Quantum-mechanical treatment of strong electron-atom collision contributions to the shift and width of hydrogen lines

Axel Könies and Sibylle Günter
Fachbereich Physik, Universität Rostock, Universitätsplatz 1, 18051 Rostock, Germany
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A quantum-mechanical theory based on a Green's function technique has been applied to calculate the shifts and the widths of hydrogen lines. Strong collision contributions have been treated via partial summation of the corresponding perturbation series. Therefore, the developed theory contains no arbitrary cutoff parameters. The calculated widths and shifts have been compared to those given by a close-coupling approach [K. Unnikrishnan and J. Callaway, Phys. Rev. A **44**, 3001 (1991); **43**, 3619 (1991)], semiclassical results of the unified theory, and Griem's cutoff procedure [H. R. Griem, Phys. Rev. A **38**, 2943 (1988)] for the perturbation theory. Electronic contributions to widths and shifts of the hydrogen lines up to main quantum numbers $n \leq 4$ without arbitrary cutoff parameters have been calculated.

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I. INTRODUCTION

The most successful theoretical approach to the electronic contribution to the shift of hydrogen spectral lines until now has been given by Griem [3,4]. With the help of the proposed semiclassical theory, a lot of line-shift calculations have been carried out. For hydrogen lines, this theory had to be extended to the shift contributions resulting from $\Delta n = 0$ interactions [5], which are due to quantum-mechanical effects [6]. Because of the applied second-order perturbation theory, however, this theory is restricted to weak emitter-perturber interactions only. The corresponding integrals for shifts and widths diverge for small impact parameters. To avoid such divergencies, a cutoff procedure has been applied. Thereby, a minimal impact parameter has been chosen in such a way that the unitarity of the corresponding scattering matrix is preserved. Unfortunately, the resulting shifts depend strongly on the choice of such a cutoff parameter. Further, the amount of strong collision contributions to the shift remains questionable.

Of course, there are some other ways to avoid divergencies for strong collisions. As is well known, the unified theory [7–11] includes strong collisions without a perturbation expansion. Due to the applied no-quenching approximation, however, the main contributions to the shift (due to $\Delta n \neq 0$ interactions) cannot be calculated within this theory. Another way to deal with strong collisions is to make use of Baranger's relation between shift and width of an atomic level and the scattering phase shifts [12–14]. Thus, the phase shifts for electron scattering at excited atomic levels have to be calculated. For the hydrogen lines L_α, L_β, and H_α, this has been done by Unnikrishnan and Callaway who include the states $1s$, $2s$, $2p$, $3s$, $3p$, and $3d$ in the corresponding close-coupling equations. The other energy levels have been treated via an optical potential [15,1,2]. The resulting line shifts (including electronic as well as ionic shift contributions) are much smaller than corresponding experimental ones. This is especially true for the H_α line. The authors suspected that they would have to include additionally the $n = 4$ states explicitly in the close-coupling equations in order to reach a better agreement between theoretical and experimental line shifts.

Convergent expressions for shifts and widths even within a low-order perturbation expansion can be reached using a quantum-mechanical many-particle theory. The inclusion of quantum-mechanical effects removes the divergence for strong collisions, whereas many-particle effects are responsible for the convergence at large impact parameters. Nevertheless, contributions from strong collisions remain overestimated [16]. In a previous paper [17], a quantum-mechanical treatment of strong collision contributions has been given by one of the authors. This approach is similar to that given by Dharma-wardana [18], who calculated an all-order mass operator within a one-particle Green's function approach. Introducing two-particle Green's functions, shift and width of the hydrogen L_α line have been calculated. Thereby, a low-order perturbation expansion has been avoided via partial summation of the corresponding T matrix, which describes the full radiator-perturber interaction.

The aim of this paper is to apply the theory developed in [17] to calculate the electronic contributions to shifts and widths of several hydrogen lines. The results will be compared to those given by other theories. The comparison with experimental data would require the inclusion of ion effects and the calculation of full line profiles as done in [19]. Full line shifts of the H_α, H_β, and P_α lines will be given in a forthcoming paper.

