

Absorption and Bremsstrahlung Cross Sections of Nitrogen for Slow Electrons

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Cross sections are found for nitrogen and singly ionized nitrogen in their ground states. Our results indicate that the screening of the nucleus has a negligible effect upon the nitrogen-ion cross sections. The inclusion of polarization and exchange forces in the analysis reduces the cross sections of the nitrogen atom by approximately an order of magnitude.

THE CROSS SECTION

THE bremsstrahlung and absorption by a low temperature ($T < 20\,000^\circ\text{K}$) tenuous plasma is of current interest from both diagnostic and applicative standpoints. The theoretical treatment that has been accorded the cross sections are summarized in the review article by Alder *et al.*¹ The bremsstrahlung cross section in the electric dipole approximation is

$$\sigma^b(\Delta k^2, k_i) = \frac{32}{3} Z_1^2 \left(\frac{e^2}{\hbar c} \right) \left(\frac{\hbar}{mc} \right)^2 \frac{1}{k_i^3 k_f} \frac{B^v}{\Delta k^2} (\text{cm}^2), \quad (1)$$

while the absorption cross section, with the usual normalization, is

$$\sigma^a(\Delta k^2, k_i) = \frac{256\pi^2}{3} Z_1^2 \left(\frac{e^2}{\hbar c} \right) \left(\frac{\hbar^2}{m\epsilon^2} \right)^5 \frac{1}{k_i^2 k_f} \frac{B^v}{(\Delta k^2)^3} (\text{cm}^5), \quad (2)$$

where

$$k_f^2 = k_i^2 \pm \Delta k^2 \quad (3)$$

with the upper sign holding for absorption and the lower sign for emission. k_i and k_f are the initial and final momenta of the electron expressed in atomic units with $v/c = 190\,737.3\Delta k^2$. The B function is defined by

$$B^v(\Delta k^2, k_i) = \sum_{l=1}^{\infty} l \{ |M_{l, l-1}^v|^2 + |M_{l-1, l}^v|^2 \} \quad (4)$$

with the matrix elements

$$M_{l_i l_f}^v(k_i, k_f) = \int_0^{\infty} \chi_{l_i}(k_i r) \frac{dv}{dr} \chi_{l_f}(k_f r) dr, \quad (5)$$

where the superscript v indicates the potential. The radial functions χ_l are solutions of the radial wave equation

$$\left[\frac{d}{dr^2} + k^2 + 2v(r) - \frac{l(l+1)}{r^2} \right] \chi_l = 0 \quad (6)$$

with the boundary conditions $\chi_l(0) = 0$ and $\chi_l \sim 1$.

For certain applications it is convenient to average the absorption cross section (2) over a Maxwellian distribution of initial electron energies, i.e.,

$$\sigma(\Delta k^2, \theta) = \int_0^{\infty} \sigma^a(\Delta k^2, k_i) f(k_i^2) d(k_i^2), \quad (7)$$

¹ K. Alder, A. Bohr, T. Huus, B. Mottelson, and A. Winther, *Rev. Mod. Phys.* **28**, 432 (1956).

where

$$f(k_i^2) = 197.85\theta^{3/2} k_i \epsilon^{-31.3275\theta k_i^2}, \quad \theta = 5040/T.$$

We assume a potential of the form

$$v(r) = v_{\text{HF}}(r) - v_p(r) \quad (8)$$

where v_{HF} is the unperturbed Hartree-Fock potential² and v_p is an effective polarization potential with the exchange perturbation included. For the ion, it is clear that the polarization and exchange forces may be neglected. For the nitrogen atom we include a strong polarization potential³

$$v_p = -4.315/(r^2 + 1.2)^2 \quad (9)$$

and one somewhat weaker³ in a second calculation

$$v_p = -3.542/(r^2 + 1.74)^2. \quad (10)$$

RESULTS

The radial wave functions of Eq. (6) are readily found by using the Runge-Kutta method of order four with point to point accuracy of h^5 . The solutions may be carried out to large r due to the well-behaved derivatives of the χ_l . The functions were evaluated with 0.02 intervals $0 \leq r \leq 2.0$, with 0.05 intervals $2.0 \leq r \leq 5.5$, with 0.10 intervals $5.5 \leq r \leq 45.5$ and with 0.50 intervals $45.5 \leq r \leq 745.5$. It is of course necessary to extend the calculation for the neutral atom only to the point where there is no significant contribution to the matrix elements.

