We believe that this size effect is not due merely to a limiting of the electron mean free path by imperfections or the surface. One of us[4] has shown experimentally that T_1 is relatively insensitive to quantities of impurities sufficient to shorten the mean free path to a value comparable to particle diameters used in the present experiment. These experiments on impure superconductors also tend to rule out the possibility that we are observing a spin diffusion limited flow of energy to nuclei having a large quadrupolar specific heat as a result of lattice imperfections.[9]

It would obviously be interesting to study other properties of these small particles.

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Inelastic Electron-Atom Collisions under Near-Resonance Conditions: Analysis of Transitions Involving Strong Coupling*

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A method has been devised to calculate the cross sections of inelastic electron-atom collisions under near-resonance conditions. This method (referred to as the method of resonance distortion) consists of solving the limiting exact-resonance problem as the zeroth-order approximation and using this solution to obtain the first-order solution by an iteration procedure, and is particularly suitable for treating optically allowed transitions produced by electron impact where the coupling between the initial and final states is strong and of long-range type. Application of this method has been made to a schematic model with an isotropic inverse-square interaction potential and to the problem of electron-atom collisions with $ns \rightarrow np$ transition. The general results indicate that (i) for weak coupling the collision strengths calculated by the resonance-distortion scheme reduce to those calculated by the method of distorted waves, (ii) the resonance-distortion method and Seaton's B'II method give nearly equal partial cross sections for large l, and (iii) at very low l, the B'II partial cross sections are substantially larger than those determined from the resonance-distortion method. The total cross sections for the $3s \rightarrow 3p$ transition in Na have been calculated by the resonance-distortion method for various incident electron energies, and the results show better agreement with experiment than do those of the Born approximation and of Seaton's version of the modified Born approximation.

I. INTRODUCTION

In the treatment of the inelastic collisions between electrons and atoms, the Born approximation, which consists of using the wave function of a free particle to obtain the first-order solution of the Schrödinger equation, is quite extensively employed.[1,2] However, when there exists a strong coupling between the initial and the final states of the atomic system, the Born approximation generally yields poor results.[3–7] The reasons for the failure of the usual Born approximation have been discussed by Seaton and modifications of the approximate method have been proposed.[4–7] The problem of the calculation of inelastic collision cross sections becomes more complicated when the change of energy in the atom is rather small (near resonance), because in such cases the expansion of the total cross section in terms of the phase shifts of the partial waves do not always converge rapidly and accurate calculations of more partial-wave cross sections are needed. In this paper we shall present a method for the calculation of cross sections for inelastic collisions under near-resonance conditions. In essence this is an iteration procedure in which we use the solution of the exact resonance problem as the zeroth-order approximation.

Consider an electron with linear momentum $\hbar\mathbf{k}_0$ 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 $\mathbf{r}'$ and the potential energy between the electron and the atom by $V(\mathbf{r},\mathbf{r}')$. If the wave func-

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[1] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, England, 1949), 2nd ed.
[2] H. S. W. Massey, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 36, p. 233.
[3] H. S. W. Massey, Rev. Mod. Phys. **28**, 199 (1956).
[4] M. J. Seaton, Proc. Phys. Soc. (London) **68**, 457 (1955).
[5] M. J. Seaton, Rev. Mod. Phys. **30**, 70 (1958).
[6] M. J. Seaton, Proc. Phys. Soc. (London) **77**, 174 (1961).
[7] M. J. Seaton, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic Press Inc., New York, 1962), p. 374.

tion of the system is written as[1]

$$\Psi(\mathbf{r},\mathbf{r}')=\sum_i F_i(\mathbf{r})\psi_i(\mathbf{r}'), \quad (1)$$

the Schrödinger equation may be decomposed into

$$(\nabla^2+k_i^2)F_i(\mathbf{r})=\sum_j U_{ij}(\mathbf{r})F_j(\mathbf{r}), \quad (2)$$

where

$$U_{ij}(\mathbf{r})=(2M/\hbar^2)V_{ij}(\mathbf{r})$$

$$=(2M/\hbar^2)\int\psi_i^*(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\psi_j(\mathbf{r}')d\mathbf{r}', \quad (3)$$

$$k_i^2=k_0^2+2M(E_0-E_i)/\hbar^2. \quad (4)$$

Here we have neglected the effect of electron exchange. This point will be discussed in Sec. VIII. The solutions of these differential equations are subject to the asymptotic conditions

$$F_0(\mathbf{r})\sim\exp(i\mathbf{k}_0\cdot\mathbf{r})+r^{-1}f_0(\theta,\phi)\exp(ik_0r),$$
$$F_i(\mathbf{r})\sim r^{-1}f_i(\theta,\phi)\exp(ik_ir). \quad (5)$$

In collision-induced transitions $0\rightarrow n$ for which the coupling between two states is strong, it is often permissible to treat only two equations, i.e.,

$$(\nabla^2+k_0^2-U_{00})F_0=U_{0n}F_n, \quad (6)$$

$$(\nabla^2+k_n^2-U_{nn})F_n=U_{n0}F_0. \quad (7)$$

In case of exact resonance, viz., $U_{00}=U_{nn}$, $E_0=E_n$, these two equations may be decoupled,[1] and for some special cases of U_{00}, U_{nn}, and U_{0n}, exact solutions of F_0 and F_n can be found. For problems involving near resonance, it is no longer possible to decouple F_0 and F_n, and our approximate method consists of inserting in Eq. (7) the $F_0^{(0)}$ obtained from the limiting exact-resonance problem and solving for F_n from Eq. (7). It is interesting to compare this procedure with the method of distorted waves[1] in which one solves for F_0 by omitting the $U_{0n}F_n$ term in Eq. (6) and then uses this F_0 in Eq. (7) to determine F_n. Thus, our method and the method of distorted waves represent two different iteration approaches; the former assumes a close coupling solution as the zeroth-order approximation and the latter starts with zero coupling. Detailed applications of our method, which will be referred to as the method of resonance distortion, are described in the following sections.

II. APPROXIMATE FORMS OF THE INTERACTION POTENTIAL

In this paper we shall be concerned primarily with the special class of electron-atom collisions which involves (i) strong coupling, (ii) a long-range interaction potential, and (iii) near resonance, although our iteration scheme is not restricted to this type of problem. It has been pointed out by Seaton[6] that certain collision-induced transitions of the type n', l, $m'\rightarrow n$, $l\pm1$, m show strong coupling with long-range interactions. In many instances, if we are dealing only with single excitation, the wave function of the atom can be represented approximately by the one-electron orbital of the excited electron $\psi_{nlm}(\mathbf{r}')=R_{nl}(r')Y_{lm}(\hat{r}')$. [This is, of course, not always valid, especially for the cases where the exchange effects of the atomic electrons must be taken into consideration, e.g., He($2\,^3S\rightarrow 2\,^3P$). However, extension of the treatment in this section to these cases can be made very easily and will not be considered here.] Choosing $\mathbf{k}_0$ as the axis of quantization and using atomic units, we have, according to Eq. (3),

$$U_{n0}(\mathbf{r})=2\int\psi_{nlm}^*(\mathbf{r}')(-1/r+1/|\mathbf{r}-\mathbf{r}'|)\psi_{n'l'm'}(\mathbf{r}')d\mathbf{r}'$$

$$=\sum_{\lambda=0}^{\infty}(8\pi/2\lambda+1)y_\lambda(nl,n'l'|r)$$

$$\times\sum_{\mu=-\lambda}^{\lambda}h_{\lambda\mu}(lm,l'm')Y_{\lambda\mu}^*(\hat{r}), \quad (8)$$

where

$$h_{\lambda\mu}=\int Y_{lm}^*(\hat{r}')Y_{\lambda\mu}(\hat{r}')Y_{l'm'}(\hat{r}')d\hat{r}',$$

and

$$y_\lambda(nl,n'l'|r)=(1/r^{\lambda+1})\int_0^r R_{nl}(r_0)r_0^{\lambda+2}R_{n'l'}(r_0)dr_0$$

$$+r^\lambda\int_r^\infty R_{nl}(r_0)r_0^{1-\lambda}R_{n'l'}(r_0)dr_0\sim s_\lambda(nl,n'l')/r^{\lambda+1}. \quad (9)$$

The long-range behavior is apparent from the fact that for large r

$$y_1(n\ l\pm1,n'l|r)\sim s_1(n\ l\pm1,n'l)/r^2, \quad (10)$$

where s_1^2 is the line strength, i.e.,

$$s_1(n\ l\pm1,n'l)=\int_0^\infty R_{n\ l\pm1}(r_0)R_{n'l}(r_0)r_0^3dr_0. \quad (11)$$

In a similar way we can calculate $U_{00}(\mathbf{r})$ and $U_{nn}(\mathbf{r})$. These functions diverge at $r=0$ and drop rapidly toward zero for increasing r.

Near-resonance occurs for transitions between the same n, i.e., $nl\rightarrow n\ l\pm1$. Here, a significant contribution to the total cross section comes from the partial waves of large l, and the effects of U_{ij} at small distances are unimportant. Thus in the $ns\rightarrow np$ transition we shall make the simplification of replacing the true interaction potentials by

$$U_{00}=U_{nn}=0,$$
$$U_{0n}=(2M/\hbar^2)\tfrac{2}{3}\pi^{1/2}Y_{1m}(\theta,\phi)s/r^2. \quad (12)$$

The same set of potential functions was used by Seaton in deriving the close-coupling formula[4] and the modified version of Bethe's approximation.[6] Throughout the

calculation 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 resonance-distortion method (see Sec. VIII).

