Nonrelativistic Partial-Wave Scattering of Electrons by Ionized Atoms~

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A nonrelativistic partial-v ave analysis of scattering of electrons by positive and negative ions has been made. Differential cross sections for $O^{\pi}({}^2P)$, Na⁺(¹S), and Ne⁺(²P) were calculated for incident electron energies between 1 and 40 keV. In the case of $\text{Na}^{+}({}^{1}S)$ the low energy $\langle \times 1000 \text{ eV} \rangle$ behavior of the differential cross section is investigated, and the influence of exchange effects are discussed. Born-approximation calculations were also carried out and compared with the partial-wave results. Throughout the work, analytical Hartree-Pock wave functions were used to describe the scatterer, and from these functions the static potential was calculated from Poisson's equation.

I. INTRODUCTION

Recently Hanson et al ¹ have reported the first results for electron scattering from an ionic molecule (N_2^+) . Extensions of this work may make it possible to determine the structure of molecular ions by gas-phase electron diffraction.

It is well known that, in the analysis of electrondiffraction data for the structure of neutral molecules, accurate partial-wave atomic scattering factors are essential. Anticipating that a similar need will arise in the case of ionic molecules, this study has been carried out to obtain partialwave scattering factors for ionic atoms and to see how accurate first Born descriptions of the scattering process really are.

The elastic scattering of electrons by an ionized atom differs from the elastic scattering of an electron by a neutral atom owing to the presence of the repulsive or attractive unscreened Coulomb field acting on the scattered electron at large distances from the nucleus. The effect of the Coulomb field, modifying the scattering process and the form of the wave function, is not simply additive to that of the corresponding neutral atom. However, in the framework of the first Born approximation they are additive.² Partial wave $(p, w,)$ treatments of the scattering process yields results significantly different from those of the Born approximation. These differences appear to be larger than the corresponding differences in the case of neutral atoms.

In the following sections, we will first discuss the theoretical aspects of the problem and then the nature of the potential, and finally the results obtained will be presented and will be compared with other authors' approaches.³

II. THEORY

The problem of scattering of electrons by ions, in this case ionized atoms, falls in the well-known general category of scattering by a modified Coulomb field or "Coulomb admixtures. "4 If Z' is the valence of a particular ion, the scattering potential for an ionized atom will behave asymptotically like $Z'e^2/r$ but will depart from it at some distance close to the nucleus where the screening of the electron cloud becomes more important. For the well-known case of scattering by a pure coulombic potential, we should remember that the scattering amplitude $A_c(k, \theta)$ can be expressed $as^{2,4-6}$

$$
A_C(k, \theta) = (\eta / 2k \sin^2 \frac{1}{2}\theta)
$$

× exp(- *i*η ln sin² $\frac{1}{2}$ θ + *i*π + 2*i*σ₀) (2.1)

with $\eta = \mu ZZ' e^2/(\hbar^2 k)$,

$$
\sigma_0 = \arg \Gamma(1+i\eta),
$$

and $\sigma_I = \arg \Gamma(l + 1 + i\eta)$.

In the above σ_l is the Coulomb phase shift.⁴ The differential cross section is given by

$$
\frac{d\sigma}{d\Omega} = |A_C(\theta)|^2 = \frac{\eta^2}{4k^2 \sin^4 \frac{1}{2}\theta} = \frac{4k^2 \eta}{s^4} \quad . \tag{2.2}
$$

In the Coulomb case, the wave function $\Psi(r, \theta)$ which describes the scattering is required to have the asymptotic form4

$$
\Psi(r, \theta) \sim \exp\{i[kz + \eta \ln k(r - z)]\}
$$

$$
+ A_c(\theta)r^{-1} \exp\{i[kr - \eta \ln 2kr]\}
$$
 (2.3)

for $|\eta^2/k(r - z)| \ll 1$.