The unit asymptotic normalization of the neutral atom wave functions is accomplished by matching the un-normalized solution, $X_l(kr)$, to linear combinations of

$$P_l(kr) = kr j_l(kr), \quad Q_l(kr) = kr n_l(kr)$$

which are solutions of Eq. (6) with $v(r) = 0$. Thus

$$\chi_l(kr) = X_l(kr) / (a_l^2 + b_l^2)^{1/2},$$

where

$$X_l(kr) = a_l P_l(kr) + b_l Q_l(kr).$$

The normalization for the ion is analogous except the

² D. R. Hartree and W. Hartree, *Proc. Roy. Soc. (London)* **A193**, 299 (1948); and E. Clementi, IBM Research Laboratory, San Jose, California (private communication).

³ P. Hammerling, W. W. Shine, and B. Kivel, *J. Appl. Phys.* **28**, 760 (1957); and M. M. Klein and K. A. Brueckner, *Phys. Rev.* **111**, 1115 (1958).

TABLE I. Phase shifts of the radial functions for the nitrogen atom (radians).

k	$v_p=0$			$v_p=-4.315/(r^2+1.2)^2$			$v_p=-3.542/(r^2+1.74)^2$		
	δ_0	δ_1	δ_2	δ_0	δ_1^a	δ_2	δ_0	δ_1	δ_2
0.05	6.106	0.217(-3)	0.1(-6)	3.076	-0.278(-3)	-0.4(-6)	3.128	-0.182(-3)	-0.3(-6)
0.10	5.934	0.174(-2)	0.2(-5)	3.011	-0.216(-2)	-0.15(-4)	3.117	-0.142(-3)	-0.11(-4)
0.15	5.769	0.595(-2)	0.11(-4)	2.950	-0.695(-2)	-0.113(-3)	3.113	-0.453(-2)	-0.86(-4)
0.20	5.616	0.143(-1)	0.44(-4)	2.893	-0.154(-1)	-0.453(-3)	3.120	-0.995(-2)	-0.345(-3)
0.25	5.473	0.286(-1)	0.129(-3)	2.842	-0.277(-1)	-0.130(-2)	3.138	-0.176(-1)	-0.985(-3)
0.30	5.343	0.509(-1)	0.312(-3)	2.798	-0.435(-1)	-0.297(-2)	3.171	-0.271(-1)	-0.226(-2)
0.35	5.223	0.834(-1)	0.651(-3)	2.763	-0.618(-1)	-0.582(-2)	3.216	-0.374(-1)	-0.442(-2)
0.40	5.113	0.1291	0.122(-2)	2.736	-0.817(-1)	-0.102(-1)	3.271	-0.475(-1)	-0.769(-2)
0.45	5.013	0.1912	0.210(-2)	2.720	-0.1018	-0.162(-1)	3.330	-0.559(-1)	-0.122(-1)
0.50	4.920	0.2730	0.340(-2)	2.712	-0.1208	-0.238(-1)	3.388	-0.613(-1)	-0.179(-1)
0.60	4.754	0.5047	0.759(-2)	2.719	-0.1513	-0.433(-1)	3.480	-0.578(-1)	-0.322(-1)

^a The negative sign indicates shift away from the origin. Numbers in parentheses indicate the power of 10 by which the preceding number is to be multiplied.

un-normalized solution is matched to linear combinations of the Coulomb wave functions $F_l(kr)$ and $G_l(kr)$ which are solutions of Eq. (6) with $v(r)=r^{-1}$. Since these functions are not extensively tabulated for small k , they were computed.⁴ The normalization for each χ_l was performed at four different sets of points on an appropriate interval and the four quantities $(a_l^2+b_l^2)^{1/2}$ agreed to the sixth decimal place.

The effect of polarization on electron-nitrogen scattering is seen from the phase shifts shown in Table I. The phase shifts for the ion are shown in Table II.