III. SCHEMATIC MODEL

Before proceeding to the solution of Eqs. (6) and (7) with potential functions (12), it is instructive to consider a schematic model in which it is assumed

$$U_{00}=U_{nn}=0,$$
$$U_{0n}=-A/r^2, \tag{13}$$

with A being an adjustable parameter. With Eqs. (13) as the interaction potentials it is possible to obtain exact solutions for F_0 and F_n in the limiting case of exact resonance. The U_{0n} in the schematic model can be thought of as representing some kind of angular average of the U_{0n} in Eqs. (12). With the proper value of A, the schematic model may be expected to give the same total cross section as that produced by the angular-dependent potential. This indeed has been demonstrated by Seaton.[4]

1. Exact Resonance

In the case of exact resonance ($E_0=E_n$), it is possible to decouple Eqs. (6) and (7) by introducing[1]

$$F^{\pm}=F_0\pm F_n, \tag{14}$$

which satisfy the differential equations

$$(\nabla^2+k_0^2\pm A/r^2)F^{\pm}=0. \tag{15}$$

With the usual partial-wave expansion

$$F^{\pm}(\mathbf{r})=r^{-1}\sum_l i^l(2l+1)F_l^{\pm}(r)P_l(\cos\theta), \tag{16}$$

where θ is the angle between $\mathbf{r}$ and $\mathbf{k}_0$, we obtain

$$\left[\frac{d^2}{dr^2}+k_0^2-(p_\pm^2-\tfrac{1}{4})/r^2\right]F_l^{\pm}(r)=0,$$
$$p_\pm=[(l+\tfrac{1}{2})^2\mp A]^{1/2}, \tag{17}$$

and

$$F_l^{\pm}=a_\pm(\pi r/2k_0)^{1/2}J_{p_\pm}(k_0r). \tag{18}$$

Here $J_{p_\pm}(k_0r)$ is the Bessel function of the first kind of order $p_\pm$, and $a_\pm$ are constant coefficients. At a large distance it is required that

$$F_{0,l}=\tfrac{1}{2}(F_l^{+}+F_l^{-})\sim\sin(k_0r-\tfrac{1}{2}l\pi)+c_{0,l}\exp(ik_0r),$$
$$F_{n,l}=\tfrac{1}{2}(F_l^{+}-F_l^{-})\sim c_{n,l}\exp(ik_0r), \tag{19}$$

which are satisfied by choosing

$$a_+\exp(\tfrac{1}{2}ip_+\pi)+a_-\exp(\tfrac{1}{2}ip_-\pi)=2i\exp(\tfrac{1}{2}il\pi-\tfrac{1}{4}i\pi),$$
$$a_-=a_+\exp[\tfrac{1}{2}i\pi(p_+-p_-)]. \tag{20}$$

The solutions of $F_{0,l}$ and $F_{n,l}$ can then be obtained from Eqs. (18) and (20), e.g.,

$$F_{0,l}=\tfrac{1}{2}i^{l+1}(\pi r/2k_0)^{1/2}\exp(-\tfrac{1}{4}i\pi)[J_{p_+}(k_0r)\times\exp(-\tfrac{1}{2}ip_+\pi)+J_{p_-}(k_0r)\exp(-\tfrac{1}{2}ip_-\pi)]. \tag{21}$$

The partial cross section corresponding to excitation can be calculated from $F_{n,l}$ as

$$Q_l(0\to n)=\pi k_0^{-2}(2l+1)\sin^2\tfrac{1}{2}\pi(p_+-p_-). \tag{22}$$

Here $\frac{1}{2}\pi p_+$ and $\frac{1}{2}\pi p_-$ may be identified with the conventional partial phase shifts η_l and δ_l.[8] In the case of exact resonance with the schematic model, the total cross section diverges. This divergence is removed when the energy difference of the two states ΔE is taken into consideration. Also, it may be added that the solution presented here is valid only when $p_\pm$ are both real.[9] For the very small values of l where $(l+\frac{1}{2})^2<A$, the partial cross sections must be determined by other means.

2. Inexact Resonance

When $E_0\neq E_n$, the two differential equations in Eqs. (6) and (7) can no longer be completely decoupled. A partial-wave expansion analogous to Eq. (16) gives

$$\left[\frac{d^2}{dr^2}+k_n^2-l(l+1)/r^2\right]F_{n,l}=-AF_{0,l}/r^2. \tag{23}$$

Making use of a standard variation of parameters procedure,[1] one obtains

$$F_{n,l}\sim k_n^{-1}\exp i(k_nr-\tfrac{1}{2}l\pi)\int_0^\infty(\tfrac{1}{2}\pi k_nr)^{1/2}J_{l+\frac{1}{2}}(k_nr)\times(-A/r^2)F_{0,l}(r)dr=c_{n,l}\exp(ik_nr). \tag{24}$$

The collision amplitude is then given simply by

$$f_n(\theta)=k_n^{-1}\sum_l(2l+1)\times\left[\int_0^\infty(\tfrac{1}{2}\pi k_nr)^{1/2}J_{l+\frac{1}{2}}(k_nr)(-A/r^2)F_{0,l}(r)dr\right]\times P_l(\cos\theta). \tag{25}$$

As a first-order approximation, we simply replace $F_{0,l}$ in the integrand of Eq. (25) by $F_{0,l}^{(0)}$ calculated for the case of exact resonance. Upon inserting $F_{0,l}^{(0)}$ from Eq. (21) into Eq. (25), we determine the inelastic collision amplitude to be

$$f_n(\theta)=-\tfrac{1}{4}A\pi(k_0k_n)^{-1/2}\times\exp(-\tfrac{1}{4}i\pi)\sum_l i^l(2l+1)[I_l^{+}\exp(-\tfrac{1}{2}ip_+\pi)+I_l^{-}\exp(-\tfrac{1}{2}ip_-\pi)]P_l(\cos\theta), \tag{26}$$

[8] See Ref. 1, p. 148.
[9] See Ref. 1, p. 40.

where

$$I_l^{\pm}=\int_0^{\infty} J_{l+\frac{1}{2}}(k_n r)J_{p_\pm}(k_0 r)r^{-1}dr.$$

It follows then in a straightforward manner that the partial cross sections for the schematic model under conditions of near-resonance are given by

$$Q_l(0\rightarrow n)=\pi k_0^{-2}(\tfrac{1}{2}\pi A)^2(2l+1)[(I_l^{+})^2+(I_l^{-})^2 +2I_l^{+}I_l^{-}\cos\tfrac{1}{2}(p_+-p_-)\pi]. \quad (27)$$

It may be easily shown that if one lets $k_0=k_n$, $Q_l(0\rightarrow n)$ reduces to the partial cross section for exact resonance, which was given in Eq. (22). It may also be shown that for large values of l, $Q_l(0\rightarrow n)$ approaches

$$Q_l(0\rightarrow n)=\pi k_0^{-2}(\pi A)^2(2l+1) \times\left|\int_0^{\infty} J_{l+\frac{1}{2}}(k_0 r)J_{l+\frac{1}{2}}(k_n r)r^{-1}dr\right|^2, \quad (28)$$

which is equivalent to the partial cross section gotten by applying the Born approximation to the schematic model.[4] It should also be pointed out that if A is reduced to zero in the zeroth order, then $F_0^{(0)}$ becomes simply $\exp(i\mathbf{k}_0\cdot\mathbf{r})$, and the first-order result $Q_l(0\rightarrow n)$ becomes identical to that determined by the Born approximation for all l. This may be seen most easily by taking $p_+=p_-=l+\frac{1}{2}$ in Eqs. (26) and (27).

The integrals involved may be evaluated in terms of hypergeometric functions ${}_2F_1$, which in turn may be determined by their power-series representation. We have then[10]

$$I_l^{\pm}=\tfrac{1}{2}(k_n/k_0)^{l+\frac{1}{2}}\Gamma\{(a_\pm)/\Gamma(a_\pm+b_\pm+1)\Gamma(1-b_\pm)\} \times{}_2F_1[a_\pm, b_\pm; a_\pm+b_\pm+1; (k_n/k_0)^2], \quad (29)$$

where

$$a_\pm=\tfrac{1}{2}(p_\pm+l+\tfrac{1}{2}),$$
$$b_\pm=\tfrac{1}{2}(l+\tfrac{1}{2}-p_\pm),$$
$$a_\pm+b_\pm+1=l+\tfrac{3}{2}.$$

Typical curves, representing partial cross sections for $A=3.0$ and different energy separations ΔE, are given in Fig. 1. The values of Q_l are seen to increase steadily with decreasing ΔE, the maximum occurring for $\Delta E=0$. It is important to notice that these partial cross sections remain below the maximum allowed by conservation. The partial cross sections for $l=0$ and $l=1$ are not shown since they cannot be calculated by this scheme.

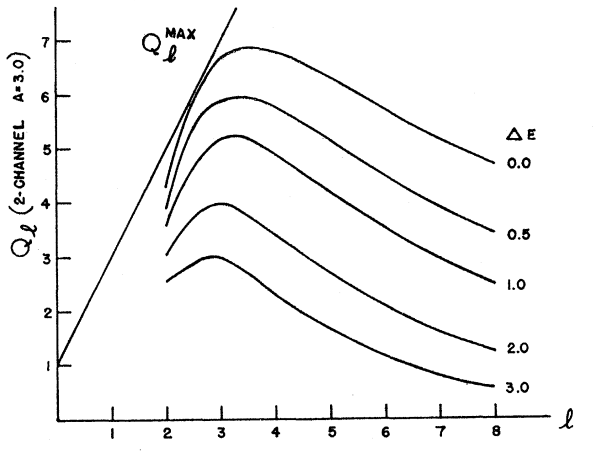

FIG. 1. Partial cross sections Q_l for different values of ΔE(eV) and $A=3.0$ calculated by using the schematic model.

IV. ATOM-ELECTRON COLLISIONS

We shall now return to the solution of atom-electron collisions by means of the resonance-distortion method. In particular, we shall consider the transition $ns\rightarrow np$. Since U_{0n} is now angular-dependent, when we express the total wave function in terms of the products of the atomic wave function and the F function of the colliding electron followed by a partial-wave expansion of F, an infinite set of coupled differential equations for the partial-wave amplitudes will result. Percival and Seaton[11] have suggested that considerable simplification can be achieved by taking advantage of the fact that the total angular momentum of the atomic and colliding electron is a constant of motion. Denoting the angular momentum quantum numbers of the atomic and the colliding electron as l_1m_1 and lm, respectively, we shall construct eigenfunctions of the total angular momentum $L\,M$ as

$$\psi_\nu(\mathbf{r}_1,\hat{r})=\textstyle\sum_{m_1m} C_{m_1mM}^{l_1lL}\psi_{n_1l_1m_1}(\mathbf{r}_1)Y_{lm}(\hat{r}), \quad (30)$$

where ν stands for the group of quantum numbers $n_1l_1lL\,M$, and C is the Clebsch-Gordan coefficient. The wave function of the whole system is then expanded as

$$\Psi(\nu'|\mathbf{r}_1,\mathbf{r})=r^{-1}\textstyle\sum_\nu F_\nu(\nu'|r)\psi_\nu(\mathbf{r}_1,\hat{r}). \quad (31)$$

The index ν' is introduced to remind us that the system represented by this wave function was initially in a state characterized by ν'. In other words, the asymptotic form of $F_\nu(\nu'|r)$ for $r\rightarrow\infty$ is

$$F_\nu(\nu'|r)\sim k^{-\frac{1}{2}}\{\exp[-i(kr-\tfrac{1}{2}l\pi)]\delta_{\nu\nu'} -\exp[i(kr-\tfrac{1}{2}l\pi)]S_{\nu\nu'}\}, \quad (32)$$

in terms of the S matrix, or alternatively

$$F_\nu(\nu'|r)\sim k^{-\frac{1}{2}}\{\sin(kr-\tfrac{1}{2}l\pi)\delta_{\nu\nu'} +\cos(kr-\tfrac{1}{2}l\pi)R_{\nu\nu'}\}, \quad (33)$$

where the S and R matrices are related by the equation

$$\mathbf{S}=(\mathbf{1}+i\mathbf{R})/(\mathbf{1}-i\mathbf{R}), \quad (34)$$

[10] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, London, England, 1944), 2nd ed., p. 404.

