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Measurement and Calculation of the Stark-Broadening Parameters for the Resonance Lines of Singly Ionized Beryllium*

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The electron-impact-broadened profile of the resonance doublet of singly ionized beryllium ($2s$-$2p$, $\lambda = 3130.4$ and 3131.1 Å) has been measured using an electromagnetically driven shock tube and a rapid-scanning Fabry-Perot spectrometer. For the conditions $N_e = 10^{17}$ cm^{-3} and $T = 19\,000$°K, we found the Lorentz half-width of each line in the doublet to be 0.035 Å ± 15%. For comparison with theory, we did both a quantum-mechanical (using the close-coupling method) and a semiclassical calculation, obtaining the values 0.015 and 0.042 Å, respectively. Possible reasons for the discrepancy are discussed.

I. INTRODUCTION

From previous measurements[1] on calcium and magnesium, we have concluded that although the agreement between measured and calculated Stark widths was good, there was still a significant discrepancy, particularly with the results obtained using the quantum-mechanical (close-coupling)[2] theory. In a more recent paper[3] it was shown that the semiclassical theory agrees quite well with measurements of Stark parameters of singly ionized atoms so that we now wanted to find a definitive test for the quantum theory. To this end, we chose a first ion which was nonhydrogenic, namely, singly ionized beryllium (lithiumlike). Its resonance doublet can be measured and provides a simple atomic system with which to work (one electron outside of a closed shell) so that we might determine whether or not there is a fundamental problem with the application of current quantum-mechanical theories to broadening of spectral lines.

Our notation is that i, f refer to the initial and final energy levels, respectively, and that i', f' are nearby states which perturb (in the perturbation-theory sense) the i, f levels. We also use the usual definition of shift and width, namely, the shift is the distance of the profile maxima from the position of the unperturbed lines ($N_e \to 0$) which should be the same (to the accuracy of our experiment) for both lines in the doublet, and the width is one-half of the separation between the two half-intensity points of *each* component of the spectrum (referred to as the "half-width").

II. LINE-PROFILE MEASUREMENTS

The apparatus and experimental procedure are similar to those used in a previous experiment[1] so that we merely summarize the equipment, the diagnostic procedures, and the apparatus used to scan the line profiles of interest and discuss, primarily, the differences from the previous arrangement.

A. Light Source

To obtain the desired conditions ($N_e \simeq 10^{17}$ cm^{-3} and $T \simeq 20\,000$ °K) where electron impacts are the predominant broadening mechanism for "isolated" lines, we used an electromagnetically driven shock tube [see Fig. 1(a)]. The background gas was 95% helium and 5% molecular hydrogen at a filling pressure of 1–2 Torr. The beryllium was introduced by dusting the quartz tube with $BeCl_2$ powder. The shock wave then picked this up enroute to the reflector. This produced a plasma in local thermodynamic equilibrium, at the desired conditions, which lasted 10–20 μsec. A slight (15% from tube center to tube wall) nearly linear inhomogeneity in the electron density was allowed for in the data reduction.

B. Measurement Apparatus

To measure the narrow Be^+ resonance lines (~0.04 Å), we used a rapid-scanning Fabry-Perot spectrometer[1,4–6] which gave us a scanning time for one complete profile of 1–2 μsec. This was limited, primarily, by the available light and not by any physical limitation of the spectrometer itself, such as the breaking strain of the piezoelectric crystal. This time was short compared to relevant times for variations in the plasma (we used this as a criterion for selecting profiles to be reduced).

The etalon used was made of fused silica and was 1 in. in diameter and 6 mm thick (each mirror). The plates were front-coated with a dielectric coating to yield a reflectivity, at the wavelengths of interest (3131 Å), of 83%, a transmission of 12%, and an absorption of 5%. They were back-coated with a $\frac{1}{2}$% antireflection coating. Other parameters of interest [see Fig. 1(b)] are the diameter of the aperture stop (3 mm), the scanning aperture ($P = 0.5$ mm), the focal length of the final lens ($F = 200$ mm), and the dispersion of the monochromator which was about 16 Å/mm.

