

Electron Excitation Cross Section of the $3^2S \rightarrow 3^2P$ Transition of Sodium*

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The cross section of the $3^2S \rightarrow 3^2P$ transition of sodium produced by electron impact has been calculated by performing a numerical integration of the set of three-channel differential equations. By means of this numerical procedure, it is no longer necessary to replace the nondiagonal matrix elements of the interaction potential by their asymptotic forms and to neglect the diagonal part of the interaction-potential matrix, as was done in the previous calculations. The cross sections calculated by this numerical scheme are smaller than those of the previous work, and the difference can be ascribed to the use of the true interaction potentials rather than their asymptotic forms. An outline of the general formulation of the numerical method for an n -channel case is given.

INTRODUCTION

IN a previous paper we have reported calculation of the cross section for the $3^2S \rightarrow 3^2P$ transition of Na by electron impact.¹ Owing to the complexity of the coupled differential equations, several simplifying approximations were made.¹⁻³ The diagonal parts of the interaction potential were set to zero while the nondiagonal term which connects the initial and the final state was replaced by its asymptotic form at large distances [see Eqs. (12) and (66) of Ref. 1]. Also, an iteration procedure in which the limiting case of exact resonance is taken as the zeroth-order approximation, was used to solve the coupled differential equations. 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.^{1,4} Instead, these two partial cross sections were simply taken as equal to one-half of the upper limit values as imposed by the conservation law. To improve this calculation we have used a numerical procedure to solve the coupled differential equations. In this way we can avoid making the various assumptions described before. A brief outline of the numerical procedure and the results of the calculation will be given in this paper.

METHOD OF SOLUTION OF THE COUPLED EQUATIONS

We shall adopt the usual notation for an electron-atom collision, i.e., \mathbf{r} and \mathbf{r}_1 for the radius vectors of the colliding electron and the atomic electron, respectively, and $\psi_{n_1 l_1 m_1}(\mathbf{r}_1)$ for the wave function of the atomic electron. If the exchange effect is neglected, the total wave function may be expanded in terms of eigenfunctions of the total angular momentum LM of the

system (coupled representation) in the form⁵

$$\Psi(\nu' | \mathbf{r}_1, \mathbf{r}) = r^{-1} \sum_{\nu} F_{\nu}(\nu' | r) \psi_{\nu}(\mathbf{r}_1, \hat{r}), \quad (1)$$

where ν stands for the group of quantum numbers $n_1 l_1 l' L M$ and where the basis functions are the Clebsch-Gordan combinations of $\psi_{n_1 l_1 m_1}$ and the partial waves (spherical harmonics) of the incident electron,

$$\psi_{\nu}(\mathbf{r}_1, \hat{r}) = \sum_{m_1 m} C_{m_1 m M}^{l_1 l L} \psi_{n_1 l_1 m_1}(\mathbf{r}_1) Y_{lm}(\hat{r}). \quad (2)$$

The index ν' serves to identify the initial state $n_1' l_1' l' L M$. In the S -matrix notation, the amplitude function $F_{\nu}(\nu' | r)$ behaves asymptotically as

$$F_{\nu}^S(\nu' | r) \sim k^{-1/2} \{ \exp[-i(kr - \frac{1}{2}l\pi)] \delta_{\nu\nu'} - \exp[i(kr - \frac{1}{2}l\pi)] S_{\nu\nu'} \}, \quad (3)$$

or alternatively

$$F_{\nu}^R(\nu' | r) \sim k^{-1/2} \{ \sin(kr - \frac{1}{2}l\pi) \delta_{\nu\nu'} + \cos(kr - \frac{1}{2}l\pi) R_{\nu\nu'} \}, \quad (4)$$

where the S and R matrices are diagonal in L and M and are related by

$$\mathbf{S} = (\mathbf{1} + i\mathbf{R})(\mathbf{1} - i\mathbf{R})^{-1}. \quad (5)$$

The cross section can be expressed in terms of the collision strength and the T matrix as

$$Q(n_1' l_1' \rightarrow n_1 l_1) = \pi k'^{-2} \Omega(n_1 l_1, n_1' l_1') / (2l_1' + 1),$$

$$\Omega(n_1 l_1, n_1' l_1') = \sum_{l' L} (2L + 1) |T(n_1 l_1 l L, n_1' l_1' l' L)|^2, \quad (6)$$

$$\mathbf{T} \equiv \mathbf{1} - \mathbf{S} = -2i\mathbf{R} / (\mathbf{1} - i\mathbf{R}).$$

The set of coupled differential equations for F is obtained by substituting Eq. (1) into the Schrödinger equation resulting in

$$\left[\frac{d^2}{dr^2} - \frac{l_{\nu}(l_{\nu} + 1)}{r^2} + k_{\nu}^2 \right] F_{\nu}(\nu' | r) = \sum_{\mu} U_{\nu\mu}(r) F_{\mu}(\nu' | r), \quad (7)$$

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¹ N. F. Lane and C. C. Lin, Phys. Rev. **133**, A947 (1964).