It is well known that $\Psi(r, \theta)$ can be written generally as

$$
\Psi(r,\theta) = \sum_{l=0}^{\infty} (2l+1)i \int e^{i\sigma l} L_l(r) P_l(\cos\theta) , (2.4)
$$

where $L_l(r)$ becomes

$$
(kr)^{-1}\sin(kr-\eta\,\ln2kr-\tfrac{1}{2}l\pi+\sigma_1)
$$

at large r . Thus in the case of a modified Coulomb field, $L_l(r)$ will have the form

$$
L_{\tilde{l}}(r) \sim (kr)^{-1} \sin(kr - \frac{1}{2}l\pi - \eta \ln 2kr + \sigma_{\tilde{l}} + \delta_{\tilde{l}}), \quad (2.5)
$$

where δ_l is an additional phase shift due to the departure from pure Coulombic scattering at small distances from the nucleus. By an analysis similar to that for atomic scattering, $4,6$ one can define a scattering amplitude due to the screening effects as

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$$
A'(k, \theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i(\delta_{\tilde{l}} + 2\sigma_{\tilde{l}})} \sin \delta_{\tilde{l}} P_{\tilde{l}}(\cos \theta).
$$
\n(2.6)

It is convenient to define the total amplitude for ionic scattering $A(k, \theta)$ as

$$
A(k, \theta) = A_{c}(k, \theta) + A'(k, \theta),
$$

where $A(k, \theta)$ may be rewritten as

$$
A(k, \theta) = A_{\alpha}(k, \theta)(1+B)
$$

with⁶

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$$
B = (1/\eta) \sin^2 \frac{1}{2} \theta \exp(i\eta \ln \sin^2 \frac{1}{2}\theta)
$$

\n
$$
\times \sum_{l=0}^{\infty} (2l+1) \exp[2i(\sigma_l - \sigma_0)]
$$

\n
$$
\times [\exp(2i\delta_l) - 1] P_l(\cos \theta).
$$
 (2.7)

Further a cross-section ratio $R(\theta)$ may be defined as

$$
R(\theta) = |A(k, \theta)/A_{c}(k, \theta)|^{2} = |1 + B|^{2}
$$
 (2.8)

which shall prove useful in comparing screening effects in ionic scattering. It should be kept in mind that the differential cross section now contains an interference term which strongly depends on whether the field is attractive or repulsive. This will be particularly true at low energies and at small scattering angles. Also note that the wave vector and electron mass used in the Schrödinger equation have been corrected for relativistic effects, and in doing so partial account is taken of relativistic effects. Notice that at 40 keV, $v/c \sim 0.3$ and a correction for the wave vector and mass of the electron makes a $(5-6%)$ change on the phase shift for $l = 0$.

III. DESCRIPTION OF THE CALCULATIONS

A. Wave Functions and Potentials

Nonrelativistic analytic Hartree-Fock (H-F) wave functions for the neutral elements and some ions with atomic numbers up to 36 are available. ⁷ In all of the calculations presented here for ions, use was made of the H- F results to calculate the scattering potential. It should be noted that use of least-squares fits of the numerical potential values would introduce, in some case, an appreciable amount of error into the calculations.^{8,9}

B. Partial-Wave Calculations

The Schrödinger equation for our particular system is given by

$$
\left[-\left(\hbar^2/2\mu\right)\nabla^2 + V\right]\Psi = E\Psi \quad , \tag{3.1}
$$

where $\mu = m_i m_t / (m_i + m_t)$

with m_i and m_f being, respectively, the masses

 $\frac{1}{k} \sum_{i=1}^{\infty} (2l+1)e^{i(\delta_{\tilde{l}}+2\sigma_{\tilde{l}})} \sin \delta_{\tilde{l}} P_{\tilde{l}}(\cos \theta).$ Of the incident and target particles. The energy
laboratory energy by laboratory energy by

$$
E = E_{1ab} m_t / (m_i + m_t).
$$

Throughout this work the unit of length is the angstrom (\AA), and the Bohr radius is taken as a_0
= 0.529 167 \AA .¹⁰ The static scattering potential $= 0.529 167 \text{ Å}.$ ¹⁰ The static scattering potentia field¹¹ will be taken as

$$
V(r) = -Ze^2/r + e^2 \int d\vec{r} \rho(\vec{r})/|\vec{r} - \vec{r}'|,
$$

where $\lim V(r) = Z'e^2/r$, (3.2)

and $\rho(\vec{r})$ is the first-order electronic density. A separation of variables of the three-dimensional Schrödinger equation leads us to the usual radial equation

$$
\left[\frac{d^2}{dr^2} + k^2 + V(r) - \frac{l(l+1)}{r^2}\right] \Psi_l(r) = 0 , \qquad (3.3)
$$