Instrumental broadening was caused primarily by the reflectivity of the etalon with a slight effect due to dynamic bowing. The instrument finesse (ratio of the free spectral range to the instrument width) in the slow scanning ($\tau \sim 5$ sec) mode was $N = 16$–17 and in the fast scanning ($\tau \simeq 1$ μsec) was $N = 15$–16. All other effects, such as changes in finesse due to changes in etalon spacing, were negligible compared to these two effects. Since the measurement of the instrument profile in the fast-scanning mode at low densities was very difficult owing to the transition being a closely spaced doublet rather than a single line, we found the instrument profile in the slow scanning mode. At worst, this introduced an error of 0.5% (see Table I).

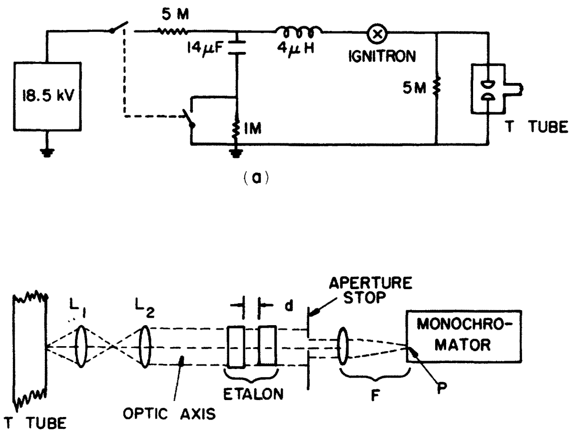

FIG. 1. (a) Schematic of the T-tube system used to produce the beryllium ions in a homogeneous plasma with $T \sim 19\,000$ °K and $N_e \sim 10^{17}$ cm^{-3}. (b) Optical system used with the Fabry-Perot spectrometer. d is the etalon spacing, F is the focal length of the final lens, and P is the diameter of the scanning aperture.

TABLE I. Measured values of the beryllium resonance linewidths. These are the values of the Lorentz width for the singly ionized beryllium resonance lines at $\lambda = 3130.4$ and 3131.1 Å. The results are normalized to $N_e = 10^{17}$ cm^{-3}. The individual values have been corrected for other broadening mechanisms, but in runs 1 and 2 the percent errors are only shot-to-shot fluctuation errors, whereas the final error includes a correction for an inhomogeneity in the electron density. The corrections for other broadening mechanisms are (i) resonance broadening ~0%, (ii) van der Waals broadening ~−5%, (iii) ion (quasistatic) broadening ~−1%, (iv) inhomogeneity of the plasma ~+8%, (v) dynamic bowing of the Fabry-Perot plates $\lesssim -0.5\%$: final correction ~−2%.

Run	Profiles used	w_l (Å)	T (°K) (±20%)
1	4	0.033 ± 6%	17 000
2	9	0.035 ± 12%	20 000
3	5	0.037 ± 20%	20 000
Final	18	0.035 ± 15%	19 000

C. Data Reduction

The result of an experiment is a set of profiles for several values of the etalon spacing [d, see Fig. 1(b)], with each value of d having profiles at several electron densities corresponding to different times in the life of the plasma. After allowing for the instrument profile (obtained by scanning a monochromatic source) and Doppler profile we obtain a set of Lorentz half-widths w_l which, when normalized to $N_e \simeq 10^{17}$ cm^{-3}, should be self-consistent.

The data reduction is accomplished by convolving a Fourier series (which is used to represent the instrument profile[1]) with a Voight profile (used to represent the atomic emission line). These integrations can be performed analytically. We then obtain the following function which can be "fitted" to the experimental data:

$$\phi_{\text{theor}}(x) = \sum_j c_j \frac{\frac{1}{2}A_0 + \sum_m A_n \cos(n\pi x_j) \exp[-n\pi l - (\frac{1}{2}n\pi g)^2]}{\frac{1}{2}A_0 + \sum_m A_n \exp[-n\pi l - (\frac{1}{2}n\pi g)^2]}, \quad (1)$$