² A. Salmona and M. J. Seaton, Proc. Phys. Soc. (London) **77**, 617 (1961).

³ M. J. Seaton, Proc. Phys. Soc. (London) **77**, 174 (1961).

⁴ N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1949), 2nd ed., p. 40.

⁵ I. C. Percival and M. J. Seaton, Proc. Cambridge Phil. Soc. **53**, 654 (1957).

where

$$U_{\nu\mu}(r) = \int \psi_{\nu}^*(\mathbf{r}_1, \hat{r}) [|\mathbf{r}_1 - \mathbf{r}|^{-1} - r^{-1}] \psi_{\mu}(\mathbf{r}_1, \hat{r}) d\mathbf{r}_1 d\hat{r}, \quad (8)$$

subject to the asymptotic boundary condition given in Eqs. (3) or (4). For the numerical treatment of this problem, it is preferable to use Eq. (4) in order to avoid manipulating with complex numbers. The S matrix and the cross section contain all of the R matrix elements; thus, it is necessary to effectively go through the solution n different times where n is the number of channels considered, permuting the initial status successively from channel to channel.

To facilitate the numerical work we shall rewrite $F_{\nu}(\nu' | r)$ in a matrix notation as F_{ij} with the second index designating the initial channel. The differential equations are now

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i(l_i+1)}{r^2} \right] F_{ij} = \sum_{k=1}^n U_{ik} F_{kj}, \quad (9)$$

$$\mathbf{F} = 0 \quad \text{for } r=0, \quad (10)$$

$$\mathbf{F} \sim \mathbf{H}^{(2)} \mathbf{K}^{-1} + \mathbf{H}^{(3)} \mathbf{K}^{-1} \mathbf{R}, \quad (11)$$

where \mathbf{K} , $\mathbf{H}^{(2)}$, and $\mathbf{H}^{(3)}$ are diagonal $n \times n$ matrices defined as

$$\begin{aligned} K_{ij} &= k_i^{1/2} \delta_{ij}, \\ H_{ij}^{(2)} &= \sin(k_i r - \frac{1}{2} l_i \pi) \delta_{ij}, \\ H_{ij}^{(3)} &= \cos(k_i r - \frac{1}{2} l_i \pi) \delta_{ij}. \end{aligned} \quad (12)$$

A method suitable to the solution of linear, second-order differential equations is that due to Numerov.⁶ The standard formula relating the second difference of a function and of its second derivative to the second derivative itself is given to the second order by

$$\delta^2 F_{ij} = (\delta r)^2 [F_{ij}'' + \frac{1}{12} \delta^2 (F_{ij}'')], \quad (13)$$

where δr is the tabular interval. To make use of this equation we note that

$$\delta^2 F_{ij}(r_n) = F_{ij}(r_{n+1}) - 2F_{ij}(r_n) + F_{ij}(r_{n-1}), \quad (14)$$

$$\delta r = r_{n+1} - r_n. \quad (15)$$

To simplify the notation, Eq. (14) will be written as

$$\delta^2 \mathbf{F}_n = \mathbf{F}_{n+1} - 2\mathbf{F}_n + \mathbf{F}_{n-1}. \quad (16)$$

Rewriting Eq. (9) as

$$\mathbf{F}'' = \mathbf{G}\mathbf{F}, \quad (17)$$

$$G_{ij} = [l_i(l_i+1)/r^2 - k_i^2] \delta_{ij} + U_{ij}, \quad (18)$$

and substituting Eqs. (16) and (17) in (13), we get

$$\begin{aligned} \mathbf{F}_{n+1} &= [\mathbf{1} - \frac{1}{12} (\delta r)^2 \mathbf{G}_{n+1}]^{-1} \\ &\times \{ [2\mathbf{1} + \frac{1}{6} (\delta r)^2 \mathbf{G}_n] \mathbf{F}_n - [\mathbf{1} - \frac{1}{12} (\delta r)^2 \mathbf{G}_{n-1}] \mathbf{F}_{n-1} \}. \end{aligned} \quad (19)$$

⁶ D. R. Hartree, *The Calculation of Atomic Structures* (John Wiley & Sons, Inc., New York, 1957), p. 71.