[11] I. C. Percival and M. J. Seaton, Proc. Cambridge Phil. Soc. 53, 654 (1957).

and the S matrix is diagonal in L and M. When Eq. (31) is substituted into the Schrödinger equation, one obtains a series of differential equations for F_ν. However, F_ν and $F_{\nu'}$ are coupled together only if ν and ν' correspond to the same values of L and M.

Upon introducing the T matrix defined by

$$\mathbf{T}\equiv\mathbf{1}-\mathbf{S}=-2i\mathbf{R}/(\mathbf{1}-i\mathbf{R}), \tag{35}$$

one can express the cross section for the $n_1'l_1'\rightarrow n_1l_1$ transition as

$$\begin{aligned}Q(n_1'l_1'\rightarrow n_1l_1)&=\pi k'^{-2}\Omega(n_1l_1,n_1'l_1')/(2l_1'+1)\\&=\pi k'^{-2}\sum_{ll'L}(2L+1)\\&\quad\times|T(n_1l_1lL,n_1'l_1'l'L)|^2/(2l_1'+1),\end{aligned} \tag{36}$$

where $\Omega(n_1l_1,n_1'l_1')$ is the collision strength for the transition $n_1'l_1'\rightarrow n_1l_1$.

Let us now consider an $ns\rightarrow np$ transition and neglect the interactions with all other states. To obtain a given total angular momentum L, one can take three different combinations of l_1 and l as follows:

$$\begin{aligned}&(1)\ l_1=0,\quad l=L\\&(2)\ l_1=1,\quad l=L-1\\&(3)\ l_1=1,\quad l=L+1.\end{aligned} \tag{37}$$

Three coupled differential equations then result corresponding to these three channels. If we designate the F function of channels (1), (2), and (3) by F_1, F_2, and F_3, these equations are

$$\left[\frac{d^2}{dr^2}+k_0^2-L(L+1)/r^2\right]F_1=L^{1/2}\beta r^{-2}F_2-(L+1)^{1/2}\beta r^{-2}F_3, \tag{38}$$

$$\left[\frac{d^2}{dr^2}+k_n^2-L(L-1)/r^2\right]F_2=L^{1/2}\beta r^{-2}F_1, \tag{39}$$

$$\left[\frac{d^2}{dr^2}+k_n^2-(L+1)(L+2)/r^2\right]F_3=-(L+1)^{1/2}\beta r^{-2}F_1, \tag{40}$$

where

$$\beta=2s_1(np,ns)/[3(2L+1)]^{1/2}. \tag{41}$$

The collision strength is

$$\Omega(np,ns)=\textstyle\sum_L(2L+1)\{|T_{12}|^2+|T_{13}|^2\}, \tag{42}$$

where the indices 1, 2, 3 refer to the respective channels.

1. Zeroth-Order Approximation

The zeroth-order solution is obtained by setting $k_0=k_n$ in Eqs. (38), (39), and (40). When this is done, the three differential equations can be decoupled by a linear transformation.[6] This can be seen by writing the three equations in matrix form as

$$r^2\left(\frac{d^2}{dr^2}+k_0^2\right)\mathbf{F}=\mathbf{AF}, \tag{43}$$

where $\mathbf{F}$ is a vector with components F_1, F_2, F_3, and $\mathbf{A}$ is the square matrix

$$\mathbf{A}=\begin{bmatrix}L(L+1) & L^{1/2}\beta & -(L+1)^{1/2}\beta\\ L^{1/2}\beta & L(L-1) & 0\\ -(L+1)^{1/2}\beta & 0 & (L+1)(L+2)\end{bmatrix}. \tag{44}$$

To solve Eqs. (43) we diagonalize $\mathbf{A}$ by means of the transformation $\mathbf{X}$, so that Eq. (43) becomes

$$r^2[(d^2/dr^2)+k_0^2]\mathbf{G}=\mathbf{aG}, \tag{45}$$

where $\mathbf{a}=\mathbf{X}^{-1}\mathbf{AX}$ and $\mathbf{G}=\mathbf{X}^{-1}\mathbf{F}$. The eigenvalues of $\mathbf{a}$ are

$$\begin{aligned}a_1&=L(L+1),\\a_2&=L^2+L+1-(2L+1)x,\\a_3&=L^2+L+1+(2L+1)x,\end{aligned} \tag{46}$$

where

$$x=[1+\beta^2/(2L+1)]^{1/2}, \tag{47}$$

and the matrix $\mathbf{X}$ is

$$\mathbf{X}=\begin{bmatrix}\xi_1 & \xi_2 & \xi_3\\ L^{1/2}\beta\xi_1/2L & L^{1/2}\beta\xi_2/(2L+1)(1-x) & L^{1/2}\beta\xi_3/(2L+1)(1+x)\\ (L+1)^{1/2}\beta\xi_1/2(L+1) & (L+1)^{1/2}\beta\xi_2/(2L+1)(1+x) & (L+1)^{1/2}\beta\xi_3/(2L+1)(1-x)\end{bmatrix}, \tag{48}$$

where

$$\begin{aligned}\xi_1^2&=4L(L+1)/[4L(L+1)+\beta^2(2L+1)],\\\xi_2^2&=\beta^2/2(\beta^2+2L+1-x),\\\xi_3^2&=\beta^2/2(\beta^2+2L+1+x).\end{aligned} \tag{49}$$

The procedure now is to choose solutions to the decoupled equations having the proper asymptotic behavior and then transform back to $\mathbf{F}$. To investigate the asymptotic behavior, we note that

$$G_i=\textstyle\sum_j(\mathbf{X}^{-1})_{ij}F_j=\sum_j X_{ji}F_j. \tag{50}$$

Considering the asymptotic form of F_j, we find that $(k_0=k_n)$

$$\begin{aligned}G_i\sim k_0^{-\frac{1}{2}}\{&X_{1i}(-2i)\sin(k_0r-\tfrac{1}{2}l\pi)\\&+X_{1i}T_{11}\exp[i(k_0r-\tfrac{1}{2}l\pi)]\\&+X_{2i}T_{21}\exp[i(k_0r-\tfrac{1}{2}l\pi)]\\&+X_{3i}T_{31}\exp[i(k_0r-\tfrac{1}{2}l\pi)]\}.\end{aligned} \tag{51}$$

Thus the solutions of G_i which conform to the proper boundary conditions are

$$G_1=-2iX_{11}(\tfrac{1}{2}\pi r)^{1/2}J_{L+\frac{1}{2}}(k_0r), \tag{52}$$

$$G_2=-2iX_{12}\exp[\tfrac{1}{2}i\pi(L-\mu_2)](\tfrac{1}{2}\pi r)^{1/2}J_{\mu_2+\frac{1}{2}}(k_0r), \quad (53)$$

$$G_3=-2iX_{13}\exp[\tfrac{1}{2}i\pi(L-\mu_3)](\tfrac{1}{2}\pi r)^{1/2}J_{\mu_3+\frac{1}{2}}(k_0r). \quad (54)$$

Here we have used the abbreviations

$$\mu_2=-\tfrac{1}{2}+[(L-\tfrac{1}{2})^2-C]^{1/2},$$
$$\mu_3=-\tfrac{1}{2}+[(L+\tfrac{3}{2})^2+C]^{1/2}, \quad (55)$$

where

$$C=(2L+1)(x-1), \quad C\geqslant(L-\tfrac{1}{2})^2.$$

The phase factors are due to the assignment of phase in the definition of the S matrix.

The functions F_1, F_2, F_3 may now be determined by transforming the G matrix to $\mathbf{F}$. In particular, for F_1 we obtain

$$F_1(r)=-2i(\tfrac{1}{2}\pi r)^{1/2}\{X_{11}^2J_{L+\frac{1}{2}}(k_0r)+X_{12}^2J_{\mu_2+\frac{1}{2}}(k_0r)\exp[\tfrac{1}{2}i\pi(L-\mu_2)]+X_{13}^2J_{\mu_3+\frac{1}{2}}(k_0r)\exp[\tfrac{1}{2}i\pi(L-\mu_3)]\}. \quad (56)$$

2. Resonance-Distortion Approximation

The approximation is now made of replacing $F_1(r)$ in Eqs. (39) and (40) by $F_1(r)$ calculated in the previous section, i.e., for the case of exact resonance. The collision strength obtained by the resonance-distortion scheme becomes

$$\Omega^{\mathrm{RD}}(np,ns)=\tfrac{4}{3}(\pi s)^2\sum_L\{L|I(L,L-1)|^2+(L+1)|I(L,L+1)|^2\}, \quad (57)$$

where

$$I(L,L\pm1)=\xi_1^2H^{(1)}(L,L\pm1)+\xi_2^2H^{(2)}(L,L\pm1)\exp[\tfrac{1}{2}i\pi(L-\mu_2)]+\xi_3^2H^{(3)}(L,L\pm1)\exp[\tfrac{1}{2}i\pi(L-\mu_3)], \quad (58)$$

and

$$H^{(i)}(L,L\pm1)=\int_0^\infty J_{p_i}(k_0r)J_{L\pm1+\frac{1}{2}}(k_nr)r^{-1}dr, \quad (59)$$

$$p_i=\mu_i+\tfrac{1}{2}, \quad (\mu_1\equiv L).$$

The integrals $H^{(i)}(L,L\pm1)$ may be expressed in terms of hypergeometric functions as[10]

$$H^{(i)}(L,L\pm1)=\tfrac{1}{2}(k_n/k_0)^{L\pm1+\frac{1}{2}}\times\{\Gamma[a_i(L\pm1)]/\Gamma[c_i(L\pm1)]\Gamma[1-b_i(L\pm1)]\}\times{}_2F_1[a_i(L\pm1),b_i(L\pm1);c_i(L\pm1);(k_n/k_0)^2], \quad (60)$$

where

$$a_i(L\pm1)=\tfrac{1}{2}[(L\pm1)+p_i+\tfrac{1}{2}],$$
$$b_i(L\pm1)=\tfrac{1}{2}[(L\pm1)-p_i+\tfrac{1}{2}], \quad (61)$$
$$c_i(L\pm1)=L\pm1+\tfrac{3}{2}.$$

It has been verified that in the limit of exact resonance ($k_0\rightarrow k_n$), the collision strength given in Eq. (57) does agree exactly with that determined by Seaton's formulas.[6] Again the results here are valid only for those values of L which satisfy the inequality in Eqs. (55).