where x_j is the reduced wavelength equal to $2(\lambda - \lambda_j)/\Delta\lambda_1$, λ_j is the wavelength of the profile maximum for the jth component, $\Delta\lambda_1$ is the free spectral range of the Fabry-Perot spectrometer, l is the reduced Lorentz width equal to $2w_l/\Delta\lambda_1$, g is the reduced Gaussian width equal to $2w_g/\Delta\lambda_1$, the A_n's are the Fourier cosine coefficients for the instrument profile (we found it unnecessary to include the Fourier sine series), and the c_j's are the relative amplitudes of each component of the spectrum (at $x_j = 0$). This equation can then be fitted to the experimental data using a nonlinear-least-squares technique. The parameters which can be varied are λ_j, c_j, l, g, and the base line of the experimental data. Figure 2 shows a comparison between $\phi_{\text{theor}}(x)$ and $\phi_{\text{expt}}(x)$. The experimental profile has been modified to allow for a time-varying continuum background. An assumption which was made was that both Lorentzian and Gaussian widths would be the same for both lines in the doublet. From quantum-mechanical arguments,[7,8] there is reason to believe that the Lorentz widths will be slightly (~6%) different, but to the accuracy of our measurements (±15%) we could not distinguish this difference.

A final point is that use of the Fourier series for the instrument profile allows for the problem of order overlap. That is, that light from successive transmission maxima are added together to form a complete measured profile, and this effect is allowed for by using a Fourier series to represent the instrument function.

D. Experimental Results

We obtain a self-consistent experiment by measuring the following data: the line profile

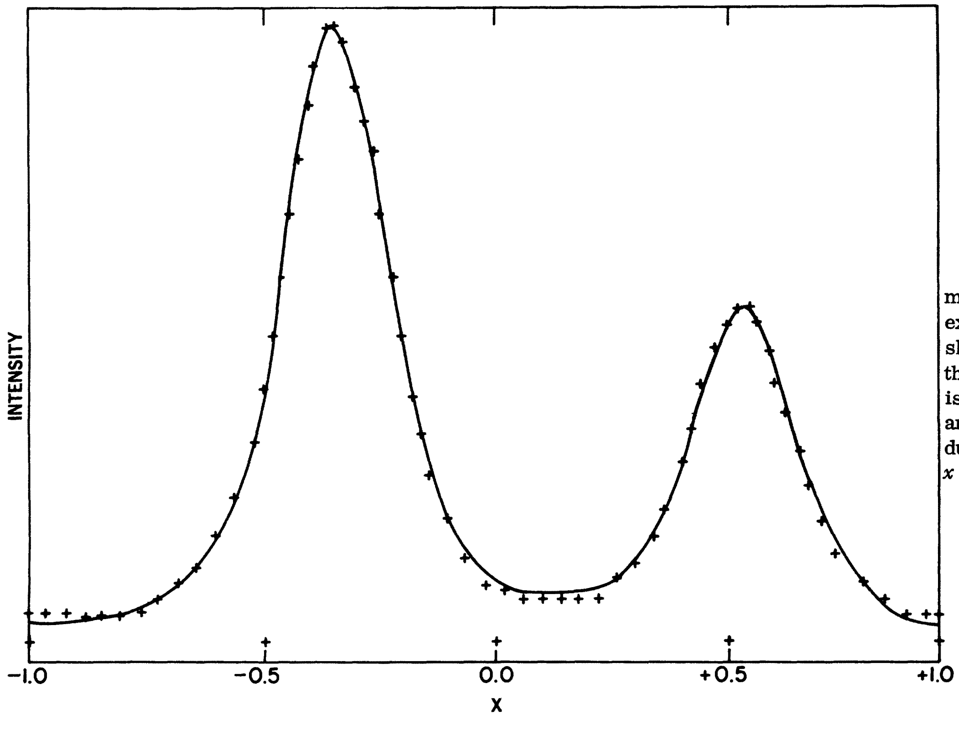

FIG. 2. Comparison of measured (+) vs fitted (–) experimental line profiles, showing the two lines in the doublet. The ordinate is arbitrary intensity units and the abscissa in the reduced wavelength scale $x = 2(\lambda - \lambda_0)/\Delta\lambda_1$.

of interest using the scanning spectrometer; a neutral helium (5016-Å) line-to-continuum ratio for a temperature measurement; and a continuum monitor (~5360 Å), which was synchronized with the scanning spectrometer, for a density measurement. The absolute calibration was checked by scanning the neutral helium line at 3889 Å. The results of the experiment are a set of Lorentz widths together with the density and temperature at which each was measured.