Once solutions are known at two points, Eq. (19) may be used as a recurrence relation to find the solution for all values of r . If the solution is started close enough to the origin, the first term of a Frobenius expansion will suffice. It is easily shown that for problems in which the matrix elements U_{ij} have no singularities of order two or greater at the origin, the solutions for small r which satisfy Eq. (1) are given by

$$\mathfrak{F}_{ij} = \bar{\alpha}_{ij} r^{l_i+1}. \quad (20)$$

In performing the numerical computation, we chose the constants $\bar{\alpha}_{ij}$ in an entirely arbitrary way. The solutions thus obtained will not in general satisfy Eq. (11) and these solutions are denoted by \mathfrak{F}_{ij} . The symbol F_{ij} is reserved for solutions with the appropriate asymptotic behavior. Since the first index in F refers to a particular differential equation in Eq. (7), it is possible to obtain the F 's from a suitable linear combination of the \mathfrak{F} 's, i.e.,

$$F_{ij} = \sum_k c_{kj} \mathfrak{F}_{ik},$$

or

$$\mathbf{F} = \mathfrak{F}\mathbf{C}. \quad (21)$$

The remaining task is to find the matrix \mathbf{C} . Using a given $\bar{\alpha}$ matrix (arbitrarily chosen) we can determine \mathfrak{F} . At large r , we write

$$\mathfrak{F} \sim \mathbf{H}^{(2)} \mathfrak{A} + \mathbf{H}^{(3)} \mathfrak{B}, \quad (22)$$

where $\mathbf{H}^{(2)}$ and $\mathbf{H}^{(3)}$ have been defined in Eqs. (12). The matrices \mathfrak{A} and \mathfrak{B} are found by matching the numerical solution to Eq. (22) for two values of r , say r_a and r_b , large enough so that Eqs. (9) may be replaced by

$$(\frac{d^2}{dr^2} + k_i^2) F_{ij} = 0. \quad (23)$$

The various matrices for $r=r_a$ and $r=r_b$ are designated as \mathfrak{F}_a , \mathfrak{F}_b , $\mathbf{H}_a^{(2)}$, $\mathbf{H}_b^{(2)}$, etc. It is easily shown that

$$\begin{aligned} \mathfrak{A} &= (\mathbf{H}_a^{(3)} \mathbf{H}_b^{(2)} - \mathbf{H}_b^{(3)} \mathbf{H}_a^{(2)})^{-1} \\ &\quad \times (\mathbf{H}_a^{(3)} \mathfrak{F}_b - \mathbf{H}_b^{(3)} \mathfrak{F}_a), \\ \mathfrak{B} &= (\mathbf{H}_a^{(2)} \mathbf{H}_b^{(3)} - \mathbf{H}_b^{(2)} \mathbf{H}_a^{(3)})^{-1} \\ &\quad \times (\mathbf{H}_a^{(2)} \mathfrak{F}_b - \mathbf{H}_b^{(2)} \mathfrak{F}_a). \end{aligned} \quad (24)$$

With the two matrices \mathfrak{A} and \mathfrak{B} available, we can determine \mathbf{C} and therefore \mathbf{R} by comparing Eqs. (21), (22) with (11),

$$\mathbf{C} = (\mathbf{K}\mathfrak{A})^{-1}, \quad (25)$$

$$\mathbf{R} = \mathbf{K}\mathfrak{B}\mathbf{C}. \quad (26)$$

THE $3^2S \rightarrow 3^2P$ TRANSITION OF Na

The numerical method of solution of the Schrödinger equation is now applied to the $3^2S \rightarrow 3^2P$ transition in Na induced by electron impact. In the approximation where the coupling with all other states is ignored, a three-channel problem results. For a given total angular

TABLE I. Partial cross sections for the $3^2S \rightarrow 3^2P$ transition in sodium.^a