II. THEORY

Starting from the relationship between optical properties and the dielectric function, a systematic approach to spectral line shapes based on a Green's function technique has been developed [16,20–23]. A diagram tech-

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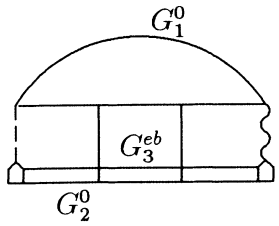
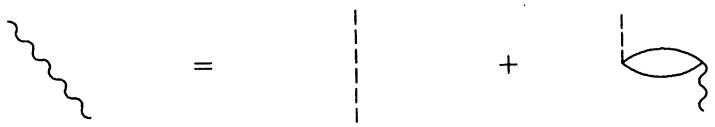
nique has been applied to carry out the perturbation expansion in a very systematic manner. It has been shown that shift and asymmetry may be derived from the self-energy, which describes the perturbation of the radiator due to the plasma environment. Allowing also for strong perturber-radiator interaction, the corresponding self-energy is given by the following diagram:

$\Sigma_2 =$ 

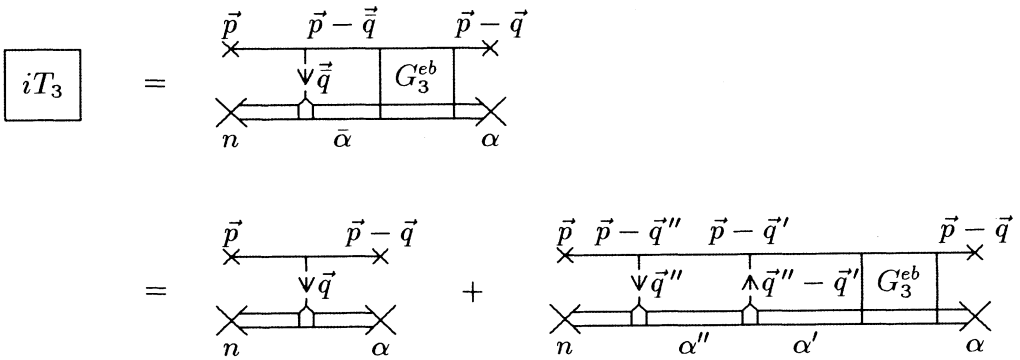
(1)

where G_1^0 and G_2^0 represent the free one- and two-particle propagator, respectively. For the screened potential the well-known relation



$$iV^S(\vec{q},\omega) = iV(\vec{q}) + iV(\vec{q})\Pi^{\mathrm{RPA}}(\vec{q},\omega)V^S(\vec{q},\omega) \tag{2}$$

holds, where $V(q)$ is the pure Coulomb potential and Π^{RPA} is the polarization function in random-phase approximation (RPA). The three-particle Green's function G_3^{eb} represents the full perturber-radiator interaction by considering a special scattering channel for the interaction between a two-particle bound state and a perturber. Within the ladder approximation, a Dyson equation may be written for the static part of the interaction in (1),



(3)

Of course, it is impossible to find the exact solution of this three-particle scattering problem. An approximate solution may be found if one considers only those parts of G_3^{eb} which describe elastic scattering. That results in setting $\vec{q}=\vec{q}'$ in Eq. (3). Furthermore, the principal quantum numbers of the states $\bar{\alpha}$, α', and α are the same within this approximation. In calculations for isolated lines, the approximations introduced above allow us to find a solution for the three-particle T matrix T_3^{eb} directly from Eq. (3). When dealing with overlapping lines, however, one has to carry out the sum over all degenerate states $\bar{\alpha}$ and α' which have the same principal quantum number as α. We assumed here, however, that the Green's function G_3^{eb} is diagonal in the quantum numbers, too. Neglecting further any correlations between Stark and Doppler broadening, for the three-particle T matrix T_3^{eb} one finds the approximate solution

$$T_3^{e,b} \approx \frac{i}{e}\frac{M_{n\alpha}^{(o)}(-\vec{q})V(q)}{1+iA(n,\alpha,\vec{p},\vec{q})} . \tag{4}$$

The self-energy which includes strong-collision contributions is therefore given by

$$\Sigma(E_n) = -\frac{2}{e^2}\sum_{\alpha}\int\frac{d\vec{q}}{(2\pi)^3}\int\frac{d\vec{p}}{(2\pi)^3}V^2(q)f_e(E_p)\frac{|M_{n\alpha}(\vec{q})|^2}{E_\alpha^o - E_n + E_{\vec{p}-\vec{q}} - E_p}\frac{1}{1+iA(n,\alpha,\vec{p},\vec{q})} , \tag{5}$$

with

$$A(n,\alpha,\vec{p},\vec{q}) = \frac{1}{e}\sum_{\alpha''}\int\frac{d\vec{q}''}{(2\pi)^3}\frac{M_{n\alpha''}^{(o)}(-\vec{q}'')M_{\alpha''\alpha}^{(o)}(\vec{q}''-\vec{q})}{M_{n\alpha}^{(o)}(-\vec{q})}\frac{V(q'')V(\vec{q}''-\vec{q})}{V(q)}\frac{1}{E_n+E_p-E_{\vec{p}-\vec{q}''}-E_{\alpha''}} . \tag{6}$$