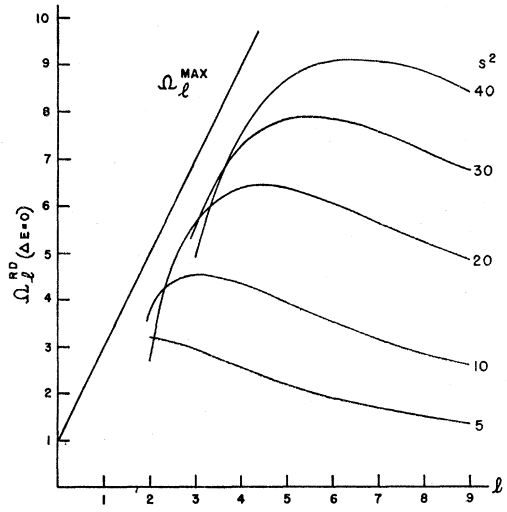

FIG. 2. Collision strengths Ω_l^{RD} in the case of exact resonance for several values of the line strength s^2.

V. GENERAL RESULTS

In the previous section a technique was presented whereby inelastic cross sections for collision-induced transitions under near-resonance conditions could be determined. It is now wished to investigate the general behavior of these cross sections for different degrees of coupling and resonance and to compare them with the results obtained from other methods of calculation.

1. Effect of the Magnitude of Coupling

In Fig. 2 the collision strength for $ns\rightarrow np$ transition with *exact* resonance is given for several values of the line strength s^2 (s^2 is a measure of the strength of coupling). The cross sections with $l=0$ and 1 cannot be calculated by the scheme outlined in the previous section, since they violate the inequality in Eqs. (55). It has been shown that for exact-resonance collisions, as one increases the strength of coupling (from weak coupling), the transfer probability first increases rapidly, then reaches a certain saturation stage, and finally behaves in an oscillatory manner.[12] For a given l, such saturation and oscillation behavior can be seen from the convergence of the points corresponding to larger values of s along each vertical line in Fig. 2. (Here we have replaced the expansion index L by l in order to facilitate comparisons with other works.) This can be illustrated more clearly in Fig. 3, where $\Omega_l^{\mathrm{RD}}/(2l+1)$ is plotted against s^2 for $l=2, 3, \cdots, 6$. The saturation effect is more pronounced for low values of l since partial waves with small l correspond classically to a small impact parameter and therefore stronger interaction. Thus the curve for $l=2$ in Fig. 3 passes through a maximum around $s^2=10$, while the $l=3$ collision strength does not reach the highest value

[12] See Ref. 1, p. 149.

until $s^2=25$, and the collision strengths for higher l require even stronger coupling for complete saturation. This saturation effect is also responsible for keeping the collision strengths below the conservation limit (see Fig. 2).

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 4 shows the variation of $\Omega_l^{RD}/(2l+1)$ with respect to s^2 for an energy separation of the initial and final states (ΔE) of 2.0 eV.

2. Effect of ΔE

In Fig. 5 is displayed the collision strength Ω_l^{RD} in terms of l for several different ΔE with $s^2=19.3$. As ΔE is decreased, the collision strength curves are found to move up steadily, at first, and finally converge upon the $\Delta E=0$ curve in an oscillatory fashion. Vertical sections of these curves are plotted against $(\Delta E)^{-1}$ in Fig. 6. All the computations were made for a particular

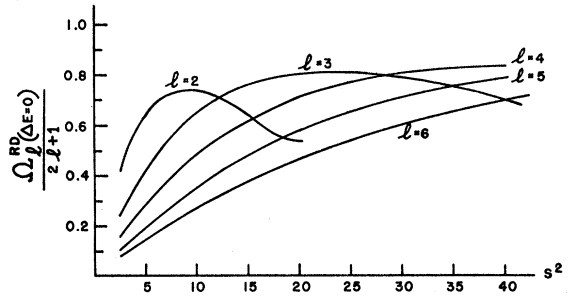

FIG. 3. Values of $\Omega_l^{RD}/(2l+1)$ for different l and $\Delta E=0$ in terms of the line strength s^2.

value of E of 13.6 eV; in general, the collision strengths depend on E and ΔE solely through $z=(k_n/k_0)^2=(E-\Delta E)/E$. This fact enables us to use Figs. 5 and 6 for several different sets of E and ΔE by means of Table I. Figure 6 illustrates that for low values of l, reduction of ΔE leads to saturation and oscillatory behavior of Ω_l^{RD} analogous to Fig. 3.

TABLE I. Values of ΔE(eV) corresponding to given values of E(eV) and z.

	E(eV)							
z	3.4	6.8	10.2	13.6	17.0	20.4	23.8	27.2
0.9632	0.125	0.25	0.375	0.50	0.625	0.75	0.875	1.0
0.9265	0.25	0.50	0.75	1.0	1.25	1.5	1.75	2.0
0.8897	0.375	0.75	1.125	1.5	1.875	2.25	2.625	3.0
0.8529	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
0.8162	0.625	1.25	1.875	2.5	3.125	3.75	4.375	5.0
0.7794	0.75	1.5	2.25	3.0	3.75	4.5	5.25	6.0
0.7426	0.875	1.75	2.625	3.5	4.375	5.25	6.125	7.0
0.7059	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0
0.6324	1.25	2.5	3.75	5.0	6.25	7.5	8.75	10.0
0.5588	1.5	3.0	4.5	6.0	7.5	9.0	10.5	12.0
0.4853	1.75	3.5	5.25	7.0	8.75	10.5	12.5	14.0
0.4118	2.0	4.0	6.0	8.0	10.0	12.0	14.0	16.0

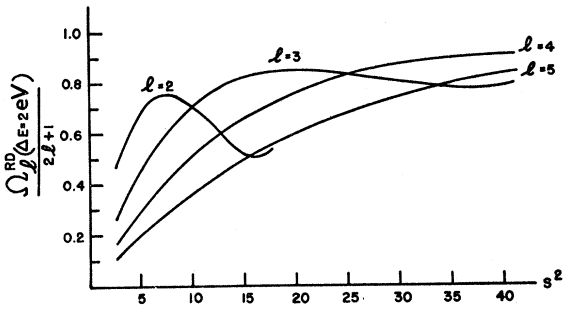

FIG. 4. Values of $\Omega_l^{RD}/(2l+1)$ for different l and $\Delta E=2.0$ eV in terms of the line strength s^2.

3. Comparison with Other Methods

The standard approximate methods for systems with weak coupling, such as Born approximation and the method of distorted waves, break down in the region where saturation is important (i.e., large s^2 or $z\approx 1$), since they give an accurate estimation of the cross sections only along the initial rise of the curves[12] of $\Omega_l/(2l+1)$ versus s^2. Thus when these methods are used for cases with strong coupling, they may produce partial cross sections which violate the conservation limit[4,6]

$$Q_l \leqslant \pi k_0^{-2}(2l+1). \tag{62}$$

It may be seen in Fig. 3 that a weak-coupling approximation applied to $l=2$ is valid only for relatively small line strengths ($s^2=7.5$ is considered small for near-resonance optically allowed transitions).

One method which has been devised so as to satisfy the conservation rule is that of Born II.[6] The method consists of replacing the R matrix which was defined in Eq. (34), by the B matrix, which for the particular case of three channels is given in atomic units by

$$B_{ij}=-\tfrac{1}{2}\pi\int_0^\infty J_{l+\frac{1}{2}}(k_i r)U_{ij}(r)J_{l'+\frac{1}{2}}(k_j r)r dr, \tag{63}$$

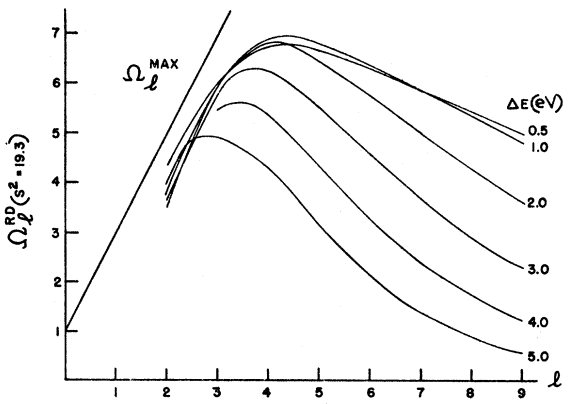

FIG. 5. Collision strengths Ω_l^{RD} with $s^2=19.3$ for several values of ΔE(eV).

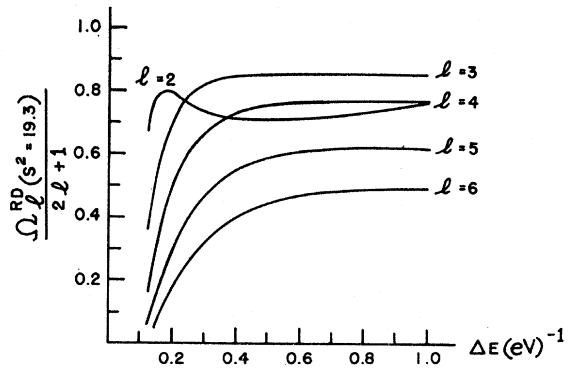

FIG. 6. Values of $\Omega_l^{RD}/(2l+1)$ for different l and $s^2=19.3$ in terms of $\Delta E(\text{eV})^{-1}$.

where

$$U_{12}=2f_1(0l1l-1;l)y_1(np,ns),$$
$$U_{13}=2f_1(0l1l+1;l)y_1(np,ns), \tag{64}$$

and

$$f_1(0l1l-1;l)=[l/3(2l+1)]^{1/2},$$
$$f_1(0l1l+1;l)=-[(l+1)/3(2l+1)]^{1/2}. \tag{65}$$

In the approximation of keeping only the asymptotic parts of the potentials (corresponding to the Bethe approximation), we have

$$U_{11}=U_{22}=U_{33}=0,$$
$$U_{12}=l^{1/2}\beta/r^2, \quad U_{13}=-(l+1)^{1/2}\beta/r^2 \tag{66}$$

and

$$B_{12}=-\tfrac{1}{2}\pi l^{1/2}\beta\int_0^\infty J_{l+\frac{1}{2}}(k_0r)J_{l-\frac{1}{2}}(k_nr)r^{-1}dr, \tag{67}$$

$$B_{13}=-\tfrac{1}{2}\pi(l+1)^{1/2}\beta\int_0^\infty J_{l+\frac{1}{2}}(k_0r)J_{l+\frac{3}{2}}(k_nr)r^{-1}dr, \tag{68}$$

where

$$\beta=2s_1(np,ns)/[3(2l+1)]^{1/2}. \tag{69}$$

Accordingly, the partial collision strength will be denoted by $\Omega_l^{B'II}$,

$$\Omega_l^{B'II}=4(2l+1)\{[(B_{12})^2+(B_{13})^2]/[1+(B_{12})^2+(B_{13})^2]\}. \tag{70}$$