l	Q_l in units of πa_0^2														
	$E=4.210$ eV			$E=7.364$ eV			$E=10.520$ eV			$E=16.832$ eV			$E=23.144$ eV		
	Num	RD	B'II	Num	RD	B'II	Num	RD	B'II	Num	RD	B'II	Num	RD	B'II
0	0.01	...	3.18	0.72	...	1.50	0.94	...	0.93	0.54	...	0.51	0.33	...	0.35
1	0.87	...	6.19	1.66	...	3.64	1.49	...	2.62	0.65	...	1.68	0.31	...	1.24
2	15.96	11.79	16.14	6.02	6.54	9.17	2.62	4.31	6.41	0.99	2.69	4.02	0.52	2.04	2.93
3	12.31	11.44	16.43	10.06	10.17	11.67	6.22	7.58	8.37	2.44	4.80	5.26	1.16	3.49	3.81
4	7.94	7.84	10.83	9.52	10.03	11.08	7.16	8.25	8.52	3.72	5.50	5.52	2.03	4.02	4.02
5	4.58	4.52	5.98	7.90	8.18	9.13	6.82	7.44	7.73	4.23	5.29	5.27	2.63	3.93	3.89
6	2.48	2.45	3.08	6.13	6.26	7.01	5.98	6.29	6.61	4.21	4.80	4.81	2.88	3.65	3.62
7	1.30	1.29	1.55	4.59	4.65	5.18	5.01	5.18	5.47	3.92	4.25	4.29	2.88	3.32	3.30
8				3.37	3.40	3.76	4.11	4.21	4.46	3.53	3.72	3.78	2.74	2.98	2.98
9				2.45	2.46	2.70	3.33	3.39	3.59	3.12	3.24	3.30	2.53	2.68	2.69
10							2.68	2.72	2.88	2.73	2.82	2.88	2.30	2.40	2.41
11							2.15	2.18	2.30	2.39	2.45	2.50	2.08	2.15	2.16
12							1.73	1.74	1.83	2.08	2.12	2.17	1.88	1.92	1.94
13										1.81	1.84	1.89	1.69	1.72	1.74
14										1.57	1.60	1.64	1.52	1.55	1.57
15													1.37	1.39	1.41

^a Num, RD, and B'II stand for the numerical method used in this work, the resonance-distortion approximation, and the B'II approximation, respectively.

momentum L , the three coupled states are

- (i) $l_1=0(3s)$, $l=L$,
- (ii) $l_1=1(3p)$, $l=L-1$,
- (iii) $l_1=1(3p)$, $l=L+1$,

where l is the partial wave angular momentum of the colliding electron. To determine the U matrix, the usual hydrogenic wave function with an effective charge of 2.92 was used. This value was chosen so that at large distances the U matrix elements reduce to the same form as those used in the previous works. In order to increase the accuracy of the solutions, the first four terms in a Frobenius expansion were used to start the numerical solution instead of the first term given in Eq. (20). In carrying out the solution it was found satisfactory to use an integration step size of $\delta r=0.1$ and to match the asymptotic expression at $r_A=250$ and $r_B=250.1$.

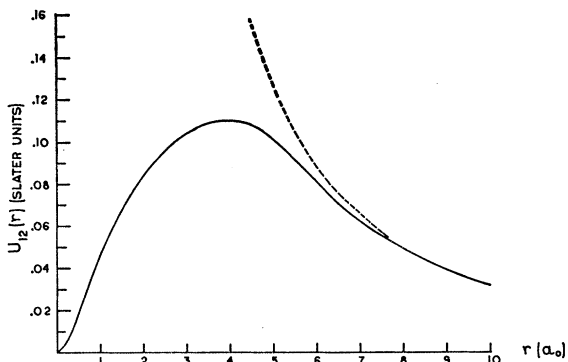


FIG. 1. Comparison of the matrix element $U_{12}(r)$ for $l=2$ as calculated using hydrogenic functions with $Z=2.92$ (solid curve) and the asymptotic form used in B'I, B'II, and RD (dashed curve). Both are in Slater atomic units.

Partial cross sections have been calculated for five incident energies and the results obtained by this numerical procedure, by the resonance-distortion method, and by Seaton's modified version of the Bethe approximation (B'II) are listed in Table I for comparison. The values⁷ of Q_l^{Num} are smaller than Q_l^{RD} of $Q_l^{\text{B'II}}$ and agree better with Q_l^{RD} . For low energies, Q_l^{RD} and Q_l^{Num} agree quite well with each other; in fact, Q_l^{RD} is closer to Q_l^{Num} than it is to $Q_l^{\text{B'II}}$. At higher energies, Q_l^{Num} deviates considerably from Q_l^{RD} and $Q_l^{\text{B'II}}$. This is understandable since in both the resonance-distortion and B'II calculations, the matrix elements U_{12} and U_{13} were replaced by their asymptotic form while the other elements of U which are of shorter range were neglected. For a particular value of l , the classical distance of closest approach is given by

$$r_i^2 = l(l+1)/k^2,$$

which increases with decreasing 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

TABLE II. Total inelastic cross sections for the $3^2S \rightarrow 3^2P$ transition in Na.

