

including one angular-momentum-dependent term. However, the formulations are basically different, and it is not surprising that there is no direct connection between their higher-order terms and those described here. In the Koelling-Freeman approach the approximations are applied directly to the HF operator rather than to the exchange energy density.

The exchange approximation including higher-order inhomogeneity corrections is of interest in that it does lead to angular-momentum-dependent exchange operators in the variationally derived single-particle approximation. In applications of these exchange approximations to atomic and crystalline systems, it should be realized that the large inhomogeneity corrections which occur particularly in regions of low electron density and

near the nucleus may be a serious error and are mathematical in their origin. Obviously, what is needed is a better range parameter. In lieu of this, the cutoff procedure of Herman *et al.*^{2,15} may be used. An alternative procedure applicable to the low-density region can be obtained by generalizing a scheme described recently by Liberman.¹⁸

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long-range parts affected by the identity plus a convergence condition effectively breaks the lattice sums into two rapidly converging series. The particular success of the Ewald scheme as opposed to known alternatives in the application to lattice sums motivates its use in this context. The short-range (first) term in the identity involves the error-function complement (erfc) which is defined $\text{erfc}(x) = (2/\pi^{1/2}) \int_x^\infty e^{-t^2} dt$.

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Effect of Time Ordering in the Unified Theory

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Using a previously developed unified theory of spectral line broadening, the effects of time ordering over the complete line profile are investigated. The results of calculations for the Lyman- α line are presented.

In a recent paper,¹ a theoretical treatment of spectral line broadening in plasmas has been developed using classical-path methods. The expression for the line shape derived in this treatment unifies certain aspects of the impact,² one-electron,³ and relaxation theories,⁴ and under certain

conditions is valid from the line center to the far line wings. Line profile calculations on the basis of this unified theory have been made for hydrogen.⁵ The effects of time ordering were not included in these calculations. In order to determine the effects of time ordering on the Stark broadening

of hydrogen profiles, numerical calculations have recently been made within the framework of the impact theory, yielding results valid near the line center.^{6,7} The purpose of the present work is to determine the effect of time ordering over the entire profile by making classical-path calculations with the unified theory and including time ordering. Only an outline of the calculations and the main results will be presented; a detailed account of the current work is given elsewhere.⁸

The general expression for the line shape obtained in the unified theory is given as

$$I(\omega) = -\frac{1}{\pi} \left(\text{Im} \sum_{a a' b} (\vec{d}_{a' b} \cdot \vec{d}_{b a}) \rho_{a'} \times \int_0^\infty P(E) \langle a | [\Delta\omega - \mathcal{L}(\Delta\omega)]^{-1} | a' \rangle dE \right), \quad (1)$$

where we have explicitly indicated the average over ion fields. $P(E)$ is the distribution function for the low-frequency component of the fluctuating microfields in the plasma,⁹ $\Delta\omega = \omega - \omega(E)$ [$\omega(E)$ being the Stark component shifted due to the static ion fields], and ρ is the atomic density matrix. The \mathcal{L} operator is defined within the impact approximation (not to be confused with the impact theory which makes the completed collision assumption) by the following expression:

$$\mathcal{L}(\Delta\omega) = -i\Delta\omega \int_0^\infty e^{it\Delta\omega} \langle U_1 - 1 \rangle_{\text{av}} dt \Delta\omega. \quad (2)$$

U_1 is the time-development operator for a binary collision and the bracket $\langle \dots \rangle_{\text{av}}$ denotes the thermal average over perturber states. The usual collision variables (ρ_0, v, t_0) were used in evaluating the thermal average and the effects of incomplete collisions were included.¹⁰ The time-development operator may be given by the familiar time-ordered exponential

$$U(t+t_0, t_0) = \mathcal{O} \exp \left(-\frac{i}{\hbar} \int_{t_0}^{t+t_0} V(t') dt' \right). \quad (3)$$

Differentiating with respect to t_0 , we obtain, for Lyman α ,

$$\begin{aligned} & \frac{i\hbar \partial}{\partial t_0} \langle 2lm | U | 2l'm' \rangle \\ &= \sum_{LM} [\langle 2lm | V(t+t_0) | 2LM \rangle \langle 2LM | U | 2l'm' \rangle \\ & \quad - \langle 2lm | U | 2LM \rangle \langle 2LM | V(t_0) | 2l'm' \rangle]. \end{aligned} \quad (4)$$