The B'I (usual Bethe approximation) partial cross section may be expressed in terms of these matrix elements as

$$Q_l^{B'I}=\pi k_0^{-2}4(2l+1)[(B_{12})^2+(B_{13})^2]. \tag{71}$$

For purposes of comparison, calculations of $\Omega_l^{B'II}$ have been made for $E=13.6$ eV, $s^2=19.3$, and several values of the energy separation ΔE. The results are shown in Fig. 7. From Fig. 8 we see that for $l>3$, the partial cross sections calculated by the resonance-distortion method and by B'II agree quite well with each other for ΔE as large as 3.0 eV. However, for $l=2$ and $l=3$, they are found to differ considerably. This can be ascribed to the fact that the method B'II tends to overestimate the collision strength for small l, since

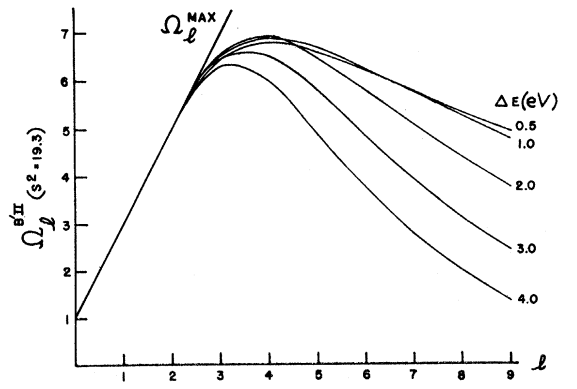

FIG. 7. Bethe II collision strengths $\Omega_l^{B'II}$ with $s^2=19.3$ for several values of ΔE(eV).

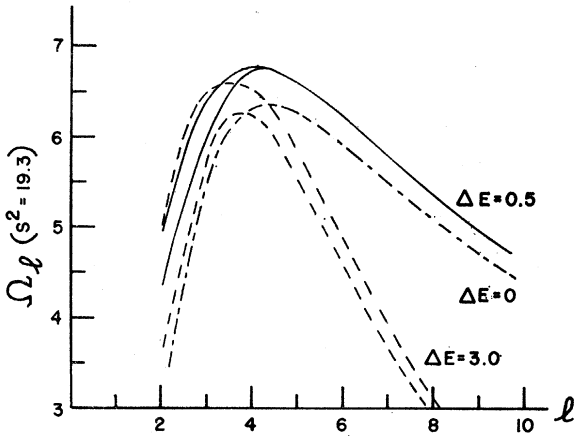

FIG. 8. Collision strengths Ω_l^{RD} for $\Delta E=0$, 0.5, 3.0 eV and $\Omega_l^{B'II}$ for $\Delta E=0.5$, 3.0 eV. The upper of the two solid and of the two dashed curves correspond to the Bethe II method, and the lower, the resonance-distortion method.

in the limit of $\Delta E=0$, $Q_l^{B'II}$ does exceed the corresponding partial cross section obtained from the exact calculation for $l=2$ and 3.[6] Furthermore, Fig. 6 shows that for these low values of l and for $\Delta E<3.0$ eV, Ω_l^{RD} is quite insensitive to ΔE. Because of the insensitivity of the collision strength with respect to ΔE and the fact that for $\Delta E=0$ the resonance-distortion result is exact for the particular potentials chosen, it appears likely that the resonance-distortion method gives more accurate partial cross sections for small l than does B'II.

VI. APPLICATION—$3\,^2S\rightarrow 3\,^2P$ TRANSITION OF Na BY ELECTRON IMPACT

An excellent example of a near-resonance and strong-coupling situation is the $3\,^2S\rightarrow 3\,^2P$ transition in Na, which has an energy separation $\Delta E=2.104$ eV and a

rather large line strength $s^2=19.0$. Since this transition is optically allowed, the coupling matrix element V_{0n} 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[13] have discussed this problem and made calculations based on the modified Bethe approximations B'II and B'III, which are found to satisfy conservation conditions. Previously, Seaton had investigated, by a close-coupling technique,[4] proton and electron impact on Na, giving rise to this transition; 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.[14]

Partial cross sections have been calculated for several values of the incident electron energy k_0^2 using the resonance-distortion method, Bethe I, and Bethe II approximations. Since for large values of l, say $l>l_0$, the coupling is weak, we find that the partial cross sections Q_l^{RD}, $Q_l^{\mathrm{B'I}}$, and $Q_l^{\mathrm{B'II}}$, all coincide. The total cross sections may then be determined by utilizing the "tail" of B'I as

$$Q^{\mathrm{RD}}=Q^{\mathrm{B'I}}-\sum_{l=0}^{l_0}Q_l^{\mathrm{B'I}}+\sum_{l=2}^{l_0}Q_l^{\mathrm{RD}}+Q', \quad (72)$$

$$Q^{\mathrm{B'II}}=Q^{\mathrm{B'I}}-\sum_{l=0}^{l_0}Q_l^{\mathrm{B'I}}+\sum_{l=0}^{l_0}Q_l^{\mathrm{B'II}}, \quad (73)$$

where

$$Q^{\mathrm{B'I}}=\pi k_0^{-2}(8s^2/3)\ \ln[(k_0+k_n)/|k_0-k_n|], \quad (74)$$

and Q' represents the sum of the s and p cross sections, which must be determined in some other manner (see Secs. III, IV, and V). Numerical values for Q_l^{RD} and $Q_l^{\mathrm{B'II}}$ are given in Tables II and III for several values of the incident energy and several l; all cross sections are in units of πa_0^2. A comparison of the partial cross sections Q_l^{RD}, $Q_l^{\mathrm{B'I}}$, $Q_l^{\mathrm{B'II}}$, and $\frac{1}{2}Q_l^{\max}$ is given in Figs. 9 and 10 for incident electron energies 10.520 and 33.660 eV, respectively. As is, of course, to be expected, the major contribution to the cross section in the case of $E=10.520$ eV is due to a few intermediate values of l; while for $E=33.660$ eV, the contribution is more uniformly distributed among several different l. One may also notice that Q_l^{RD}, $Q_l^{\mathrm{B'I}}$, and $Q_l^{\mathrm{B'II}}$ all approach the same value for large l, the convergence being faster for small E.

In calculating cross sections by the resonance-distortion and Bethe methods, all of the hypergeometric functions needed, except those for $E=33.660$ eV, were evaluated by means of the series representation[15]

$${}_2F_1(a;b;c;z)=\sum_{n=0}^{\infty}[(a)_n(b)_n/(c)_n n!]z^n, \quad (75)$$

TABLE II. Partial cross sections in units of πa_0^2 of the $3s-3p$ transition of Na calculated by the method of resonance distortion.

	E(eV)					
l	4.210	7.364	10.520	16.832	23.144	33.660
2	11.79	6.54	4.31	2.69	2.04	1.51
3	11.44	10.17	7.58	4.80	3.49	2.40
4	7.84	10.03	8.25	5.50	4.02	2.74
5	4.52	8.18	7.44	5.29	3.93	2.70
6	2.45	6.26	6.29	4.80	3.65	2.54
7	1.29	4.65	5.18	4.25	3.32	2.34
8	0.66	3.40	4.21	3.72	2.98	2.15
9	0.34	2.46	3.39	3.24	2.68	1.96
10	0.17	1.77	2.72	2.82	2.40	1.79
11	0.09	1.27	2.18	2.45	2.15	1.64
12	0.04	0.91	1.74	2.12	1.92	1.50
13	0.02	0.65	1.39	1.84	1.72	1.38
14	0.01	0.47	1.11	1.60	1.55	1.27
15	0.006	0.33	0.89	1.39	1.39	1.17

TABLE III. Partial cross sections in units of πa_0^2 of the $3s-3p$ transition of Na calculated by B'II method.

	E(eV)					
l	4.210	7.364	10.520	16.832	23.144	33.660
0	3.18	1.50	0.93	0.51	0.35	0.23
1	6.19	3.64	2.62	1.68	1.24	0.86
2	16.14	9.17	6.41	4.02	2.93	2.01
3	16.43	11.67	8.37	5.26	3.81	2.61
4	10.83	11.08	8.52	5.52	4.02	2.75
5	5.98	9.13	7.73	5.27	3.89	2.67
6	3.08	7.01	6.61	4.81	3.62	2.51
7	1.55	5.18	5.47	4.29	3.30	2.32
8	0.77	3.76	4.46	3.78	2.98	2.13
9	0.38	2.70	3.59	3.30	2.69	1.95
10	0.19	1.93	2.88	2.88	2.41	1.79
11	0.10	1.37	2.30	2.50	2.16	1.64
12	0.05	0.98	1.83	2.17	1.94	1.50
13	0.02	0.69	1.46	1.89	1.74	1.38
14	0.01	0.49	1.16	1.64	1.57	1.27
15	0.006	0.35	0.92	1.42	1.41	1.17

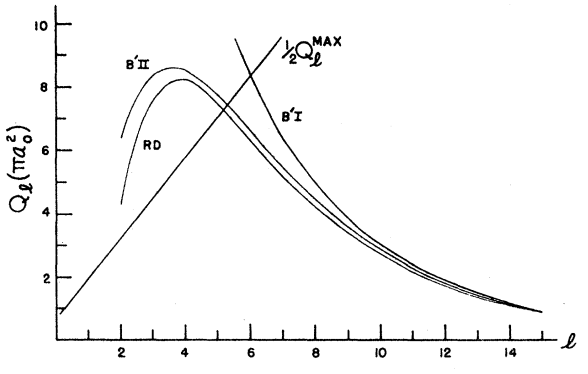

FIG. 9. Partial cross sections Q_l^{RD}, $Q_l^{\mathrm{B'I}}$, $Q_l^{\mathrm{B'II}}$, and $\frac{1}{2}Q_l^{\max}$ for Na ($3^2S\rightarrow 3^2P$) by electron impact, where $\Delta E=2.104$ eV and $s^2=19.0$ for an incident energy of $E=10.520$ eV.

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

[14] W. Christoph, Ann. Physik **23**, 51 (1935); I. P. Zapesochnyi and L. L. Shimon, Opt. Spectr. **13**, 355 (1962).

[15] A. Erdelyi, *Higher Transcendental Functions, I* (McGraw-Hill Book Company, Inc., New York, 1953), p. 56.

TABLE IV. Total cross sections in units of πa_0^2 and partial sums of Q_l for the $3s-3p$ transition of Na.