E (eV)	Q in units of πa_0^2			
	Num	RD	B'II	B'I
4.210	46.8	47.1	64.9	288.63
7.364	58.7	61.7	71.6	231.87
10.520	57.2	62.9	68.9	189.12
16.832	48.9	57.7	60.5	139.19
23.144	42.1	51.6	53.3	111.26

⁷ Here we have replaced the index L by l in order to facilitate comparison with other works as was done in Ref. 1.

behavior of the elements $U_{ij}(r)$ near the origin. As an illustration, a plot of $U_{12}(r)$ used in this work along with its approximate asymptotic form which was used for the resonance-distortion and B'II calculations, is shown in Fig. 1. It is interesting to note that the total cross sections calculated by the Born approximation are always smaller than those from the Bethe method B'I, and are even smaller than the B'II cross sections at energies above 20 eV. Here again replacing the interaction potential matrix elements by their asymptotic inverse-square form results in an increase of the cross sections.

Since the B'I approximation is valid for large values of l , this may be used in conjunction with the partial cross sections in Table I to calculate total inelastic cross sections. In Table II are given total cross sections calculated by means of our numerical method, resonance-distortion, B'I, and B'II approximations. Comparison of the theoretical excitation functions with the experimental data⁸ is shown in Fig. 2. The results

⁸ G. Haft, Z. Physik 82, 73 (1933); W. Christoph, Ann. Physik 23, 51 (1935); D. R. Bates, A. Fundaminsky, and H. S. W.

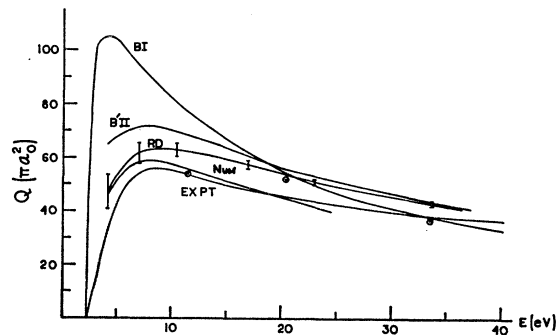


FIG. 2. Total cross sections for the $3s \rightarrow 3p$ transition in Na calculated by the methods BI, B'II, RD, and Num, and absolute measurements of Christoph, designated by the circled points, and relative measurements of Haft, represented by the curve EXPT. The Born cross section (BI) was given by Bates *et al.* (Ref. 8).

of the numerical method show better agreement with experiment than do those of the previous calculations.

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Matrix Elements of a Fermion System in a Representation of Correlated Basis Functions*

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The ground state and low excited states of liquid He^3 (and other fermion systems) can be constructed from a set of basis functions

$$\Psi(|\mathbf{n}\rangle) = \psi_0^B \Phi(|\mathbf{n}\rangle)$$

in which ψ_0^B is the ground-state boson-type solution of the Schrödinger equation and the model functions $\Phi(|\mathbf{n}\rangle)$ are Slater determinants suitable for describing states of the noninteracting Fermion system. Diagonal and nondiagonal matrix elements of the identity and the Hamiltonian operator are evaluated by a cluster-expansion technique. An orthonormal basis system is constructed from $\Psi(|\mathbf{n}\rangle)$ and used to express the Hamiltonian operator in quasiparticle form: a large diagonal component containing constant, linear, quadratic, and cubic terms in free-quasiparticle occupation-number operators and a nondiagonal component representing the residual interactions involved in collisions of two and three free quasiparticles.

I. INTRODUCTION

SIMPLE correlated trial functions have proved useful in the study of nuclear matter and the He^3 and He^4 liquids.¹⁻³ The theory begins with a model function Φ

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⁵ R. Abe, Progr. Theoret. Phys. (Kyoto) 19, 57, 407 (1958).

⁶ F. Y. Wu and E. Feenberg, Phys. Rev. 122, 739 (1961).

⁷ H. W. Jackson and E. Feenberg, Ann. Phys. (N. Y.) 15, 266 (1961).

⁸ K. Kumar, *Perturbation Theory and Nuclear Many Body Problem* (Interscience Publishers, Inc., New York, 1962), Chap. V.

describing a state of the N -particle system in the absence of interactions. The model is adapted to the presence of strong short-range repulsive interactions by introducing a symmetrical positive valued correlation factor $\exp \frac{1}{2} S(1, 2, \dots, N)$ which vanishes when any two particles approach closely. The resulting trial function is

$$\Psi = e^{S(1, 2, \dots, N)/2} \Phi(1, 2, \dots, N). \quad (1)$$

A linear combination of such correlated trial functions provides the possibility of a close approach to exact solutions of the many-particle problem. Construction of a suitable trial (or basis) system may start from a set of normalized orthogonal model functions Φ_n , generated by properly symmetrized products of single-particle orbitals. In the applications the functions Ψ_n are used to construct matrix elements of the identity and the Hamiltonian operator. One recognizes that the functions