Shift and Broadening of Neutral Helium Spectral Lines in Dense Plasmas

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Abstract. Shift and broadening of isolated neutral Helium lines 7281 Å (2\textsuperscript{1}P \rightarrow 3\textsuperscript{1}S), 6678 Å (2\textsuperscript{1}P \rightarrow 3\textsuperscript{1}D), and 4713 Å (2\textsuperscript{3}P \rightarrow 4\textsuperscript{3}S) in a dense plasma are investigated. Based on a quantum statistical theory using thermodynamic Green's functions, where the electronic contributions to the shift and width are considered. Dynamical screening of the electron-atom interactions are included. Compared to the width, the electronic shift is more affected by dynamical screening. This effect is increased at high density. A cut-off procedure for strong collisions is used. The effect of the ions are taken into account in a quasi-static approximation, with both the quadratic Stark effect and the quadrupole interaction. The results for shift and width agree well with theoretical calculations and experimental data.

1. Introduction
Line profile calculations are a powerful method for both laboratory and astrophysical plasmas, e.g. to determine the internal parameters or to understand the microscopic processes within the plasma [1, 2].

Helium spectral lines are important for plasma diagnostics in laboratory such as shock wave tube or pulsed arc plasmas, in stellar atmospheres, and also to interpret theoretical approach. The influence of the surrounding electrons and ions in a plasma lead to a modification of the spectral line. In particular, time-dependent electric fields generated by the surrounding charges modify the spectral line via the Stark effect. In this context, screening as an important collective effect in a plasma has to be taken into account. The influence of electrons and ions can be treated separately due to the difference in mass and mobility. A traditional impact approximation can be used for electrons, while almost stationary heavy ions are treated in a quasi static ion approximation due to static micro fields [3].

In this work, the theoretical approach to spectral line shapes of non-ideal plasmas is presented in section 2. In section 3, the shift and full width at half maximum (FWHM) for non-overlapping isolated He I lines 7281 Å, 6678 Å, and 4713 Å are illustrated and discussed.

2. Theory
A quantum statistical approach has been advanced to account in a systematic way for medium modifications of spectral line shapes. Here, we give a short review of the most important results. For details, we refer to Refs. [4, 5].
The electronic shift and width of spectral lines are calculated with the help of thermodynamic Green’s functions. In this way, the pressure broadened profile $I^\text{pr}$ is obtained in the quasi-static approximation by averaging over the ionic micro fields [6]
\[
I^\text{pr}(\Delta \omega) = \frac{[\omega_0]^4}{8\pi^3 c^3} \exp\left(-\frac{\hbar \omega_0}{k_B T}\right) \left(1 + \frac{\Delta \omega}{\omega_0}\right)^4 \exp\left(-\frac{\hbar \Delta \omega}{k_B T}\right) \times \sum_{i',f,f'} e^2 \langle i|\mathbf{r}|f\rangle \langle f'|\mathbf{r}|i'\rangle \int_0^\infty dE P(\beta) \Im \langle i|(fL^{-1}(\Delta \omega, \beta))f'|i'\rangle .
\]
(1)

Where $\Delta \omega$ is the frequency deviation from the unperturbed transition frequency $\omega_0$ of the initial $i$ and final $f$ atomic states. The ionic micro fields are incorporated via the Hooper field distribution function $P(\beta)$ and $\beta = E/E_0$ is the normalized field strength [7]. Medium modification given via the function $L$
\[
L(\Delta \omega, \beta) = \hbar \Delta \omega - \Re (\Sigma_i(\Delta \omega, \beta) - \Sigma_f(\Delta \omega, \beta)) - i \Im (\Sigma_i(\Delta \omega, \beta) + \Sigma_f(\Delta \omega, \beta)) + i \Gamma_f^{\text{el}} ,
\]
(2)

