortion method [27] in the case of the three-channel problem, but our results are for the two-channel problem. Numerical values of $\sigma_l^{RD}, \sigma_l^{B'II}, \sigma_l^{SM}$ are given in Table 2 for two values of the incident energy and several values of l. All cross sections are in units πa_0^2. As expected, the major contribution to the cross section in the case of $E = 10.52$ eV is due to a few intermediate values of l, while for $E = 33.66$ eV, the contribution is more uniformly distributed among several different l. In fact, σ_l^{SM} are closer to σ_l^{RD} for $l = 2$ at $E = 10.52$ eV and for $l = 2, 3$ at $E = 33.66$ eV, than they are to $\sigma_l^{B'II}$. At high values of l, σ_l^{SM} deviates considerably from σ_l^{RD} and $\sigma_l^{B'II}$. This is understandable since both in the resonance-distortion and B'II calculations, the three-channel problem is used where the matrix elements U_{12} and U_{13} were replaced by their asymptotic form which depends on the angular momentum l, while the other elements of $\mathbf{U}$, which are of shorter range, were neglected. Our model is for the two-channel problem, where the interaction potential matrix elements are replaced by their asymptotic inverse square forms, which are independent of l.

TABLE 2. Partial cross sections, in units of (πa_0^2), *of the* 3s−3p *transition of* Na *calculated by the Bethe method* $(\sigma_l^{B'II})$, *and resonance distortion method* (σ_l^{RD}), *and numerical technique* (σ_l^{SM}) *for two values of the incident energy, for line strength* $s^2 = 19.0$, *and* $\Delta E = 2.104$ eV.

	$E = 10.52$ eV			$E = 33.66$ eV		
l	σ_l^{RD}	$\sigma_l^{B'II}$	σ_l^{SM}	σ_l^{RD}	$\sigma_l^{B'II}$	σ_l^{SM}
2	4.31	6.41	4.76	1.51	2.01	1.82
3	7.58	8.37	4.58	2.40	2.61	2.28
4	8.25	8.52	3.43	2.74	2.75	2.07
5	7.44	7.73	2.44	2.70	2.67	1.76
6	6.29	6.61	1.73	2.54	2.51	1.48
7	5.18	5.47	1.23	2.34	2.32	1.24
8	4.21	4.46	0.89	2.15	2.13	1.05
9	3.39	3.59	0.64	1.96	1.95	0.90
10	2.72	2.88	0.47	1.79	1.79	0.77
11	2.18	2.30	0.34	1.64	1.64	0.67
12	1.74	1.83	0.25	1.50	1.50	0.58
13	1.39	1.46	0.19	1.38	1.38	0.51
14	1.11	1.16	0.14	1.27	1.27	0.44
15	0.89	0.92	0.11	1.17	1.17	0.39

TABLE 3. Total cross sections in units (πa_0^2) *and partial sums of* σ_l *for the* 3s − 3p *transition in* Na. $(\sigma_l^{B'II})$ *Bethe method,* (σ_l^{RD}) *resonance distortion method,* σ' *for* $(l = 0, 1)$ *and* (σ_l^{SM}) *numerical technique with schematic model.*

E(eV)	$\sigma^{B'I}$	$\sigma^{B'II}$	σ^{RD}	$\sum_{l=16}^{\infty} \sigma_l^{B'I}$	$\sum_{l=2}^{15} \sigma_l^{B'I}$	σ'	σ_l^{SM}
4.208	288.63	64.9	47.1	0.0	9.4	12.9	22.3
7.364	231.87	71.6	61.7	0.9	18.4	7.4	26.7
10.520	189.12	68.9	62.9	3.6	21.2	5.2	27.9
16.832	139.19	60.5	57.7	9.6	21.1	3.2	33.9
23.144	111.26	53.3	51.7	13.2	19.2	2.5	34.9
33.660	84.48	44.4	43.5	15.6	16.0	1.6	33.2

Since the B'I approximation is valid for large values of l, this may be used in conjunction with the partial cross sections obtained by the numerical method to calculate the total cross sections, using the tail scheme in Eq. (8). Table 3 gives the total cross sections, calculated by means of the proposed schematic model, the resonance-distortion method and the Bethe approximations B'I and B'II (Seaton's modified version of the Bethe method), where the cutoff value for the tail is $l_0 = 15$. Because of the use of an approximate non-diagonal interaction potential with r^{-2} dependence over the entire range, it was not possible to calculate the partial cross sections for $l = 0$ and $l = 1$ by solving the differential equations in the usual way. Instead, these two partial cross sections were simply taken as equal to the upper limit values as imposed by the conservation law,

$$\sigma_l^{\max} = \pi k_0^{-2}(2l+1)\,, \tag{39}$$

which is represented by the straight line in Fig. 1.This is approximately the linear interpolation of the curves of partial cross sections for $l < 2$, with the s and p state contributions chosen from this conservation law and their percentage contributions relative to σ_l^{SM} are given in Table 3.

In the calculations presented in previous sections, we have made the approximation of using a special set of potential functions as given in Eqs. $(12-14)$ and neglecting the effect of the exchange between the colliding and the atomic electrons. For transition with long-range coupling, where the total cross section is distributed over a large number of σ_l, these approximations can be justified on the basis that they affect only the partial cross sections corresponding to small values of l. The use of the schematic model was merely to simplify the numerical volume. The calculation of the cross sections is not essential to the numerical technique and in fact yields an important difference with the RD and B'II approximation. Our results can be extended to phenomenological problems of scattering to include the angular-momentum coupling effects at the cost of more complication.

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PROUČAVANJE ATOMSKIH PRIJELAZA NUMEROVOM METODOM U SHEMATSKOM MODELU

Računanje parcijalnih udarnih presjeka u teoriji atomskih sudara, kad je sudar neelastičan i nema izmjene čestica, zahtijeva rješavanje sustava vezanih diferencijalnih jednadžbi. Primjenjujemo Numerovu metodu za rješavanje shematskog sustava jednadžbi koje oponašaju rješenje stvarnih problema, a se mogu egzaktno riješiti. Proučavamo 3^2S prijelaz u natriju kao odličnu primjenu uvjeta blizu rezonancije i snažnog vezanja za slučaj približenja razmatranjem dva stanja. Ishodi računa uspoređuju se s ishodima Betheovog približenja i približnog računa ometanja rezonancije. Razlika se može pripisati primjeni dvokanalnih diferencijalnih jednadžbi umjesto trokanalnih jednadžbi u drugim približenjima i pojednostavljenim razmatranjem potencijala međudjelovanja.