E(eV)	$Q^{B'I}$	$Q^{B'II}$	Q^{RD}	Q'	$\sum_{l=16}^{\infty} Q_l^{B'I}$	$\sum_{l=2}^{15} Q_l^{RD}$
4.210	288.63	64.9	47.1	6.5(13.7%)	0.0(0%)	40.66(86.3%)
7.364	231.87	71.6	61.7	3.7(6.0%)	0.9(1.5%)	57.10(92.5%)
10.520	189.12	68.9	62.9	2.6(4.1%)	3.6(5.7%)	56.69(90.2%)
16.832	139.19	60.5	57.7	1.6(2.8%)	9.6(16.6%)	46.50(80.6%)
23.144	111.26	53.3	51.6	1.2(2.3%)	13.2(25.6%)	37.24(72.1%)
33.660	84.48	44.4	43.5	0.8(1.8%)	15.6(35.9%)	27.10(62.3%)

where

$$(\rho)_n=\rho(\rho+1)(\rho+2)\cdots(\rho+n-1), \qquad (76)$$

and

$$|z|\leqslant 1.$$

For the higher energy, use was made of a formula given by Seaton.[4]

The total resonance-distortion and Bethe II cross sections calculated by means of Eqs. (72) and (73) are given in Table IV. The cutoff value for the tail is $l_0=15$ and the percentage contributions from the tail, the intermediate values of l, and $l=0$ and $l=1$ are also given in the table (i.e., % relative to Q^{RD}); the s and p cross sections were arbitrarily taken as $\frac{1}{2}Q_l^{max}$. In Fig. 11, these cross sections are compared with Born approximation as well as absolute measurements of Christoph and relative measurements of Haft (as quoted by Bates *et al.*).[16] The relative curve has been adjusted according to the absolute measurements. It is important to note that some freedom remains in the adjustment of Haft's relative measurements. Each resonance-distortion cross section in Fig. 11 is accompanied by a bar indicating the maximum and minimum values obtained by taking $Q'=0$ and $Q'=Q'_{max}$, respectively. (One may recall that in Table IV the value $\frac{1}{2}Q_{max}'$ was used.) It is clear that the form of the resonance-distortion curve is in reasonable agreement with that of the experimental curve, however we should not place too much faith in our results for small E, since in such cases, $k_0^2-k_n^2$ is no longer very small compared to k_0^2 (i.e., the kinetic energy of relative motion changes considerably during the collision) and thus our assumption of exact resonance in the zeroth order is no longer justified. It is also likely that distortion effects due to the diagonal elements U_{00}, U_{nn} will come in. Exchange effects have been neglected completely, and are expected to be important only for small l; however, since for small E, the effect of small l becomes significant, one might then expect exchange to be important.

A close-coupling technique was devised by Seaton[4] specifically for cases where exceptionally strong coupling causes the weak-coupling approximations to give much too large cross sections. In such cases, one may find a value l_0 of l, such that

$$Q_l^{BI}\approx\tfrac{1}{2}\pi k_0^{-2}(2l_0+1). \qquad (77)$$

It is found that a reasonably good approximation is

$$\begin{aligned} Q_l^{CC}&=\tfrac{1}{2}\pi k_0^{-2}(2l+1), && l<l_0\\ &=Q_l^{BI}, && l\geqslant l_0. \end{aligned} \qquad (78)$$

It is known that for large l, Q_l^{BI}, and $Q_l^{B'I}$ (standard Bethe approximation) coincide. Thus, if l_0 is suitably large, one may simplify calculation by replacing Q_l^{BI} above by $Q_l^{B'I}$. Despite the simplicity of this approach, it is actually found to give satisfactory results. Cross

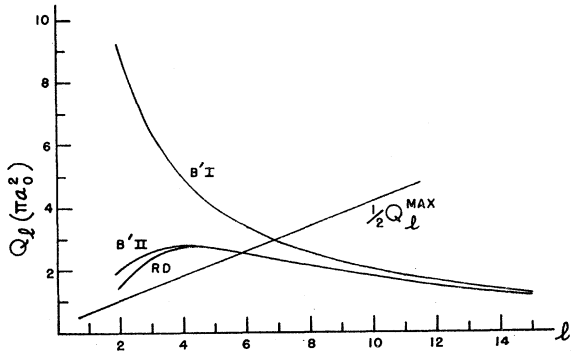

FIG. 10. Partial cross sections Q_l^{RD}, $Q_l^{B'I}$, $Q_l^{B'II}$, and $\frac{1}{2}Q_l^{max}$ for Na ($3^2S\rightarrow 3^2P$) by electron impact, where $\Delta E=2.104$ eV and $s^2=19.0$ for an incident energy of $E=33.660$ eV.

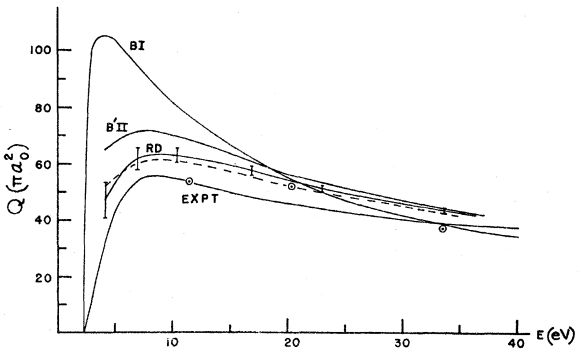

FIG. 11. Total cross sections Q^{RD}, $Q^{B'I}$, $Q^{B'II}$, and Q^{CC} for Na ($3^2S\rightarrow 3^2P$) by electron impact. The open circles refer to the absolute measurements of Christoph and the solid curve marked EXPT represents the relative measurements of Haft. The dashed curve represents Seaton's close-coupling approximation Q^{CC}.

[16] D. R. Bates, A. Fundaminsky, and H. S. W. Massey, Phil. Trans. Roy. Soc. London A243, 93 (1950); G. Haft, Z. Physik 82, 73 (1933).

sections calculated by this method (denoted by CC) are included in Fig. 11. It should be pointed out that this method is strictly limited to cases of strong coupling, its failure in other cases having been clearly demonstrated.[4]

VII. TWO-CHANNEL APPROXIMATION FOR ELECTRON-ATOM COLLISION

Attempts have been made to devise a simplified procedure for the calculation of the collision strength by the resonance-distortion method, particularly to avoid the task of solving the three-channel coupled differential equations. Here the zeroth-order solution of F_0 [denoted by $F_0^{(0)}$] is again obtained from the limiting exact-resonance case, i.e., $F_0^{(0)}$ and $F_n^{(0)}$ satisfy the equations

$$(\nabla^2+k_0^2)F_0^{(0)}=U_{0n}F_n^{(0)}, \tag{79}$$

$$(\nabla^2+k_0^2)F_n^{(0)}=U_{n0}F_0^{(0)}. \tag{80}$$

At this point we introduce an additional approximation of replacing the angular dependent $U_{0n}(\mathbf{r})$ by an angular independent potential of the form $-A/r^2$. This eliminates the three-channel coupling for the zeroth-order equations and $F_0^{(0)}$ can be obtained by a procedure analogous to that given in Sec. III. We then solve for F_n by using this form of $F_0^{(0)}$ and the original angular dependent U_{0n}. At first thought, this procedure might seem inconsistent in that we use an angular-independent interaction potential to calculate $F_0^{(0)}$, and an angular-dependent one for F_n. However, it must be remembered that $F_0^{(0)}$ can be regarded as a first-step trial function. It need not be the solution of the problem corresponding to the true potentials so long as it has sufficient resemblance to the actual solution F_0 of Eqs. (6) and (7).

The first task is to select a suitable value of A, so that $F_0^{(0)}$ gotten here will produce a satisfactory result for F_n. As suggested before, the potential $-A/r^2$ represents some kind of average of U_{0n}. Considering Eqs. (12), we can write down the asymptotic form of U_{0n} for the transitions $ns\rightarrow np m$, as

$$U_{0n}(\mathbf{r})\sim\tfrac{4}{3}\pi^{1/2}Y_1^m(\theta,\phi)s/r^2\sim U_{n0}^*(\mathbf{r}), \tag{81}$$

where θ, ϕ give the orientation of the incident particle in the atomic coordinate system. We recall that when one considers the cross section for transition to a degenerate level, one must sum the cross sections over each of the degenerate states of the level. This fact leads us to consider two averaging techniques in order to obtain an appropriate value of A. It should be remembered that the zeroth-order function $F_0^{(0)}$ need only represent one of the three degenerate states ($m=0,\pm1$), since in performing the iteration it will be used to calculate the cross section for each of the degenerate states, separately. We first take A to be determined by averaging the modulus squared of $U_{0n}^0(\mathbf{r})$ over all space as

$$(U_{0n})_{\rm rms}=-A/r^2=\tfrac{4}{3}\sqrt{\pi}\left\{\frac{1}{4\pi}\int|Y_1^0(\hat{r})|^2d\hat{r}\right\}^{1/2}sr^{-2}$$
$$=\tfrac{2}{3}s/r^2, \tag{82}$$

thus

$$A=-\tfrac{2}{3}s.$$

Alternatively, we can average the square of the matrix elements over all the m values, i.e.,

$$(U_{0n})_{\rm rms}=\{\tfrac{1}{3}(|U_{0n}^0|^2+|U_{0n}^{+1}|^2+|U_{0n}^{-1}|^2)\}^{1/2}$$
$$=\tfrac{2}{3}s/r^2, \tag{83}$$

giving the same result as Eq. (82).

Next we shall determine F_n from

$$(\nabla^2+k_n^2)F_n(\mathbf{r})=U_{n0}(\mathbf{r})F_0(\mathbf{r}), \tag{84}$$

where U_{n0} is given by Eq. (8). It is not permissible to expand $F_n(\mathbf{r})$ in terms of Legendre polynomials since such an expansion implies cylindrical symmetry. Rather, the spherical harmonics must be used, i.e.,

$$F_n(\mathbf{r})=r^{-1}\textstyle\sum_{lg}F_{n,lg}(r)Y_{lg}(\hat{r}). \tag{85}$$

The differential equation for the partial-wave amplitudes is

$$\left[\frac{d^2}{dr^2}+k_n^2-l(l+1)/r^2\right]F_{n,lg}(r)$$
$$=\sum_{l'g'}\int Y_{lg}^*(\hat{r})U_{n0}(\mathbf{r})Y_{l'g'}(\hat{r})F_{0,l'g'}(r)d\hat{r}. \tag{86}$$

The desired solution may be found by the standard variation of parameters technique, in which the Wronskian of the homogeneous solutions is chosen to be equal to one.[17] Thus we have for the partial-wave amplitudes, the asymptotic result

$$F_{n,lg}(r)\sim(-1)^l\exp(ik_nr)\sum_{l'g'}\int_0^\infty rj_l(k_nr)F_{0,l'g'}(r)dr$$
$$\times\int Y_{lg}^*(\hat{r})U_{n0}(\mathbf{r})Y_{l'g'}(\hat{r})d\hat{r}, \tag{87}$$

where

$$j_l(kr)=(\pi/2kr)^{1/2}J_{l+\frac{1}{2}}(kr),$$

and for the total inelastic function

$$F_n(\mathbf{r})\sim r^{-1}\exp(ik_nr)\sum_{lg,l'g'}(-1)^l\int_0^\infty rj_l(k_nr)F_{0,l'g'}(r)dr$$
$$\times\int Y_{lg}^*(\hat{r})U_{n0}(\mathbf{r})Y_{l'g'}(\hat{r})d\hat{r}Y_{lg}(\hat{r}). \tag{88}$$

[17] See Ref. 1, p. 107.