which contains the self energy corrections of the initial $\Sigma_i$ and final states $\Sigma_f$ and the vertex correction $\Gamma_f^{\text{el}}$ for the overlapping lines. Note, that electronic as well as ionic contributions could be occurred. Within Born approximation with respect to the perturber-radiator interaction, the electronic contribution reads
\[
\Delta_n^{\text{SE}} + i \Gamma_n^{\text{SE}} = < n|\Sigma_i(E_n^0/\hbar + \delta \omega, \beta)|n > = -\frac{1}{e^2} \int \frac{d^3q}{(2\pi)^3} V(q) \sum_{\alpha} |M_{n\alpha}(q)|^2 \times \int_{-\infty}^{\infty} \frac{d\omega}{\pi} (1 + n_B(\omega)) \frac{\Im \varepsilon^{-1}(\mathbf{q}, \omega + i0)}{\hbar \delta \omega - (E_{\alpha}(\beta) - E_n^0) - \hbar(\omega + i0) .
\]
(3)

In this expression, $n_B(\omega)$ is the Bose distribution function, $V(q)$ is the Coulomb potential, $M_{n\alpha}$ are the matrix elements of the dipole operator, and $\varepsilon(\mathbf{q}, \omega)$ is the dielectric function.

Many particle effects such as screening are contained in the inverse dielectric function, which is taken in random phase approximation
\[
\varepsilon^{\text{RPA}}(\mathbf{q}, \omega) = 1 - e^2 \int \frac{dp}{(2\pi)^3} V(q) \frac{f_\uparrow(E_p) - f_\uparrow(E_{p+\mathbf{q}})}{E_p - E_{p+\mathbf{q}} - \hbar \omega - i0} ,
\]
(4)

where $E_p = \hbar^2 p^2/2m$ is the kinetic energy of the single particle. In high frequency limit, where $\omega_{\text{pl}} < \omega_{na}$, the inverse dielectric function can be approximated as
\[
\Im \varepsilon^{-1}(\mathbf{q}, \omega) \approx -\Im \varepsilon(\mathbf{q}, \omega) ,
\]
(5)

and
\[
\Im \varepsilon^{\text{RPA}}(\mathbf{q}, \omega) \approx 2\pi \frac{V(q)}{\Omega} \sum_p |f_\uparrow(E_p) - f_\uparrow(E_{p+\mathbf{q}})| \delta(E_p - E_{p+\mathbf{q}} - \hbar \omega) .
\]
(6)

However, if the transition frequency $\omega_{na}$ becomes comparable to the electron plasma frequency $\omega_{\text{pl}} = (N_e e^2/\epsilon_0 m_e)^{1/2}$, the full expression of the inverse dielectric function has to be used. While the approximation of the inverse dielectric function leads to a linear behavior of the electronic shift contribution with respect to electron density, a nonlinear dependence of the electronic shift with increasing electron density is to be expected if the full dielectric function is used [8, 9].
Transition matrix elements $M_{\alpha\beta}$ are evaluated in dipole approximation using the Coulomb approximation method of Bates and Damgaard for the radial wave function [10, 11]. The spherical part is approximated by a linear combination of hydrogen-like wave functions.

As stated above, the electronic contribution of the self energy is evaluated in Born approximation. This overestimates the self energy. To prevent the overestimation in which the perturbation theory fails, we introduce a cut-off procedure for the q-integral in Eq. (3) by an upper cut-off parameter $q_{\text{max}}$ instead of e.g. solving the T-matrix or using the close coupling method. Following Griem [3, 11], this cut-off parameter is the inverse of the minimum limiting impact parameter ($q_{\text{max}} = 1/\rho_{\text{min}}$) [12]

\begin{equation}
\rho_{\text{min}} = \left[ \frac{2e^4}{3h^2v^2} \sum_\alpha |<n^\alpha|r|\alpha>|^2 |A(z_{\text{min}}^\alpha) + iB(z_{\text{min}}^\alpha)|^2 \right]^{1/2}, \tag{7}
\end{equation}

where $I$ and $K$ are modified Bessel functions. An appropriate strong electronic collision term for the width of neutral helium, which is introduced by Griem et al. [13], should be added to the width in Eq. (3)

\begin{equation}
\left(\frac{3}{4}\right) \frac{3}{4} N_e \int dv f(v) v \pi \rho_{\text{min}}^2, \tag{8}
\end{equation}

where $f(v)$ is the Maxwell velocity distribution function, $v$ is thermal electron velocity, and $N_e$ is the electron density.