We used a total of 18 scans for which the results are summarized in Table I; the results shown are corrected for other types of line broadening. The percent values of the other possible types of line-broadening mechanisms are also listed (relative to the uncorrected values), as is the final correction which we needed to make, and the final averaged corrected Lorentzian half-width.

III. THEORY

We have used a standard[1,3,9,10] semiclassical, as well as a detailed quantum-mechanical, close-coupling theory[2,7,8,11-13] for comparison with measurement. For the temperature ($T = 19\,000$ °K) and density ($N_e = 10^{17}$ cm^{-3}) of interest, electron-impact broadening dominates so that the intent of the theory is to calculate the following expression,[10]:

$$w + id = \left\langle if \left\| \sum_j f_j (1 - S_{i_j} S_{f_j}^{\dagger}) \right\| if \right\rangle \tag{2}$$

for the width and shift of the lines in terms of the scattering matrices S for the scattering of electrons by ions. The notation is that $\| if \rangle$ is a wave function in "doubled" line space,[10] $\sum_j f_j$ is an average over types of perturber motion, either as an integral over impact parameters for the classical case or as a sum over angular momenta for the quantum-mechanical case. In both formulations there is also an average over a Maxwell velocity distribution.

A. Semiclassical Calculation

A semiclassical calculation is done by making a perturbation expansion for S and using the first-contributing terms. This procedure does not, however, allow for "strong" collisions and it is necessary to include these in some manner.[3,9,10] A further source of error[3] seems to be the incompleteness or incorrectness of the set of available energy levels.

B. Quantum-Mechanical Calculations

The quantum calculations use a fully quantum-mechanical theory with all *relevant* perturbing levels taken into account. Unfortunately, the agreement is not as good as we had expected from our experience with calcium and magnesium.[1] If the theory adequately describes an atomic system and its interaction with a plasma, the calculations for *simpler* atomic systems should show better agreement with measured line profiles. This does not seem to be the case for the sequence calcium,[7] magnesium,[8] and beryllium, which procedes from a more complex to simpler atomic systems.

1. *Method of Calculation*

The expression for the linewidth for a transition of the form $n_f s_{1/2} - n_i p_J (J = \frac{3}{2}, \frac{1}{2})$ can be derived from the formula given by Bely and Griem[8] and can be written

$$w = \pi N_e \left(\frac{\hbar}{m}\right)^2 \sum_l \int_0^\infty \frac{f(v)}{v} (C_s + C_p + C_{sp})\, dv \ (\text{cm}^3\ \text{sec}^{-1}), \tag{3}$$

where l is the orbital angular momentum of the colliding electron. "Direct" terms C_s and C_p are given by

$$C_s = \tfrac{1}{4} \sum_{S_s^T} (2L_s^T + 1)(2S_s^T + 1)\, \mathrm{Re}(T_s^*), \tag{4a}$$

$$C_p = \tfrac{1}{12} \sum_{L_p^T S_p^T} (2L_p^T + 1)(2S_p^T + 1)\, \mathrm{Re}(T_p), \tag{4b}$$

and the mixed "interference" term C_{sp} by

$$C_{sp} = -\tfrac{1}{12} \sum_{L_p^T, S_s^T = S_p^T} (2L_p^T + 1)(2S_p^T + 1)\, \mathrm{Re}(T_s^* T_p) - \tfrac{1}{9}(2J+1)^{-1} \sum_{L_p^T, S_p^T, S_s^T} (-1)^{S_s^T + S_p^T}\, \mathrm{Re}(T_s^* T_p). \tag{4c}$$