where $\lim_{t \to \infty} \Psi_{t}(r) = 0$. $r-0$

 $r\rightarrow\infty$

Asymptotically, the solution of the radial equa-

on will match a linear combination of the regu-

r and irregular Coulomb wave functions at the

int (r_m) where the ionic potential is purely

vulombic, i.e.,¹²
 $\Psi_l(r_m)$ Asymptotically, the solution of the radial equation will match a linear combination of the regular and irregular Coulomb wave functions at the point (r_m) where the ionic potential is purely Coulombic, i.e., 12

$$
\Psi_l(r_m) = F_l(\eta, kr_m)
$$

+
$$
C_l[G_l(\eta, kr_m) + iF(\eta, kr_m)]
$$
, (3.4)

where $\eta = \mu ZZ' e^2/\hbar^2 k$

and
$$
C_l = -\frac{1}{2}i[\exp(2i\delta_l) - 1]
$$
.

Thus the scattering amplitude can be written as

$$
A(k,\theta) = A_c(k,\theta)
$$

+ $\frac{1}{k} \sum_{l=0}^{\infty} (2l+1)e^{2i\sigma_l} C_l P_l(\cos\theta)$, (3.5)

and the differential cross section is given by

$$
d\sigma/d\Omega = |A(k,\theta)|^2 \tag{3.6}
$$

To solve the Schrödinger equation numerically, a modification of Cowell 's method known as the Noumerov^{13,14} method was used. This technique is especially suitable when the second- order differential equation can be written in the form

$$
\Psi''(r) = A(r)\Psi(r), \qquad (3.7)
$$
\n
$$
\Psi'''(r) = A(r)\Psi(r), \qquad (3.7)
$$
\nre in the present case

\n
$$
A(r) = l(l+1)/r^2 - V(r) - k^2.
$$

where in the present case

$$
A(r) = l(l+1)/r^2 - V(r) - k^2.
$$

The substitution $13,14$

$$
f(r)=\Psi(r)-\frac{(h^2/12)}{A(r)\Psi(r)},
$$

with the notation

$$
f_{i-1} = f(r_{i-1})
$$
 and $f_i = f(r_i)$,

can be used with the recurrence scheme

$$
f_{i\; +\; 1} = \left(2 + \frac{h^2 A(r_i)}{1 - (h^2/12)A(r_i)}\right)f_i - f_{i\; -\; 1}\;,\qquad (3.\;8)
$$

where $f_0 = 0$, $f_1 = c$, for $l \ne 1$,

and $f_0 = -0.2c$, $f_1 = c$, for $l = 1$,

to obtain the required solutions where h is the step size, which in this case was chosen as h $=4\times10^{-4}$ Å. Integrating from the origin, C_l and/ or $\sin 2\delta_l$ and $\cos 2\delta_l$ were obtained by using two points to compare the functions $f(r)$ with the Coulombic solution written as in Eq. (3.4) after it had been modified to account for the substitution of variables used above. Further details may be variables used above. Further details may be
found in the literature.^{12–15} The caluclations of the Coulomb wave functions were performed using in most of the cases the asymptotic solutions given by Fröberg¹⁶ for F_0 and G_0 . The values of G_I for $l>0$ were obtained by use of an upwards recurrence relation. In the case of F_1 the calculations were carried out by a downwards recurrence scheme as proposed by Stegun and Abramowitz,¹⁷ since an upwards recurrence scheme would lead to inaccurate results due to numerical instability.

The calculations of the Coulomb phase shifts (σ) , were accomplished using a series solution.^{15,18} However, Lanczos's¹⁹ method to approximate the gamma function was also successfully used. The value for $l = 0$ using the latter agreed with the one obtained by the series solution to 10 significant figures (single precision using a CDC 3600). The values of the Coulomb phase shifts for $l > 0$ were obtained through upward recurrence from the value for $l = 0$ by use of the formula¹⁵

$$
\sigma_{L+1} = \tan^{-1} [\eta/(L+1)] + \sigma_L \quad . \tag{3.9}
$$

C. Potential Functions

During the calculations, two functions were used to approximate the "exact" potentials. For high energy the potential given in Eq. (3. 2) was used. The potential can be evaluated from Clementi7 H-F wave functions using the well-known relations,

$$
\frac{1}{|\vec{r} - \vec{r}'|} = \sum_{mn} \frac{4\pi}{2n+1} Y_n^{m*}(\hat{r}) Y_n^{m}(\hat{r}') \frac{\gamma \langle n \rangle}{\gamma \rangle^{n+1}},
$$
\n(3.10)

$$
\int Y_n^{m*}(\hat{r}) Y_n^{m'}(\hat{r}) d\Omega_r = \delta_{n,n'} \delta_{m,m'} .
$$
 (3.11)