$V(t)$ denotes the interaction between the radiator and perturber and was approximated by a dipole potential. A Debye cutoff [at $\rho_0 = (kT_e/4\pi n_e e^2)^{1/2}$] and a strong collision cutoff (at $\lambda = \hbar/mv$) on the radiator-perturber separation [$r = (\rho_0^2 + v^2 t^2)^{1/2}$]

were included in the potential. For values of $\rho_0 \gg 10\lambda$, where ρ_0 is the impact parameter of the collision, we find that the real parts of the matrix elements in Eqs. (4) become equal to the un-time-ordered values. This is merely a consequence of the fact that a second-order expansion of the time-development operator is valid in this region. An approximation due to Berman and Lamb¹¹ was used for impact parameters smaller than $\rho_s = 0.3\lambda$, where $\rho_s \ll \rho_w$ ($\rho_w = \sqrt{2/3}\lambda n^2$ with n the principal quantum number of the upper state). In this approximation a unitary operator is introduced which instantaneously diagonalizes the interaction potential. The coupled differential equations, indicated in Eq. (4) above, were numerically integrated in the region $0.3\lambda < \rho_0 \leq 10\lambda$. Owing to the spherical symmetry of the interaction potential, only the (200) and (21m) matrix elements of the thermal average were required. [Here we have used the notation (nlm) to denote the quantum dependence of the hydrogen levels.] For interaction times greater than $10/\omega_p$ (where ω_p is the plasma frequency) the time-development operator converges to the S-matrix limit, thus calculations in this region were made with the time-ordered S matrix. Physically this corresponds to times of interest large enough such that virtually all collisions are completed.

For comparison, the un-time-ordered time-development operator was also calculated and a difference function generated which represents the effect of time ordering. This effect is illustrated in Fig. 1 where we plot the ratio $C(t)/F(t)$ as a function of time for the required matrix elements of the thermal average. Here $C(t)$ is the thermal average of the difference function and $F(t)$ is the thermal average of the time-ordered time-development operator. The calculation is representative in that the velocity average was performed with the electron velocity distribution $f(v) = \delta(v - v_{\text{av}})$, where v_{av} is the thermal velocity [$v_{\text{av}} = (3kT_e/m)^{1/2}$]. The effect of time ordering on the thermal average was found to increase monotonically with time. The correction to the (200) matrix element approaches a constant value of about -14% for large values of time, while for the (21m) matrix elements the correction approaches +11%. The direction in which the correction occurs for these elements is in agreement with the impact calculation of Bacon, Shen, and Cooper.⁶ The influence of time ordering is still important at times of interest somewhat smaller than $1/\omega_p$; however, it eventually drops off to zero at values of $t \sim 1/\Delta\omega_c$ (the Weisskopf frequency for Lyman α is $\Delta\omega_c = 2kT_e/3\hbar$). This behavior is reflected in the Fourier transform where we find an inverse behavior in frequency space.⁸

The influence on the profile was the greatest in the line center where the intensity was found to decrease by about 12%. The half-width increases over

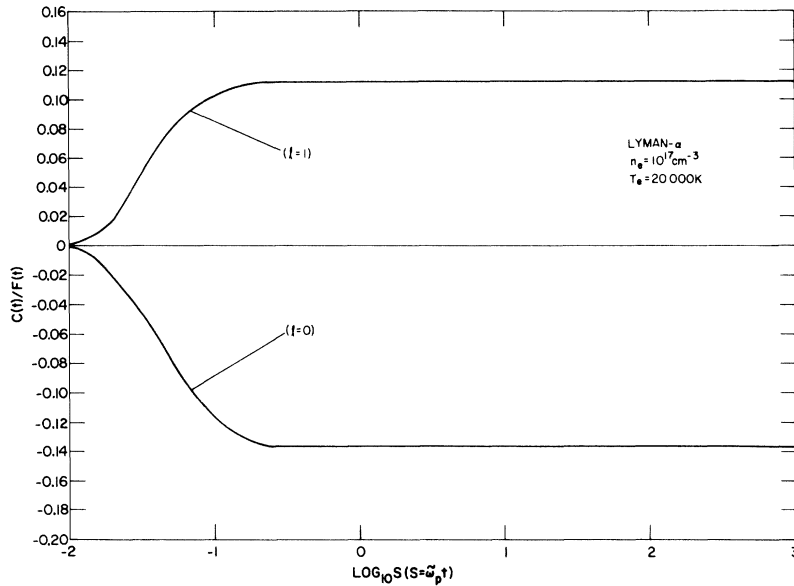


FIG. 1. Ratio of the thermally averaged difference function to the thermal average of the time-ordered time-development operator. The time scale is normalized with respect to the inverse of the plasma frequency ($s = \tilde{\omega}_p t = \sqrt{2} \omega_p t$).

the un-time-ordered result by about 14% which is in agreement with a comparison between the impact result⁶ and the calculation of Shen and Cooper.¹² As one goes toward the wings of the profile the effect of time ordering causes an increase in the intensity of the profile in the vicinity of the Stark component which is shifted due to ion fields. Beyond about $10\omega_p$, time ordering ceases to be important.