In the case of optically allowed transitions, which are often accompanied by strong coupling, $U_{n0}(\mathbf{r})$ will always include a dipole term, i.e., a term given by

$$b_\mu(l\pm1\ m, lm')Y_{1\mu}^*(\hat{r})y_1(n\ l\pm1, nl|r), \quad (89)$$

where for $ns\rightarrow np$ transitions we have

$$b_m(pm,so)=\tfrac{4}{3}\pi^{1/2}, \quad (90)$$

and for large r

$$y_1(np,ns|r)\sim s_1(np,ns)/r^2. \quad (91)$$

We replace $U_{n0}(\mathbf{r})$ in Eq. (88) by its asymptotic form, and noticing that as a result of the angular integration, $g=g'-m$ and $l=l'\pm1$, we obtain for the total collision amplitude

$$f_n{}^m(\theta,\phi)=\tfrac{4}{3}\pi^{1/2}s\sum_{l'g'}(-1)^{l'}\Big\{\int_0^\infty j_{l'+1}(k_nr)F_{0,l'g'}(r)r^{-1}dr\int Y_{l'+1,g'-m}(\hat{r})Y_{1m}(\hat{r})Y_{l'g'}(\hat{r})d\hat{r}\cdot Y_{l'+1,g'-m}(\hat{r})$$
$$-\int_0^\infty j_{l'-1}(k_nr)F_{0,l'g'}(r)r^{-1}dr\int Y_{l'-1,g'-m}{}^*(\hat{r})Y_{1m}(\hat{r})Y_{l'g'}(\hat{r})d\hat{r}Y_{l'-1,g'-m}(\hat{r})$$
$$=-2s\sum_{lg}(-1)^l\{I(l+1,lg)c^1(lg;l+1\ g-m)Y_{l+1,g-m}(\hat{r})+I(l-1,lg)c^1(lg;l-1\ g-m)Y_{l-1,g-m}(\hat{r})\}, \quad (92)$$

where we have employed the Condon and Shortley notation,[18] (see Table V)

$$c^k(lm;l'm')=(2/2k+1)^{1/2}\int_0^\pi\Theta(k,m-m')\Theta(l,m)\Theta(l',m')\sin\theta d\theta, \quad (93)$$

and where we have defined

$$I(l'\pm1,l'g')\equiv\int_0^\infty j_{l'\pm1}(k_nr)F_{0,l'g'}(r)r^{-1}dr. \quad (94)$$

The total cross section for the transition $ns\rightarrow npm$, is given by

$$Q(ns\rightarrow npm)=(k_n/k_0)\int|f_n{}^m(\theta,\phi)|^2d\Omega=(k_n/k_0)\tfrac{4}{3}s^2\sum_{lg}\{|I(l+1,lg)c^1(lg;l+1\ g-m)|^2$$
$$+|I(l-1,lg)c^1(lg;l-1\ g-m)|^2+I^*(l+1,lg)I(l+1,l+2\ g)c^1(lg;l+1\ g-m)c^1(l+2\ g;l+1\ g-m)$$
$$+I^*(l-1,lg)I(l-1,l-2\ g)c^1(lg;l-1\ g-m)c^1(l-2\ g;l-1\ g-m)\}. \quad (95)$$

In evaluating the radial integrals $I(l',lg)$, we use $F_{0,lg}{}^{(0)}(r)$ as determined for the case of exact resonance. In this section, we have made use of the expansion

$$F_0(\mathbf{r})=r^{-1}\sum_{lg}F_{0,lg}(r)Y_{lg}(\hat{r}). \quad (96)$$

Comparing this with Eq. (26) for $F_{0,l}$, we find that

$$F_{0,lg}(r)=2i^l[\pi(2l+1)]^{1/2}F_{0,l}(r)\delta_{g,0}, \quad (97)$$

where $\delta_{g,0}$ is the usual Kronecker delta. The radial integrals are found to be given by

$$I(l\pm1,l\,0)=i\pi^{3/2}(-1)^l(2l+1)^{1/2}(k_0k_n)^{-\frac{1}{2}}\exp(-\tfrac{1}{4}\pi i)$$
$$\times[H^+(l\pm1,l)\exp(-\tfrac{1}{2}ip_+\pi)+H^-(l\pm1,l)\exp(-\tfrac{1}{2}ip_-\pi)], \quad (98)$$

where we have defined

$$H^+(l\pm1,l)\equiv\frac{1}{2}\int_0^\infty J_{p+}(k_0r)J_{l\pm1+\frac{1}{2}}(k_nr)r^{-1}dr,$$
$$H^-(l\pm1,l)\equiv\frac{1}{2}\int_0^\infty J_{p-}(k_0r)J_{l\pm1+\frac{1}{2}}(k_nr)r^{-1}dr. \quad (99)$$

Making use of the coefficients given in Table V, we find for the total cross sections

$$Q(ns\rightarrow np(\pm1))=\pi k_0{}^{-2}\tfrac{4}{3}(\pi s)^2\sum_l\Big\{\frac{(l+2)(l+1)}{2(2l+3)}|G(l+1,l)|^2+\frac{l(l-1)}{2(2l-1)}|G(l-1,l)|^2$$
$$-\frac{(l+2)(l+1)}{2(2l+3)}G^*(l+1,l)G(l+1,l+2)-\frac{l(l-1)}{2(2l-1)}G^*(l-1,l)G(l-1,l-2)\Big\}, \quad (100)$$

[18] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, London, England, 1951), p. 175.

and

$$Q(ns\rightarrow np_o)=\pi k_0^{-2}\tfrac{4}{3}(\pi s)^2\sum_l\left\{\frac{(l+1)^2}{2l+3}|G(l+1,l)|^2+\frac{l^2}{2l-1}|G(l-1,l)|^2+\frac{(l+2)(l+1)}{2l+3}G^*(l+1,l)\right.$$
$$\left.\times G(l+1,l+2)+\frac{l(l-1)}{2(2l-1)}G^*(l-1,l)G(l-1,l-2)\right\},\quad(101)$$

TABLE V. Integrals of three normalized associated Legendre polynomials.

$$c^1(l,0;l+1,\pm1)=-[(l+2)(l+1)/2(2l+3)(2l+1)]^{1/2}$$
$$c^1(l,0;l-1,\pm1)=[l(l-1)/2(2l+1)(2l-1)]^{1/2}$$
$$c^1(l+2,0;l+1,\pm1)=[(l+2)(l+1)/2(2l+5)(2l+3)]^{1/2}$$
$$c^1(l-2,0;l-1,\pm1)=-[l(l-1)/2(2l-1)(2l-3)]^{1/2}$$
$$c^1(l,0;l+1,0)=(l+1)/[(2l+3)(2l+1)]^{1/2}$$
$$c^1(l,0;l-1,0)=l/[(2l+1)(2l-1)]^{1/2}$$

where we have defined

$$G(l\pm1,l)\equiv H^+(l\pm1,l)\exp(-\tfrac{1}{2}ip_+\pi)+H^-(l\pm1,l)\exp(-\tfrac{1}{2}ip_-\pi).\quad(102)$$

Since the initial state is nondegenerate, we need only sum the three cross sections above to obtain the total $ns\rightarrow np$ cross section; one finds

$$Q(ns\rightarrow np)=\pi k_0^{-2}\tfrac{4}{3}(\pi s)^2\textstyle\sum_l\{(l+1)|G(l+1,l)|^2+l|G(l-1,l)|^2\}.\quad(103)$$

The radial integrals given in Eqs. (102) may be readily evaluated in terms of hypergeometric functions[10] as

$$H^\pm(l+1,l)=\frac{1}{2}\int_0^\infty J_{p_\pm}(k_0r)J_{l+\frac{1}{2}}(k_nr)r^{-1}dr$$
$$=\tfrac{1}{4}(k_n/k_0)^{l+3/2}\{\Gamma(a_\pm)/\Gamma(c_\pm)\Gamma(1-b_\pm)\}\times{}_2F_1[a_\pm,b_\pm;c_\pm;(k_n/k_0)^2],\quad(104)$$

where

$$a_\pm=\tfrac{1}{2}(p_\pm+l+\tfrac{3}{2}),\quad b_\pm=\tfrac{1}{2}(l+\tfrac{3}{2}-p_\pm),\quad c_\pm=l+\tfrac{5}{2},\quad(105)$$

and

$$H^\pm(l-1,l)=\frac{1}{2}\int_0^\infty J_{p_\pm}(k_0r)J_{l-\frac{1}{2}}(k_nr)r^{-1}dr$$
$$=\tfrac{1}{4}(k_n/k_0)^{l-\frac{1}{2}}\{\Gamma(a_\pm')/\Gamma(c_\pm')\Gamma(1-b_\pm')\}\times{}_2F_1[a_\pm',b_\pm';c_\pm';(k_n/k_0)^2],\quad(106)$$

with

$$a_\pm'=\tfrac{1}{2}(p_\pm+l+\tfrac{3}{2}),\quad b_\pm'=\tfrac{1}{2}(l+\tfrac{3}{2}-p_\pm),\quad c_\pm'=l+\tfrac{5}{2}.\quad(107)$$

We notice that Eq. (103) is of precisely the same form as the Born cross section given by Eq. (71), except that the radial integrals are different and in the iteration result, contain the A dependence. It can be shown that for a given A and large values of l, or for small A and any values of l, the two results coincide. This is to be expected since A is a measure of the distortion of F_0, and its effect becomes much less pronounced for large l; we also find that for $A\rightarrow0$ we have $F_0^{(0)}(\mathbf{r})\rightarrow\exp(i\mathbf{k}_0\cdot\mathbf{r})$.

The criterion by which we chose the constant A is, of course, somewhat intuitive. It is based on the well-known idea that transitions in an atomic system are governed by the absolute square of the matrix elements of the external perturbation connecting the initial and the final state. Since the cross sections calculated from Eq. (103) do depend appreciably on A, the use of the two-channel approximation does introduce some uncertainty to the cross sections. Nevertheless, this "two-channel" scheme may be used as an approximate method for calculating the cross sections where more detailed calculations are impractical. Figure 12 shows reasonable agreement between the collision strengths calculated by the three-channel coupling equations and by the two-channel approximation with $A=-\frac{2}{3}s$. Also is shown the variation of the collision strengths with respect to A.