Furthermore, for a spherically symmetric system the potential expression reduces to the evaluation of the two basic types of integrals

$$
\frac{1}{r} \int_0^r r'^2 R_{lp}(r') R_{l'p'}(r') dr'
$$
 (3.12a)

and
$$
\int_{\gamma}^{\infty} r^{\prime} R_{lp}(r^{\prime}) R_{l^{\prime}p^{\prime}}(r^{\prime}) dr^{\prime} , \qquad (3.12b)
$$

where
$$
R_{lp}(r) = \frac{e^{-\xi} l p r}{(2n_p)^{1/2}}
$$
 ${(2\xi}_{lp})^{n} l p^{-\frac{1}{2}} r^{n} l p^{-1}$. (3.13)

All the integrals of the type mentioned above were
solved analytically.²⁰ solved analytically.²⁰

In the calculations for low-energy scattering, where exchange effects must be taken into account, the following expression was used to approximate the "exact" potential²¹ as

$$
V_T(r) = V(r) - V_r(r) , \t\t(3.14)
$$

where
$$
V_{\chi}(r) = \pi^{-1} [3\pi^2 \rho(r)]^{1/3}
$$
. (3.15)

Some previous work from this laboratory has shown that this approximation is valid for electron scattering by atoms in the energy range $50-600$ eV.²²

IV. RESULTS

A. High-Energy Scattering (I keV-40 keV).

It is well known that the first Born approximation, when used to describe the atomic scattering of electrons, gives a rather good approximation to the scattering amplitude, if one restricts its use to the keV energy range and to atoms of small atomic number (Z) . The results in Fig. 1 show that this is true in the case of ions, but that substantial differences exist between results using different atomic potentials.

The major difference between the first Born results and the p. w. treatment for negative ions occurs in the region of the minimum in the cross section. The Born^{2,4,5} expression for the scattered amplitude is given by

 $\frac{dg}{d\Omega}(\mathbb{A}^2)$ $\int Y_n^{m*}(\hat{r}) Y_n^{m'}(\hat{r}) d\Omega_r = \delta_{n,n'} \delta_{m,m'}$. (3. 11) 40

FIG. 1. Differential cross section for the ${}^{2}P$ state of 0⁻ using Hartree-Fock wave functions. The solid curve stands for the partial-wave treatment; the dashed curve is the Born calculation using Clementi H-F wave functions; and 0 Born results given in Ref. 3.

$$
f^{b}(s) = (2\beta_0^{-1/2}/a_0 s^2)[Z - F_{\chi}(s)] , \qquad (4.1)
$$

where $F_{\chi}(s)$ is the x-ray scattering factor

$$
F_{\chi}(s) = 4\pi \int_0^{\infty} \rho(r) j_0(sr) r^2 dr \tag{4.2}
$$

with $j_0(sr) = (\text{sinsr})/sr$,

and where $\rho(r)$ is the electron density for a particular ionized atom. From Eq. (4. 1) it is clear that the Born result has a zero in the cross section for electron scattering by negative ions. The results of this work show that the p. w. result given by Eq. (3.5) , on the other hand, has a small but nonzero value at the same s value.

The maximum and minimum in the differential cross section are a direct consequence of the fact that the scattering potential is attractive near the nucleus and repulsive further out for a negatively ionized atom.

Also in Fig. 1 the first Born calculations of Hanson and Pohler³ are compared with the present results for the first Born and p. w. values. The large discrepancy is probably due to the fact that they made use of wave functions which are solutions of Hartree-Fock equations based on the "old" Slater free-electron exchange^{23,24} expression which has since been improved by Kohn and
Sham²⁵ and Cowan *et al*,²⁶ The results of Pohle Sham²⁵ and Cowan et $al.^{26}$ The results of Pohle: and Hanson for positive ions are in much better agreement with these calculations as will be shown below.