The diagonal elements of the transition matrix $\underline{T}$ are

$$T_s = T(s\tfrac{1}{2} l\tfrac{1}{2} L_s^T S_s^T;\ s\tfrac{1}{2} l\tfrac{1}{2} L_s^T S_s^T)$$

and

$$T_p = T(p\tfrac{1}{2} l\tfrac{1}{2} L_p^T S_p^T;\ p\tfrac{1}{2} l\tfrac{1}{2} L_p^T S_p^T),$$

corresponding to the scattering of an electron with orbital angular momentum l by an ion in the s or p state, respectively. If the matrix $\underline{T}_s$ is evaluated at the energy E then $\underline{T}_p$ must be evaluated at E plus the $2s$-$2p$ excitation energy. $\underline{T}$ is given in terms of the $\underline{R}$ matrix by $\underline{T} = -2i\underline{R}(1 - i\underline{R})^{-1}$. The total spin and orbital angular momentum of the system (atom plus colliding electron) are S_s^T, S_p^T and L_s^T, L_p^T, respectively. For $\underline{T}_s$ we have $L_s^T = l$.

For the computation of the $\underline{T}$ matrix we have used

TABLE II. Partial-wave contributions (%) to the width. Exchange is *not* included in these calculations.

	T (°K)			
l	5000	10 000	20 000	40 000
0	9.4	9.3	7.5	5.9
1	31.8	31.6	28.8	23.8
2	39.8	33.3	27.5	22.9
3	15.0	19.8	25.1	27.5
4	2.9	4.2	7.0	11.0
5	0.78	1.26	2.54	5.05
6	0.17	0.41	1.05	2.53
7	0.08	0.17	0.48	1.37

a general close-coupling program written by Moores[14] which uses a noniterative technique for the solution of the system of coupled equations.

2. *Calculations*

a. Calculation without electron exchange. If the possibility of electron exchange is omitted then the $\underline{\text{T}}$ matrix is independent of the total spin S^T, the second term in the expression for C_{sp} vanishes, and both components of the multiplet have the same width. Since partial contributions to the linewidth decrease rapidly with increasing l (see Table II), in no case have we included contributions for $l \geqslant 8$.

Five atomic states ($2s2p3s3p3d$) have been included in the calculation for angular momenta $L^T = 0, 1$ and energies of the free electron[15] greater than 10.0 eV. For $L^T > 1$ the five-state calculation was used for energies above the $3d$ threshold. Below 10.0 eV, numerical difficulties prevented the program from finding a solution if both the $3p$ and $3d$ states were included. In this region we have, therefore, performed a four-state calculation, omitting either the $3p$ or $3d$ level. Below 1.35 eV similar difficulties restricted the calculation to three or two states (see Table III). It was found that in this latter region the $\underline{\text{T}}$ matrices in most cases were not sensitive to the omission of the upper states in the close-coupling method.

Just below the excitation thresholds of levels ($2p, 3s, 3p,$ and $3d$) the resonant structure of the $\underline{\text{T}}$ matrix is very dense. In these regions we have used averaged $\underline{\text{T}}$-matrix elements in the expression for the linewidth. These were found, using the prescription of Seaton,[12] by extrapolating the $\underline{\text{Y}}$ matrix below threshold and then calculating the $\underline{\chi}$ matrix. Matrix elements of $\underline{\chi}$, connecting two open channels i, k are related to $(T_{ik})_{\text{av}}$ by $(T_{ik})_{\text{av}} = \delta_{ik} - \chi_{ik}$. This method can be used if all closed channels have the same energy. A quadratic fit to $\underline{\text{Y}}$ was found to be satisfactory except for $L^T = 0, 1$ above the $2p$ level, where a more complicated expression was employed. To obtain averaged $\underline{\text{T}}$-matrix elements below the $3p$ level, we extrapolated $\underline{\text{Y}}$ from the region above the $3d$ level as the $3p$ and $3d$ levels are very close. In this case, the averaging procedure can introduce an error just below the $3p$ level, since in this case the closed channels are no longer degenerate. However, this error in $(T)_{\text{av}}$ cannot affect w much, because it occurs only a small interval of energies. Another inaccuracy could be introduced by the averaging process in the mixed term C_{sp}, if regions with dense resonances in both $\underline{\text{T}}_s$ and $\underline{\text{T}}_p$ overlap.[13] With Be$^+$ this situation does not occur. To simplify calculations, we also used averaged $\underline{\text{T}}$-matrix elements between 10.0 eV and the $3d$ threshold for $L^T > 1$.