The static ionic contribution to the ionic self energy is treated by means of the micro field concept including both quadratic and quadrapole effects. The first order perturbation term vanishes for non-hydrogenic like atoms because of nondegeneracy with respect to the orbital quantum number $l$. According to second order perturbation theory, the quadratic Stark effect is proportional to the square of the micro electric field. In the case of He I, it is given by [14]:

\begin{equation}
\Sigma_{nlm}^2(E) = \frac{9e^2n^2}{4(2l+1)} \left[ \frac{(n^2 - (l + 1)^2((l + 1)^2 - m^2))}{(2l + 3)(E_{nl} - E_{nl+1})} + \frac{(n^2 - l^2)(l^2 - m^2)}{(2l - 1)(E_{nl} - E_{nl-1})} \right], \tag{9}
\end{equation}

where $E$ is the micro electric field, $n$, $l$, and $m$ are the well known principle, orbital, and magnetic atomic quantum number, respectively.

The quadrapole Stark effect is due to the inhomogeneity of the ionic micro field. We use the expression derived by Halenka [15]

\begin{equation}
\Sigma_{nlm'}^3(E) = -\frac{5}{2\sqrt{32\pi}} \frac{eE_0}{R_0} B_\rho(\beta) <n|3z^2 - r^2|n'> . \tag{10}
\end{equation}

Here, $B_\rho(\beta)$ is the mean field gradient at a given field strength and the screening parameter $\rho = R_0/r_D$ is taken as the ratio between the mean distance and the Debye radius.

Finally, thermal Doppler broadening is taken into account by a convolution with a Maxwellian velocity distribution [6]

\begin{equation}
I(\Delta\omega) \propto \int_{-\infty}^{\infty} d\Delta\omega' \exp\left[-\frac{m_e c^2}{2k_BT}(\frac{\Delta\omega - \Delta\omega'}{\omega_0 + \Delta\omega'})^2\right] I_{\text{pr}}(\Delta\omega') . \tag{10}
\end{equation}
3. Results and discussion

The calculated FWHM and the shifts of the line 6678Å as a function of the electron density are given in Figs. 1 and 2, respectively. Doppler broadening is included according to Eq. (10). The approximation for the dielectric function, see Eq. (6), indeed leads to a linear dependence with increasing density. Dynamically screened electron-atom interactions reduce the magnitude of the shift at high densities and shows some non-linear behavior at high densities. The results have been compared with various experimental studies: i) values are obtained in a pulsed arc plasma by Pérez et al. [16] for the electron densities \( (2.0 - 6.5) \times 10^{22}\text{m}^{-3} \) and temperatures \( (1.9 - 4.3) \times 10^{4}\text{K} \). ii) experimental values have been measured in a laser produced plasma by Vujčić et al. [17] for electron densities \( (0.7 - 1.7) \times 10^{23}\text{m}^{-3} \) at a temperature \( 3 \times 10^{4}\text{K} \). iii) a repetitively pulsed low-pressure arc hydrogen-helium plasma was used by Mijatović et al. [18] in the electron densities range \( (0.25 - 0.59) \times 10^{22}\text{m}^{-3} \), electron temperatures from \( (1.93\text{ to } 2.36) \times 10^{4}\text{K} \) and gas temperatures from \( (0.5\text{ to } 1.2) \times 10^{4}\text{K} \). iv) the visible spectrum emitted by a helium plasma generated in a wall-stabilized arc has been reported by Kelleher [19] at electron density \( 1.03 \times 10^{22}\text{m}^{-3} \), electron and a gas temperature \( 2.09 \times 10^{4}\text{K} \) and \( 1.58 \times 10^{4}\text{K} \), respectively. v) measurement by Milosavljević et al. [20] was performed at electron densities \( (0.3 - 8.2) \times 10^{22}\text{m}^{-3} \) and electron temperatures \( (8 - 3.3) \times 10^{4}\text{K} \) in five different plasma discharge conditions using a linear, low-pressure, pulsed arc as an optically thin plasma source operated in a helium-nitrogen-oxygen gas mixture. Comparison with some other theoretical works have been also performed. Bassalo et al. [21] assumed in their calculations a semi-classical approach for electron collisions in plasmas and ions have been treated in the same way as Griem’s approach [3]. Furthermore, results obtained by a molecular dynamic (MD) simulation for independent and interacting particles by Gigosos et al. [22, 23] are included for electron densities range \( (0.25 - 50.0) \times 10^{22}\text{m}^{-3} \) and temperatures range \( (1.9 - 4.2) \times 10^{4}\text{K} \). In general, our calculated FWHM results for the given densities and temperatures agree well with the other theoretical and experimental values. Deviations arise for densities above \( N_e = 10^{23}\text{m}^{-3} \) in comparison with the available MD data. The discrepancy between our results and the available data is more pronounced for the shift. For low densities, the calculated shift is about half the size of the MD data, while at high densities we overestimate the shift as compared to the MD results. Concerning the high densities, the data by Gigosos already indicate the importance of strong coupling effects. Regarding the data point reported by Bassalo et al., the discrepancy might be due to neglect of the shift and width in the lower states. Instead, the matrix element is calculated via the oscillator strength of transition. Furthermore, the discrepancies might be related somehow to the ambiguous definition of the cut-off parameter. In addition, the line profile (6678Å) might be no longer isolated or the linear Stark effect might be of importance at high electron densities. Note, that an asymmetric profile of this line was already shown in our previous work [24].