In Fig. 2, the ratio $R(\theta)$ for O^- shows the departure from the Coulombic behavior of the differential cross section as a function of s. Notice that $R(\theta)$ has a minimum close to the minimum in the differential cross sections. Also $R(\theta)$ approaches unity at smaller angles which is as one would expect.

The differential cross section for scattering of high-energy electrons by positive ions (see Fig. 3) shows quite a different behavior as compared with negative ions (see Fig. 1). This is due to the nature of the potential field which for a positive ionized atom does not change sign. In Fig. 3 the differential cross section of 40-keV electrons scattered by $\text{Na}^{+}(^{1}S)$ is shown. A comparison between p. w. and different Born results is also made in Fig. 3, and again a discrepancy is found between Born results, stressing the influences which approximations in the scattered potential can have on the differential cross section. It is interesting to notice that the Born results given here are generally higher than the p. w. results. However, those given in Ref. 3 are generally lower as can be seen from Figs. 1 and 3. In Table I we compare the values for the scattered intensity as calculated with the p. w. and Born methods in this work and the Born results given in Ref. 3.

In Fig. 4 $R(\theta)$ as defined in Eq. (2.8) is plotted for $Na^{+}(1S)$ for 40- and 1-keV electrons. As is expected, $R(\theta)$ approaches unity at small angles where the scattering is mainly Coulombic. The 1-keV curve in Fig. 4 approaches unity faster (at smaller s values) than the 40-keV curve, and both ratios are always greater than unity.

FIG. 2. $R(\theta)$ for 1-keV (dashed curve) and 40-keV (solid curve) electrons scattered from $\mathrm{O}^+(\!\!{}^2P)$ is shown as a function of s. ^A minimum is observed close to the minimum in the corresponding differential cross section. The Coulombic behavior can be evidenced at small s values where $R(\theta)$ approaches unity.

Partial-wave elastic electron scattering factors are given in Tables II-IV for 40-keV electrons for $O^{-2}P$, Na⁺⁽¹S), and Ne⁺⁽¹S), from s = 0.2 to $s = 30.$

Besides the values for the scattered amplitude given by Eq. (3. 5), we also list values for the phase $\eta(s)$ given by

$$
\eta(s) = \tan^{-1}[\text{Im}f(s)/\text{Re}f(s)]
$$

which makes it possible to correct for the failure of the Born approximation²⁷ in electron scattering by molecules containing these ionized atoms. Notice that since the scattering is almost Coulombic for small s, the values for $\eta(s)$ are approximately given by

$$
\eta(s) \sim \tan^{-1}(-\eta \ln \sin^2 \frac{1}{2} \theta + 2\sigma_0)
$$

where, since $\eta < 0$ for a positive ion,

$$
\lim_{s\to 0} \eta(s) \sim \tan^{-1}(-\infty) = -\frac{1}{2}\pi.
$$

Note that the values for $\eta(s)$ have been reduced

FIG. 3. Scattered intensity of 40-keV electrons scattered on $\text{Na}^+(1\text{S})$. The solid curve stands for the partialwave results; the dashed curve is the Born approximation results; and Q represents Born results (Ref. 3) obtained using numerical Hartree-Fock Slater (Ref. 24) .

to the range $0-2\pi$.

B. Low-Energy Scattering $(< 1000 \text{ eV})$

Calculations have been carried out for energies between 40 and 500 eV for elastic electron scattering from $\text{Na}^{+(1)}S$ and $\text{Ne}^{+(1)}S$). In Fig. 5 the behavior of the $R(\theta)$ for the ¹S state of Na⁺ as a function of s for energies of the incoming electron between 40 and 500 eV is plotted without including exchange in the scattering potential. However, by analogy with atomic scattering it should

TABLE I. Differential cross section (\hat{A}^2) for 40-keV electrons scattered from the ¹S state of Na⁺.

λ^{-1}	$\bm{s^{\mathrm{a}}}$	B (Ref. 3)	Partial wave
1.	27.709	27.143	27.43
2.	4.517	4.309	4.441
5.	0.805	0.758	0.786
9.	0.176	0.171	0.171

 a This calculation using H-F wave function (Ref. 7).