One can separate contributions to the linewidth corresponding to direct terms C_s, C_p and to the mixed term C_{sp}. Furthermore, C_s and C_p can be split into two parts representing elastic and inelastic processes using the relation

$$\text{Re}(T) = \tfrac{1}{2} \sum_{l'} |T(lL^T, l'L^T)|^2$$

$$= \tfrac{1}{2} \sum_{\text{el}} |T(lL^T, l'L^T)|^2 + \tfrac{1}{2} \sum_{\text{inel}} |T(lL^T, l'L^T)|^2 .$$

TABLE III. Combinations of atomic levels used for calculating the T matrix. These are the electronic states used in calculating the T matrix via the close-coupling method for various regions of energy (of the colliding electron with respect to the ground state). Exchange is not included. The energy required for excitation of an electron from the ground state ($2s$) to the various excited states of the ion are $2p = 3.95$ eV; $3s = 10.9$ eV; $3p = 12.0$ eV; $3d = 12.1$ eV.

Region (eV)	$L^T = 0, 1$	$L^T > 1$
$E < 1.35$	$2s2p3s$	$2s2p$
$1.35 < E < 10.0$	$2s2p3s3p$ or $2s2p3s3d$	Same as for $L^T = 0, 1$
$10.0 < E < 12.1$	$2s2p3s3p3d$	$(T)_{\text{av}}$ by extrapolation of Y below ($3d$)
$12.1 < E$		same as for $L^T = 0, 1$

TABLE IV. Partial contributions to w/N_e. These calculations are for a temperature $T = 20\,000$ °K and the units are 10^{-8} cm^3 sec^{-1}. Exchange is not included.

	2s (direct term)		2p (direct term)		
l	El.	Inel.	El.	Inel.	Mixed term
0	7.64	0.02	8.02	1.38	−14.09
1	28.43	0.58	17.64	1.70	−37.05
2	3.35	0.75	4.00	4.13	−1.37
3	5.47	1.22	1.22	2.34	−0.36
4	0.68	0.68	0.35	0.98	0.00
5	0.12	0.30	0.13	0.42	0.00
6	0.04	0.13	0.06	0.18	0.00
7	0.01	0.05	0.03	0.08	0.00
Total	45.73	3.73	31.45	11.21	−52.87

The result of this separation is shown in Table IV for $T = 20\,000$ °K. The mixed term is important for the first two angular momenta and appreciably affects the total width. The inelastic contribution to the direct terms for low values of l is very small, but increases with increasing l, and for large l, inelastic contributions dominate for both the s and p levels. Table IV shows that inelastic contributions represent 38% of the *total* width and elastic contributions combined with the mixed terms yield the remaining 62%. Inelastic contributions arise almost exclusively from excitation and deexcitation of the $2p$ level. Inelastic terms representing excitation increase with increasing temperature for all l and those representing deexcitation decrease with increasing temperature for small l and increase for large l.

Total calculated half-widths, as a function of temperature, are shown in Fig. 3 and Table V. The results shown in Fig. 3 and listed in Tables II and IV were obtained using levels ($2s2p3s3p$) in the region between 1.35 and 10.0 eV. Widths calculated using the levels ($2s2p3s3d$) are somewhat lower (~10%).

b. Calculation with electron exchange. In doing the close-coupling calculations with exchange, the levels ($2s2p3s3d$) have been used for all energies. Owing to a considerable increase in computing time, $\underline{T}$-matrix elements have been computed for a much smaller number of energies than for the calculation excluding exchange, and we have made extensive use of the extrapolation procedures of the quantum-defect method. However, as shown by similar calculations performed for the nonexchange case, this simplification does not change the accuracy of the width by more than 10%. Since the effect of exchange decreases rapidly with increasing l or L^T, the calculations using exchange have been carried out only for $L^T < 4$. Contributions for higher angular momenta were taken over from the nonexchange calculations.