For the neutral atom, the integration in Eq. (5) was

carried to $r=5.5$ and with polarization included to $r=20.5$. For the ion the integration was truncated at $r=745.5$. An error bound due to the truncation was found, the greatest error being less than 24% for $k=0.05$ and $\Delta k^2=0.00005$. For most cases the error was within a few percent.

For $k \leq 0.6$ the series of Eq. (4) converges rapidly with l for the neutral atom and, to a very good approximation

$$B^I(\Delta k^2, k_i) \approx |M_{1,0}^I|^2 + |M_{0,1}^I|^2 + 2|M_{2,1}^I|^2 + 2|M_{1,2}^I|^2. \quad (11)$$

The results for absorption and emission are shown in Figs. 1 and 2. For the nitrogen ion it is necessary to use the proton result of Biedenharn⁵ to obtain the dipole

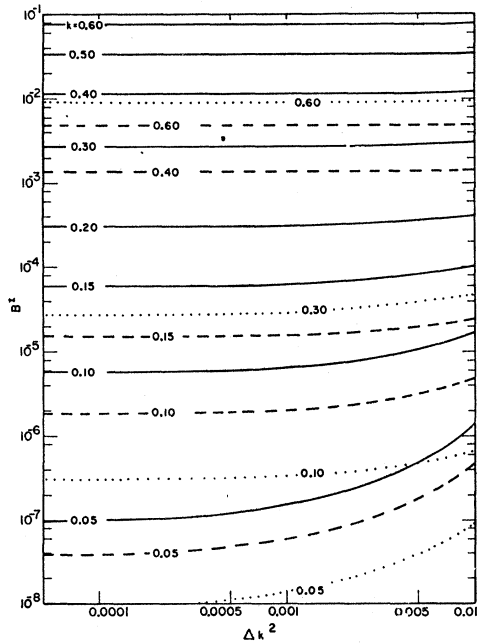


FIG. 1. The absorption function for the nitrogen atom, B^I . — $v_p=0$; --- v_p of Eq. (9); ··· v_p of Eq. (10).

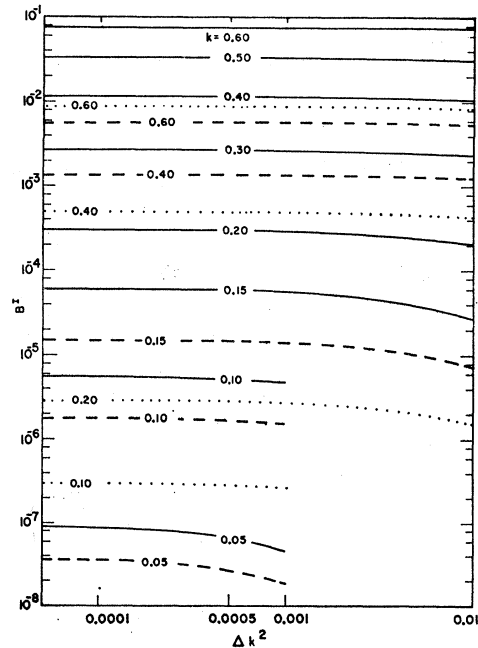


FIG. 2. The emission function for the nitrogen atom, B^I . — $v_p=0$; --- v_p of Eq. (9); ··· v_p of Eq. (10).

⁴ R. DeVore and S. Lin, Antenna Laboratory, The Ohio State University Research Foundation, Report 1565-4, 1963 (unpublished).

⁵ L. C. Biedenharn, Phys. Rev. 102, 262 (1956).

TABLE II. Phase shifts of the radial functions for the nitrogen ion (radians).

k	$N^+(^3P)$		
	δ_0	δ_1	δ_2
0.05	3.026	1.495	0.0173
0.1	3.025	1.493	0.0179
0.2	3.019	1.489	0.0202
0.3	3.009	1.481	0.0243
0.4	2.997	1.472	0.0302
0.5	2.981	1.461	0.0380
0.6	2.962	1.449	0.0478

function

$$B^{II} \approx \{b_0 - [|(1,2;0)|^2 + |(-1,2;1)|^2 + 2|(1,2;1)|^2 + 2|(-1,2;2)|^2]\} + \{|M_{0,1}^{II}|^2 + |M_{1,0}^{II}|^2 + 2|M_{2,1}^{II}|^2 + 2|M_{1,2}^{II}|^2\}. \quad (12)$$

The terms in the first set of braces are defined in Ref. 5 and represent the contribution to the nitrogen ion dipole function for $l \geq 2$. This is a good approximation as evidenced by the phase shifts of Table II. The absorption result is given in Fig. 3.