In Fig. 2, we have plotted the ratio of the profile to the Holtsmark $\Delta\lambda^{-5/2}$ wing (resulting from considering only the ions). The un-time-ordered re-

sult is also plotted along with the result obtained using a full thermal average (dotted line). As indicated above, the influence of time ordering is to lower the Lyman- α profile in the line center and to increase it in the wings, which effectively reduces the structure of the profile.

In comparing the results presented with various experiments in the high-electron-density regime, we observe the following facts: For the experiment of Elton and Griem¹³ ($\text{Ly}\alpha$, $n_e = 3.6 \times 10^{17} \text{ cm}^{-3}$, $T_e = 20\,400 \text{ K}$) the correction from time ordering

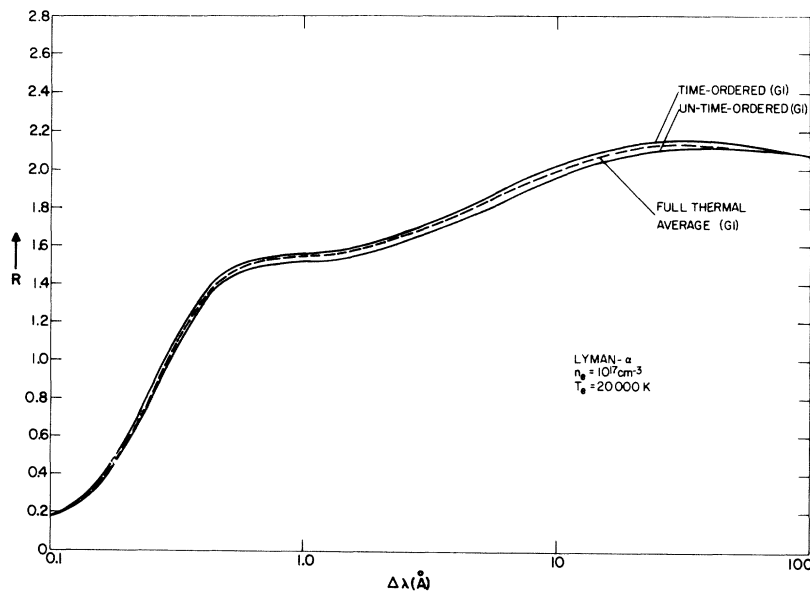


FIG. 2. Final Lyman- α profile normalized with respect to the asymptotic Holtsmark $\Delta\lambda^{-5/2}$ wing (ions only) for the time-ordered and un-time-ordered (including the case where a full thermal average is made) time-development operators ($\Delta\lambda_c = 137 \text{ \AA}$).

improves agreement between the theoretical profile and the experimental data, while in the case of the measurements of Boldt and Cooper¹⁴ ($\text{Ly}\alpha$, $n_e = 8.4 \times 10^{16} \text{ cm}^{-3}$, $T_e = 12200 \text{ K}$) the agreement becomes worse.

The main effect of time ordering, as discussed above, appears to be a decrease in intensity at the line center with a corresponding increase in the wings. This behavior was obtained in the S -matrix

limit^{6, 7} for both $\text{Ly}\alpha$ and $\text{H}\alpha$. One may therefore expect a similar behavior for other hydrogen lines (in the case of the recent measurements by Wiese, Kelleher, and Paquette¹⁵ the correction from time ordering improves agreement between the theoretical and experimental profiles).

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Group Properties of Hydrogenic Radial Functions*

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The radial wave functions of hydrogen are put into such a form that they form bases for irreducible unitary representations of an algebra isomorphic to that of $O(2, 1)$. Operators proportional to r^k are found which form bases for the adjoint representations of this algebra. Matrix elements of these operators are evaluated, and selection rules are determined by considering Kronecker products of representations of $O(2, 1)$. Differences between this approach and one previously suggested are discussed.

I. INTRODUCTION

Following Racah,¹ the angular portion of the atomic wave function has been analyzed using the powerful techniques of group theory. The radial atomic function has, on the other hand, been considered simply to be a solution to a differential equation. As a result, calculations involving the radial function lack, in general, the elegance and essential simplicity of calculations involving the angular functions.

The possibility has recently been raised of extending the use of group theory to studies of the radial wave function. Because the techniques necessary for such studies are largely unknown (or unrecognized), work has been centered on the simpler quantum-mechanical systems—the hydrogen atom (both nonrelativistic^{2,3} and relativistic⁴), the harmonic-oscillator,⁵ and the generalized Kepler problem.⁴ The radial functions of these systems must certainly be completely understood before any significant progress can be made in more com-