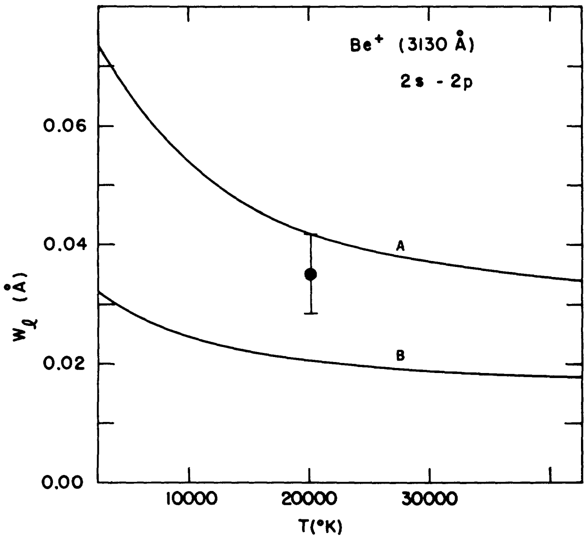

FIG. 3. Comparison of the measured value of the Lorentzian half-width vs (A) the semiclassical calculation and (B) the quantum-mechanical calculation which was done *excluding* exchange.

The results are presented in Table V. The inclusion of exchange decreases the width for

TABLE V. Comparison of calculated widths. Comparison of the effect of including two different sets of atomic levels and exchange terms in the close-coupling computer code. Results are in Ångström units and are calculated at $N_e = 10^{17}$ cm^{-3}.

			T(°K)		
Levels included		Method	5000	10 000	20 000	40 000
$2s2p3s3p$ or $2s2p3s3d$	(for details see Table III)	Without exchange	0.0320 0.0277	0.0244 0.0219	0.0205 0.0188	0.0176 0.0162
$2s2p3s3d$		With $s_{1/2}$-$p_{1/2}$ exch. $s_{1/2}$-$p_{3/2}$	0.0289 0.0275	0.0185 0.0175	0.0154 0.0147	0.0136 0.0132

higher temperatures. This effect is due primarily to larger mutual cancellation of the direct and mixed terms for angular momenta $l=0,1$, so that at $T=20\,000$ °K the major contributions to w come from the $l=2,3$ partial waves. The difference between the linewidths of the two components of the doublet is less than 6% for all temperatures considered, which justifies our use of equal Lorentzian linewidths in the experimental deconvolution.

It seems unlikely that the difference between the quantum-mechanical result and the measured value for the width can be attributed to omission of levels higher than $3d$. The difference between linewidths obtained using either the $3p$ or $3d$ level is rather small and suggests that higher levels are not very important. At temperatures below $T=40\,000$ °K inelastic collisions leading to excitation of levels ($3s, 3p$, and $3d$) are almost negligible.

On the other hand, the quantum results seem to be quite sensitive to the value of the $\underline{T}$ matrix for small angular momenta l, due to the large cancellation of direct and mixed terms in the expression for the linewidth (see Table IV). Thus, even small inaccuracies in $\underline{T}$ may produce large corresponding errors in the resulting values for the linewidth. We have obtained these same results using another computer code and computer.

IV. CONCLUSIONS

The results of the line-profile measurements and the two theoretical results are shown in Fig. 3. The agreement between the measured widths and the corresponding semiclassical calculations is quite good, whereas the agreement with quantum calculations is no better than a factor of 2. As this is the simplest atomic system (an ion with a single electron outside of a closed shell but nonhydrogenic) with which we can work, the quantum theory should be limited only by the numerical accuracy. As we still have disagreement with the experimental results (more so than with the much simpler semiclassical theory), one must conclude that either the numerical accuracy is less than one would expect from a double-precision calculation, or that some quantum-mechanical interaction has not been included. It has been pointed out[16] that the evaluation of the interference term (which decreases the width) may yield too large a value due to the lack of intermediate states[10] necessary to evaluate this term.

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