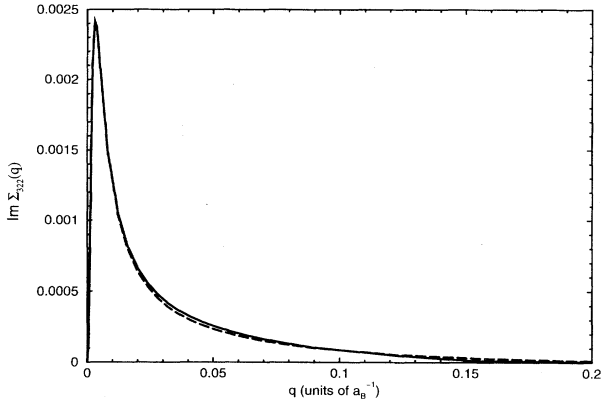


FIG. 1. Integrand of the imaginary part of the self-energy for the $\{n,l,m\}=\{3,2,2\}$ level of a hydrogen atom at an electron density of 6.4×10^{16} cm^{-3}. The result obtained from partial summation (solid line) is compared with the Born approximation result (dashed line). The perturbing level is $\{n,l,m\}=\{3,1,1\}$ ($\Delta n=0$) and the temperature is 12 000 K.

The term $[1+iA(n,\alpha,\vec{p},\vec{q})]^{-1}$ causes the deviation from the Born approximation for large q and therefore the correction for the strong-collision contribution.

We summarize now the applied approximations. In order to describe strong-collision contributions, via partial summation, an infinite sum over parts of the perturbation series is included. In spite of this approximation and the restriction to elastic scattering partly applied in Eq. (3), the resulting self-energy is correct up to the third order with respect to the interaction potential V. Furthermore, we consider the $\Delta l=0$ and $\Delta l=1$ terms of the multipole expansion of the matrix elements. That means we include monopolelike and dipolelike interactions between radiator and perturber. To avoid too much numerical effort, in computing the self-energy according to Eq. (5), instead of the correction term $A(n,\alpha,\vec{p},\vec{q})$ its average

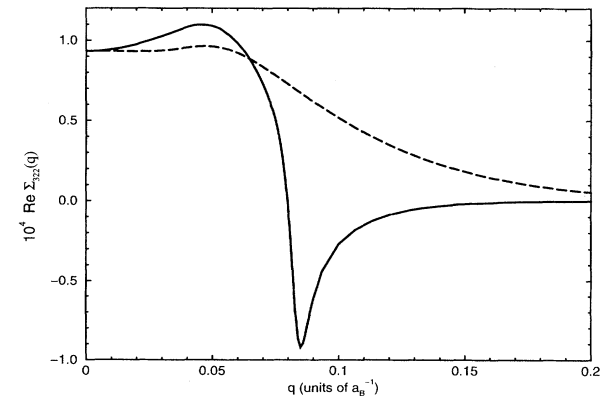


FIG. 2. Integrand of the real part of the self-energy for the $\{n,l,m\}=\{3,2,2\}$ level of a hydrogen atom at an electron density of 6.4×10^{16} cm^{-3}. The result obtained from partial summation (solid line) is compared with the Born approximation (dashed line). The perturbing level is $\{n,l,m\}=\{4,3,3\}$ ($\Delta n=1$) and the temperature is 12 000 K.

TABLE I. Electronic with (Å) of the level $\{2,1,1\}$. The electron density is 2×10^{17} cm^{-3}.

		This paper	
T (eV)	Unnikrishnan [2]	Partial summation	Born approximation
1	0.064	0.050	0.065
2	0.053	0.040	0.053
3	0.048	0.035	0.046
5	0.042	0.030	0.037

over the angles of $\vec{q}$ has been applied,

$$\overline{A}(n,\alpha,\vec{p},q)=\int d\Omega_q\, A(n,\alpha,\vec{p},\vec{q})\ , \tag{7}$$

and only the momentum transfer $\vec{q}''$ in the direction of $\vec{p}$ has been considered.