FIG. 4. Ratios $R(\theta)$ between the partial-wave differential cross sections for 1-keV (dashed curve) and 40 keV (solid curve) electrons scattered from $\text{Na}^+(^1S)$ and Rutherford scattering of electrons by a singly positive point charge.

be expected that exchange effects will be important at the lower energies. This can be seen in Fig. 6, where we compare 40-eV differential cross sections for $\text{Na}^{+}(^1S)$ without exchange and with exchange included in the scattering potential, as given by Eqs. (3.14) and (3.15) , respectively. In fact Bransden and Dalgarno²⁸ have already pointed out the importance of polarization and exchange effects for scattering of electrons at low energies for He+. In the case of negative ions the range of the exchange approximation extends to such large r values that the current numerical techniques proved to be inadequate for the calculation of the phase shifts.

In Fig. 7 exchange²¹ effects predicted by the potential given in Eqs. (3. 14) and (3. 15) are observed by comparing curves with and without exchange. The inclusion of the exchange correction in the scattering potential has obviously a strong influence in the scattered intensity of 40-eV electrons from Na+; its inclusion in the calculations seems to be necessary not only for a quantitative but also for a qualitative description of the scattering phenomena as can be seen from Figs. 6 and 7. These exchange effects seem to be more important for the ionic case than in the case of scat-

TABLE II. Partial-wave scattered amplitude $f(s)$ for 40-keV electrons scattered from $O^{(2)}P$ as a function of $s = 2k \sin \frac{1}{2}\theta$. The third column on the right gives the phase as defined in Sec. IV.

\boldsymbol{s} (\AA^{-1})	f(s) $\rm(A)$	$\eta(s)$ (rad)
0, 20	98.35	3.391
0.60	7.921	3.340
1.00	0.9175	3.193
1.20	0.2427	0.8127
1.40	0.8135	0.3695
1.60	1.146	0.3168
1.80	1.328	0.2979
2.00	1.419	0.2894
2.20	1.454	0.2854
3.00	1.337	0.2878
4.00	1.057	0.3062
5.00	0.8122	0.3315
6.00	0.6263	0.3601
7.00	0.4898	0.3901
8.00	0.3901	0.4200
9.00	0.3161	0.4491
10.00	0.2609	0.4767
13.00	0.1600	0.5492
16.00	0.1087	0.6066
19.00	0.07919	0.6534
22.00	0.06047	0.6934
25.00	0.04783	0.7280
28,00	0.03876	0.7599
32.00	0.03022	0.7977

TABLE III. Partial-wave scattered amplitude $f(s)$ for 40-keV electrons scattered from $\text{Na}^+($ ¹S) as a function of $s = 2k \sin \frac{1}{2} \theta$. The third column on the right gives the phase as defined in Sec. IV.

tering by neutral atoms.

To conclude, it should be stressed that the p. w. treatment is necessary to provide a quantitative description of ionic scattering not only at low energies but also in the keV energy range. This is especially true for negative ions in the region of the minimum in the cross section. The ex-

FIG. 5. $R(\theta)$ as defined by Eq. (2.8) is shown for partial-wave differential cross sections and Rutherford scattering for $Na^+(^1S)$ as a function of s and different electron energies from 40-500 eV. Exchange corrections between the scattered electron and the atom were not included.

FIG. 6. Partial-wave low-energy (40-eV) differential cross section for $\text{Na}^+(S)$ with (dashed curve) and without exchange (solid curve).

change effects seem to be more important for the ionic case than in the case of scattering by neutral atoms. Perhaps scattering at low energies from positive-ion beams will offer a test for the various approximations of the exchange potential. Although more difficult to accomplish experimentally the characteristic features of the cross sections for negative-ion scattering offer potentially an even more sensitive test of the atomic field.

Finally I would like to call attention to the works of Bely²⁹ in this field where problem of

FIG. 7. "Exact" differential cross sections for elastically scattered electrons from the ${}^{1}S$ state of Na⁺ with exchange (dashed curve) and without exchange {solid curve) included in the scattering potential, are compared for 250-eV electrons.

exchange is taken in consideration in the scattering of electrons by positive ions, and substantial contributions done by Seaton³⁰ in excitation of positive ions and quantum-defect methods.³¹ positive ions and quantum-defect methods.

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