A similar calculation is performed for the line 7281Å. The comparison are shown in Figs. 3 and 4. Again, the overall agreement with results published by other authors are quite well. As before, deviations are more pronounced for the shift and less for the width. Also, discrepancies are larger at higher densities. Note, that the calculation by Gigosos et al. [22, 23] covers the densities range \( (0.25 - 50.0) \times 10^{22}\text{m}^{-3} \) and temperatures range \( (1.9 - 4.2) \times 10^{4}\text{K} \), while in Ref.[25] the temperatures lie in the interval \( (1.6 - 2.5) \times 10^{4} \) with a mean value around \( (2.0 \times 10^{4})\text{K} \).}

Stark broadening calculations have been also performed for the line 4713Å, see Fig. 5. A linear dependence of the FWHM with the electron density is found. For this transition, Pérez et al. [16] have carried out measurements in the temperatures range \( (1.9 - 4.3) \times 10^{4}\text{K} \). In this case, only results for the width have been reported. We notice a good agreement of our results with these data.
Figure 1. The full width half maximum of He I line 6678Å. —— this work, ····· this work (dynamical screening), - - - - this work (Doppler broadening). A comparison is made with various theoretical and experimental data.

Figure 2. Shift of line 6678Å versus electron density. ◊ this work and ◊ this work with dynamical screening. The electron temperatures are taken according to the References given in Sec. 3.

Figure 3. Stark FWHM for He I line 7281Å as a function of electron density. ◊ this work. Comparison with some theoretical and experimental data are shown.

Figure 4. Shift of line 7281Å versus electron density. ◊ this work and ◊ this work (dynamical screening) are compared with the previous data.

4. Conclusion
Using a quantum statistical approach of spectral lines in-medium modifications, we have reported results for the shift and the broadening of neutral helium lines. The overall agreement of our calculations with experimental results as well as other theoretical studies is good, in particular for the width. It is obvious, that the line shape depends strongly on the charged perturbers density. Dynamical screening decreases the shift especially at high electron density. However, quantitative discrepancies remain to be investigated at higher electron densities. To address these shortcomings, several improvements should be considered. At high densities, pair-correlation effects are important for the micro fields and should be included by an appropriate approach. Furthermore, a microscopic description of strong collisions via partial summation of T-matrix diagrams should be used to avoid artificial cut-off parameters. Finally, the use of the Coulomb approximation for the wave functions should be improved.
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