III. RESULTS

In order to investigate the influence of strong collisions on shift and width of spectral lines, one has to look at their q integrands according to Eq. (5). For small momentum transfers q (which correspond to large impact parameters within the semiclassical theory) this integrand should be close to that obtained within a second-order Born approximation. For larger values of q the Born approximation becomes invalid. Therefore, the correction due to strong collision contributions $\overline{A}(n,\alpha,\vec{p},q)$ should become important for large momentum transfers or small impact parameters.

Figures 1 and 2 show the q integrand of the imaginary and the real part of the self-energy for the $\{n,l,m\}=\{3,2,2\}$ level of hydrogen at an electron density of 6.4×10^{16} cm^{-3}, and a temperature of 12 000 K. The main contributions to hydrogen line shifts result from virtual $\Delta n=1$ transitions whereas for the width only $\Delta n=0$ transitions are important. Therefore, for demonstration in this figure the perturbing levels are chosen to be $\{3,1,1\}$ for the imaginary part and $\{4,3,3\}$ for the real part of the self-energy.

The self-energy obtained according to Eq. (5) is compared to those resulting from a Born approximation. It becomes obvious that for large momentum transfers, deviations from the Born approximation result become important. This is especially true for the shift of the energy levels which would be overestimated within a second-order Born approximation by a factor of 2 (Fig. 2). For the width of the central component, however, the Born

TABLE II. Electronic width (Å) of the $3d$-$2p$ transition. The electron density is 10^{17} cm^{-3}.

		This paper	
T (eV)	Unnikrishnan [1]	Partial summation	Born approximation
1	4.04	3.25	4.37
2	3.38	2.67	3.41
3	3.0	2.35	2.92
5	2.75	2.14	2.62

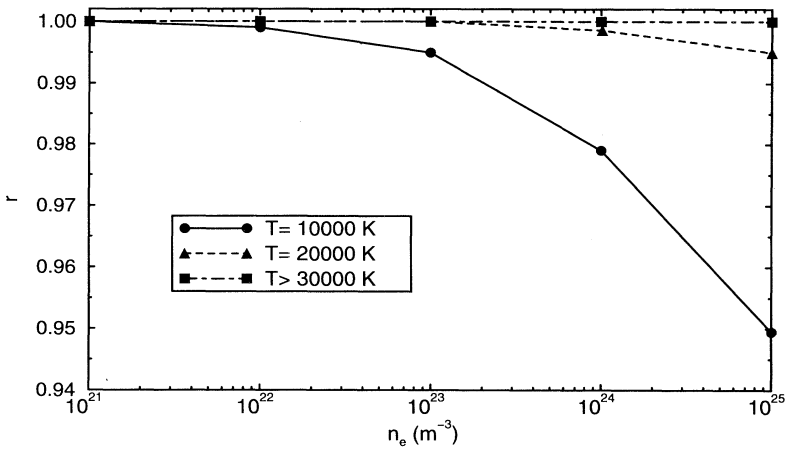


FIG. 3. Ratio $r = \mathrm{Im}\Sigma_{322-311}/\mathrm{Im}\Sigma^{\mathrm{Born}}_{322-311}$ vs the electron density n_e at different temperatures.

approximation is in better coincidence with the partial summation result. The deviation from the Born approximation for the other components is larger.

For high temperatures one would expect that nearly all collisions become weak, and the Born approximation should work very well. Figures 3 and 4 show the relations between the shift and width including strong collision contributions according to Eq. (5) and those obtained within a Born approximation. As is to be expected, for higher temperatures the theory approaches toward its limiting case—the Born approximation.

The pole structure of the q integrand in Figs. 1 and 2 is probably a result of the approximations introduced above. However, instead of the exact behavior of the q integrand, the integrals for width and shift are important for line-shape calculations.

Nevertheless, problems occur for the $\Delta n = 0$ contributions to the shift. The integrand of the imaginary part of the $\Delta n = 0$ contributions is much larger than that of the real part. Because the imaginary part and the real part of the self-energy are related via the Kramers-Kronig relation, the pole in the q integrand of the imaginary part causes a large peak in the q integrand of the real part. Since this peak leads to an overestimation of the $\Delta n = 0$ contributions to the line shift, these contributions are estimated to be the same percentage of the Born approximation result as obtained for the other shifts.