VIII. DISCUSSION

In the calculations presented in the previous sections, we have made the approximation of using a special set of potential functions as given in Eqs. (12) and of neglecting the effect of exchange between the colliding and the atomic electrons. For transitions with long-range coupling, where the total cross section is dis-

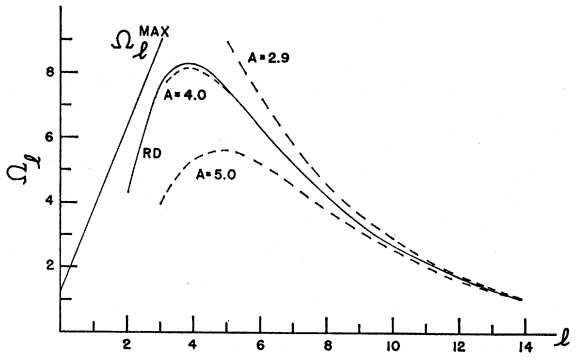

FIG. 12. Collision strengths $\Omega_l^{RD}(s^2=19.0)$ and Ω_l(2 channel, $A=2.9$, 4.0, 5.0) for Na($3^2S\rightarrow3^2P$) by electron impact with $\Delta E=2.104$eV. The value of $A=2.9$ corresponds to the relation $|A|=\frac{2}{3}|s|$.

tributed over a large number of Q_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 approximate potential functions is merely to simplify the calculation of the cross sections, and is not essential to the method of resonance distortion. In case U_{00} and U_{nn} are not set to zero, our zeroth-order solution, in the uncoupled representation,[19] is taken as the solution of

$$\begin{aligned}(\nabla^2+k_0^2-U_{00})F_0^{(0)}&=U_{0n}F_n^{(0)},\\(\nabla^2+k_0^2-U_{00})F_n^{(0)}&=U_{n0}F_0^{(0)},\end{aligned}\tag{108}$$

and the first approximation of F_n is gotten by solving

$$(\nabla^2+k_n^2-U_{nn})F_n=U_{n0}F_0^{(0)}.\tag{109}$$

We have investigated, to a certain extent, the effects of the parts of the potential functions which were neglected in Eqs. (12), on the cross sections. For electron-atom collisions, U_{00} and U_{nn} behave like $-r^{-1}\exp(-ar)$ near the origin and decay rapidly on account of the exponential factor. The radial part of $-U_{0n}$ is proportional to r^{-2} at large distances ($ns\rightarrow np$), but attains a maximum and eventually passes through the origin as r is decreased to zero. Even for elastic collision problems, the functional form of U_{00} is so complicated as to make exact solution impractical. In their studies of elastic collisions between electrons and atoms of the rare gases, Allis and Morse[20] used a potential of the form

$$\begin{aligned}V&=Z(1/r_0-1/r), && r<r_0,\\&=0, && r\geqslant r_0,\end{aligned}\tag{110}$$

which makes possible an analytic solution of the Schrödinger equation. As a trial calculation we have considered a modified schematic model with the following interaction terms:

$$\left.\begin{aligned}&U_{00}=U_{nn}=2Z(1/r_0-1/r)\\&U_{0n}=0\end{aligned}\right\}\quad r<r_0,\tag{111}$$

$$\left.\begin{aligned}&U_{00}=U_{nn}=0\\&U_{0n}=-A/r^2\end{aligned}\right\}\quad r\geqslant r_0.\tag{112}$$

We chose the parameter r_0 so that at $r=r_0$, U_{00} and U_{nn} are both very small and U_{0n} has deviated appreciably from its asymptotic inverse-square form. Once r_0 is fixed, Z can be determined in the same manner as was done by Allis and Morse.[20] For the case of *exact* resonance, the solutions of F_0 and F_n can be expressed in terms of the Coulomb wave functions[20] ($r<r_0$) and Bessel functions ($r\geqslant r_0$). We have calculated the partial cross sections (exact resonance) for the $2s\rightarrow 2p$ transitions of H at an electron energy of 13.6 eV using the two-region interaction potentials of Eqs. (111) and (112), and have repeated the same calculation with the one-region asymptotic form of Eqs. (13). It is found that the results of these two cases are different only for small l. For instance, the sum of Q_l from $l=2$ to $l=7$ varies by about 10%. Thus for transitions involving a long-range interaction, the introduction of the two-region potential alters the total cross section only slightly.

The exchange effect of the electrons can be incorporated into the formulation of the method of resonance distortion. If we consider only the interaction of two states, ψ_0 and ψ_n, the total wave function is now expanded as

$$\begin{aligned}\Psi(1,2)=&F_0(\mathbf{r})\psi_0(\mathbf{r}')+F_n(\mathbf{r})\psi_n(\mathbf{r}')\\&+[G_0(\mathbf{r}')\psi_0(\mathbf{r})+G_n(\mathbf{r}')\psi_n(\mathbf{r})],\end{aligned}\tag{113}$$

in the uncoupled representation. Upon introducing

$$\begin{aligned}F_{0,\pm}&=F_0\pm G_0,\\F_{n,\pm}&=F_n\pm G_n,\end{aligned}\tag{114}$$

we obtain the differential equations for the scattering amplitudes as[2]

$$[\nabla^2+k_0^2-U_{00}]F_{0,\pm}(\mathbf{r})\pm\int K_{00}(\mathbf{r},\mathbf{r}')F_{0,\pm}(\mathbf{r}')d\mathbf{r}'$$

$$=U_{0n}F_{n,\pm}(\mathbf{r})\mp\int K_{0n}(\mathbf{r},\mathbf{r}')F_{n,\pm}(\mathbf{r}')d\mathbf{r}',\tag{115}$$

$$[\nabla^2+k_n^2-U_{nn}]F_{n,\pm}(\mathbf{r})\pm\int K_{nn}(\mathbf{r},\mathbf{r}')F_{n,\pm}(\mathbf{r}')d\mathbf{r}'$$

$$=U_{n0}F_{0,\pm}(\mathbf{r})\mp\int K_{n0}(\mathbf{r},\mathbf{r}')F_{0,\pm}(\mathbf{r}')d\mathbf{r}',\tag{116}$$

where U_{00}, U_{nn}, and U_{0n} are given by Eq. (8), and

$$\begin{aligned}K_{00}(\mathbf{r}_1,\mathbf{r}_2)&=\psi_0^*(\mathbf{r}_1)\psi_0(\mathbf{r}_2)(k_0^2-2/r_{12}-2E_0),\\K_{nn}(\mathbf{r}_1,\mathbf{r}_2)&=\psi_n^*(\mathbf{r}_1)\psi_n(\mathbf{r}_2)(k_n^2-2/r_{12}-2E_n),\\K_{0n}(\mathbf{r}_1,\mathbf{r}_2)&=\psi_n^*(\mathbf{r}_1)\psi_0(\mathbf{r}_2)(k_n^2-2/r_{12}-2E_0)\\&=K_{n0}^*(\mathbf{r}_2,\mathbf{r}_1).\end{aligned}\tag{117}$$

The zeroth-order solutions, which will be denoted as $F_{0,\pm}^{(0)}$ and $F_{n,\pm}^{(0)}$, are taken as the solutions of the limiting exact-resonance problem, ignoring exchange. Under these limiting conditions, Eqs. (115) and (116) reduce to Eqs. (108) and (109), and $F_{0,\pm}^{(0)}$ and $F_{n,\pm}^{(0)}$ become identical to the functions $F_0^{(0)}$ and $F_n^{(0)}$, respectively. We then replace $F_{0,\pm}$ in Eq. (116) by $F_{0,\pm}^{(0)}$ and solve for $F_{n,\pm}$. A similar iteration procedure can be used if one expands $\Psi(1,2)$ in terms of basis functions of the coupled representation.[11]

Finally we wish to discuss the applicability of the

[19] Uncoupled representation refers to the expansion of the total wave function as a linear combination of products of the atomic wave functions and the colliding electron functions F. In the *coupled* representation, on the other hand, the wave function is expanded according to Eq. (31).

[20] W. P. Allis and P. M. Morse, Z. Physik **70**, 567 (1931); P. M. Morse, Rev. Mod. Phys. **4**, 577 (1932).

method of resonance distortion and its relation to other approximate methods of solving collision problems. First of all, the method of resonance distortion is restricted to problems involving near-resonance, since the limiting case of exact resonance is taken as the zeroth-order approximation. This method is most suitable for cases where the coupling between the initial and final states is strong. We can illustrate the nature of this method through a partial-wave analysis. The partial cross sections corresponding to large l for the strong coupling case reduce to the Born partial cross sections, because partial waves of large l are classically equivalent to distant impacts and at large distances, U_{00}, U_{nn}, and U_{0n} are sufficiently small so that the Born approximation is applicable. At lower l the "effective" coupling becomes so large that the use of the Born approximation and the method of distorted waves, which are valid for weak coupling, is not always justifiable. It is in this region of l (called "low-l region") that the method of resonance distortion is useful. For collision-induced transitions with a long-range interaction potential, where the contribution from the partial cross sections in the "low-l region" constitutes a substantial part of the total cross section (e.g., Table IV), we may expect the method of resonance distortion to yield more accurate results than the usual Born approximation.

For very weak coupling, the results of the method of resonance distortion approach those of the method of distorted waves. This can be seen from Eqs. (108) and (109). When U_{0n} becomes very small, $F_0^{(0)}$ in Eq. (109) is nearly equal to the zeroth-order solution in the method of distorted waves, which is defined by

$$(\nabla^2+k_0^2-U_{00})(F_0^{(0)})_{\mathrm{DW}}=0.$$

The difference in F_n as calculated by these two zeroth-order functions should be small compared to F_n itself.

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Analytical Self-Consistent Field Functions for Cr^+, Cr and Its Excited States*

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(Received 7 October 1963)

Self-consistent field calculations by the expansion method were carried out for Cr^+, Cr and some of its excited states. The results represent closely the absolute Hartree-Fock solutions. The wave functions were calculated with the requirement to satisfy exactly the cusp condition so that they can be considered to be particularly accurate in the immediate vicinity of the nucleus. The differences in calculated energy levels are compared with experiment.

INTRODUCTION

THE self-consistent field (SCF) expansion method of Roothaan[1–3] was applied on a number of cases.[4–9] In this paper the application is carried out for Cr^+, Cr and some of its excited states. Vector coupling coefficients $J_{\lambda\mu\nu}$ and $K_{\lambda\mu\nu}$ were taken from the tables calculated recently.[10]

The computation was done on an IBM 7090 computer with a modification of the previously established program.[8]

RESULTS AND DISCUSSION

The notation and the units used are the usual ones and are identical with those employed in a recent work.[7]

Some of the important results are presented in

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[1] C. C. J. Roothaan, Rev. Mod. Phys. **23**, 69 (1951).
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