To effect the integration in Eq. (7), the k space was partitioned into intervals of length 0.025 for $0.05 \leq k \leq 0.20$ and 0.05 for $0.20 \leq k \leq 0.50$. This adequately covers the distribution for the temperature of interest. The averaged cross sections for absorption are shown in Fig. 4.

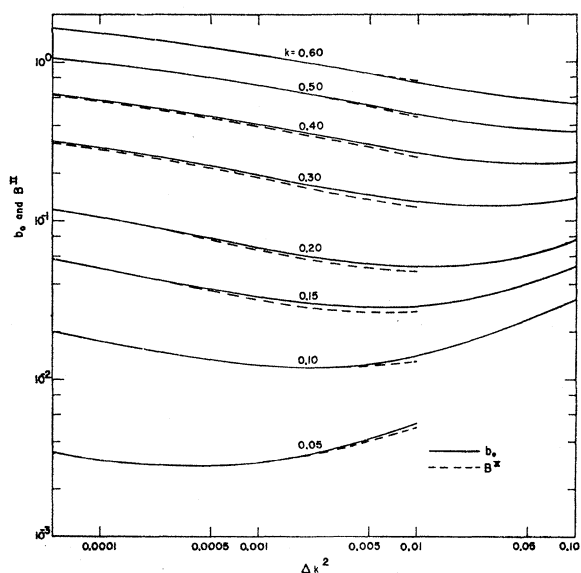


FIG. 3. The absorption function for the nitrogen ion B^{II} , and the function b_0 , for the hydrogen ion.

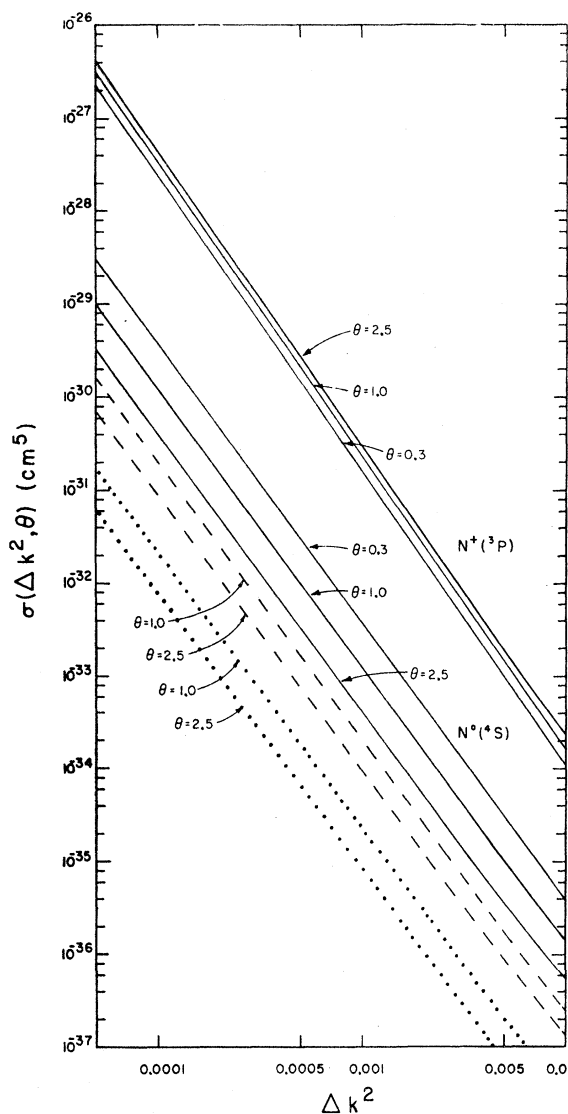


FIG. 4. The averaged absorption cross sections for different temperatures for the nitrogen ion and atom. — $v_p=0$; - - - v_p of Eq. (9); ···· v_p of Eq. (10).

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