Unnikrishnan and Callaway [1,2] calculated the S-matrix elements for electron-atom scattering from close-coupling equations. All states of the hydrogen atom up to $n = 3$ were treated exactly whereas the upper states were approximated by an optical potential using 12 pseudostates. Therefore we shall compare our results with this calculation.

For the width of the L_α line ($n = 2$) the close-coupling results agree within a few percent with those given by the Born approximation (Table I). From the partial summation we obtain somewhat smaller values, which approach the Born approximation at higher temperatures. At high temperatures the close-coupling width even exceeds the Born approximation. It is not obvious which physical reason should cause such an effect. Also for the $3d$-$2p$

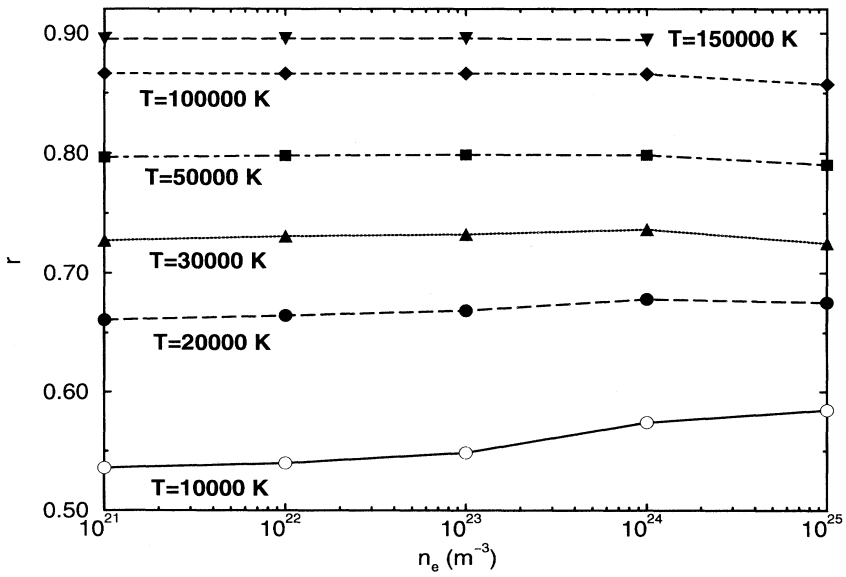


FIG. 4. Ratio $r = \mathrm{Re}\Sigma_{322-433}/\mathrm{Re}\Sigma^{\mathrm{Born}}_{322-433}$ vs the electron density n_e at different temperatures.

TABLE III. FWHM (Å) of the L_α and the H_α line (static ion approximation). The electron density is 10^{17} cm^{-3}.

	Simulation		MMM	"Unified theory"		This paper	
T (K)	[25]	[26]	[27,28]	[7]	Others	$0 \le \Delta l \le 1$	$\Delta l = 1$
L_α							
10 000	0.062	0.065	0.060	0.053	0.058[a]	0.0672	0.065
H_α							
10 000	6.84		6.14	6.11	7.40[b]	7.17	6.77

[a]Reference [29]
[b]Reference [30].

(central component of H_α) transition one may observe the same qualitative behavior (Table II) but larger deviations.

Most of the other theories give the full line profiles rather than "purely" theoretical values of the electronic width. Some of them, such as the computer simulations or the model-microfield method (MMM), are even in principle unable to give single constituents of the profile. Therefore we compare the full width at half maximum (FWHM) of both the L_α and the H_α line profiles in static ion approximation (Table III) with other theories. This quantity is very sensitive to differences in the electronic width. Our theory yields—as would the close-coupling approach—significantly larger half-widths than the semiclassical theories. (From an extrapolation of the data of Unnikrishnan and Callaway we estimate the corresponding half-width of the H_α line to be approximately 8.32 Å.)

Obviously this interesting result is due to the consequent quantum-mechanical treatment of the electron-atom-scattering problem in the theory presented and the phase-shift calculations. Within semiclassical approaches ("unified theory," computer simulation, MMM, Griem's theory) the interaction between perturber and radiator is reduced to the interaction between the atom and a field caused by the perturber. The dipole approximation, which is usually applied, neglects all other parts of a multipole expansion of the interaction term. The difference between semiclassical and our quantal results arises from the $\Delta l = 0$ transitions, which are contained in the quantum-mechanical theories (see Table III).

Considering the shift of the central L_α component, one finds an excellent agreement between the partial summation result and the scattering phase-shift calculation for temperatures above 20 000 K (Table IV). However, for 10 000 K the deviation is near 30%. The numerous approximations used in both theories may be the reason.

On the other hand, the line shifts given by Unnikrishnan and Callaway for the H_α line are too small (Table V). The latter is true not only in comparison with our results but also in comparison with the experiment [2]. As already suspected by the authors, this drawback is probably an effect of the optical potential approximation for the atomic states with $n > 3$. The main contributions to the shift of a level with $n = 3$ arise from perturbations by the levels with $n \ge 4$, which are obviously underestimated by the optical potential approximation. The results for the linewidths should not be affected, since $\Delta n \neq 0$ contributions to the linewidth are negligible.

As already mentioned, our theory needs no cutoff parameters. For comparison, we may define, however, a maximal transition momentum at which the integrand of the Born approximation has to be cut off in order to obtain the same result as follows from our partial summation of the perturbation series. Assuming that, in principle, the transition momentum is the inverse impact parameter ($q \approx 1/\rho$), it is also possible to define a minimal impact parameter. It should be noted, however, that we may find a cutoff parameter only for a special atomic state, but not for a spectral line, as done by Griem [3,4]. In order to compare both results we assumed that Griem's impact parameter for a spectral line is equal to that for the upper atomic state of the considered transition. Such minimal impact parameters are compared with those given by Griem for various atomic states in Table VI. It is apparent that the cutoff parameters agree quite well for 12 000 K. As it becomes obvious from Table VII, this coincidence becomes poor for higher tem-

TABLE IV. Electronic shift (Å) of the level $\{2,1,1\}$. The electron density is 2×10^{17} cm^{-3}.

	Unnikrishnan	This paper	
		Partial	Born
T (eV)	[2]	summation	approximation
1	0.0087	0.012	0.030
2	0.011	0.011	0.025
3	0.011	0.011	0.022
5	0.011	0.010	0.018

TABLE V. Electronic shift (Å) of the $3d$-$2p$ transition. The electron density is 10^{17} cm^{-3}.

	Unnikrishnan	This paper	
		Partial	Born
T (eV)	[1]	summation	approximation
1	0.414	0.518	1.47
2	0.262	0.524	1.09
3	0.228	0.511	0.91
4	0.221	0.492	0.79

TABLE VI. "Cutoff" parameter $\rho_{\min}/a_B$ for the $\Delta n=1$ transition of the hydrogen atom at an electron density of 10^{17} cm^{-3} and a temperature of 12 000 K.

Atomic level	This paper	Griem
$n=2$	7.30	9.20
$n=3$	16.24	15.34
$n=4$	27.86	21.47

TABLE VII. "Cutoff" parameter $\rho_{\min}/a_B$ for the $\Delta n=1$ transition of the hydrogen atom at the level $n=3$, an electron density of 10^{17} cm^{-3}, and different temperatures.

T/K	This paper	Griem
12 000	16.24	15.34
50 000	15.53	7.87
100 000	15.20	5.57

peratures. Griem's minimal impact parameter decreases faster with the temperature. Thus, our shifts are smaller than those given by Griem, which is in good agreement with experiment [24].

IV. CONCLUSIONS

A full quantum-mechanical theory has been applied to calculate hydrogen line shifts. In order to be able to deal with weak as well as strong collisions, the electron-emitter interaction has been treated via partial summation of the corresponding perturbation series. Thus, the theory developed contains no arbitrary parameters. The calculated shifts for the $n=2$ levels agree well with the results given by Unnikrishnan and Callaway, whereas for the $n=3$ levels the results for the line shift are larger than those of the phase-shift calculations. Keeping in mind that the shifts caused by the ions of the plasma reduce the resulting line shifts, this is in agreement with experimental results.

For higher temperatures, the shifts obtained from this theory are smaller than those given by Griem, which is in agreement with experimental results. The linewidths obtained exceed those of semiclassical theories because the virtual $\Delta l=0$ (monopole) contributions are automatically included in quantum-mechanical theories. However, they are smaller than those given by Unnikrishnan and Callaway. These comparisons serve as a test of the theory. The final purpose of this theory is the calculation of asymmetric and shifted line profiles from first principles. The inclusion of the ion-radiator interaction into the calculation of the profile will be the subject of a forthcoming paper.

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