

an analysis of the two limits may be easier for Eq. (6) than for Eq. (14). Another is that only the diagonal elements of the T matrix enter in Eq. (6) whereas off-diagonal elements of S are required in Eq. (14). However, off-shell matrix elements

of T occur in Eq. (6) with only on-shell elements of S appearing in Eq. (14) (with above reservations).

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Classical-Path Calculation of the Impact-Broadening Operator for the Stark Broadening of H_α

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The impact-broadening operator Φ for the hydrogen line H_α is calculated by solving numerically for the S matrices using the straight-line classical-path approximation. All contributing multipoles in the perturber- (free-electron-) atom interaction [$V(t)$] are included; time ordering of the operators in the S matrices is retained. The matrix elements are compared with previous approximations based on the same model; the effects on the H_α line profile are considered.

In a previous paper¹ we numerically calculated the S matrices used to compute the impact-broadening operator $\Phi_{nn'}$ for the Stark broadening of the hydrogen-line Lyman α using the classical-path approximation. All contributing multipoles in the free-electron-atom interaction were included and time ordering of the operators in the S matrices was retained.

In this report we apply the same techniques to the hydrogen line H_α and compare the results with previous calculations using the same approximation. (Details may be found in Ref. 2.) For ease of comparison, the $\Phi_{nn'}$ matrix elements are expressed in the form (note the different sign convention as compared with Ref. 1)

$$\text{Re}\Phi_{nn'} = C [E_1(y_{\text{min}}) - K] \mathcal{R}, \quad \text{Im}\Phi_{nn'} = C \mathcal{I}, \quad (1)$$

where

$$C = \frac{-\lambda_0^2 \hbar^2 N^{1/3} (2m/kT)^{1/2}}{2.61e \text{ cm}^2}$$

and

$$\mathcal{R} = [\vec{r}_n \cdot \vec{r}_n + \vec{r}_n \cdot \vec{r}_n - 2\vec{r}_n \cdot \vec{r}_n],$$

$$E_1(y_{\text{min}}) = -0.577 - \ln y_{\text{min}} - \sum_{n=1}^{\infty} \frac{(-1)^n y_{\text{min}}^n}{nn!},$$

$$y_{\text{min}} = (4\pi N/3m)(e\hbar n^2/kT)^2.$$

With this definition of $\Phi_{nn'}$, the line profile in reduced units α ($\alpha = -\Delta\lambda/F_0$) is given by (see, for ex-

ample, Ref. 3)

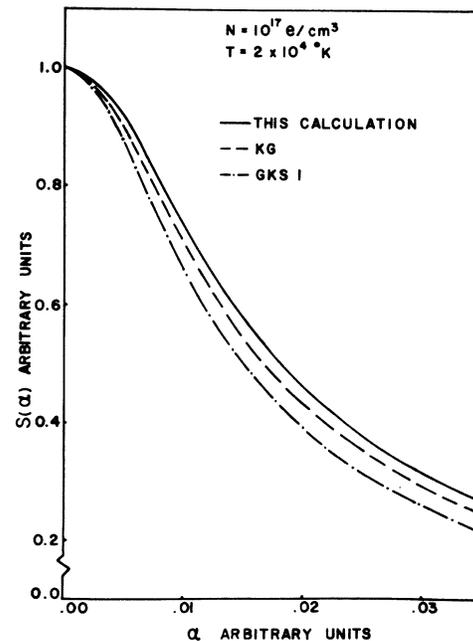


FIG. 1. Comparison of H_α profiles. The SC and BE curves are not shown. The SC curve lies almost exactly on top of the KG curve and the BE(GKSII) curve is slightly narrower than the KG curve.

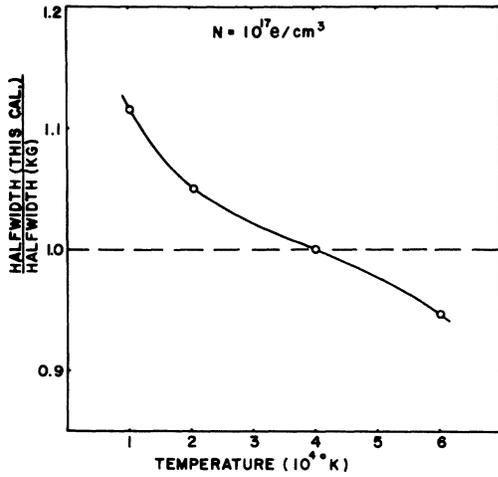


FIG. 2. The ratio of the half-widths of this calculation to the KG half-widths as a function of temperature for $N = 10^{17} e/cm^3$.

$$S(\alpha) = \frac{A_{nm'}}{\pi} \int_0^\infty W_r(f) df \operatorname{Re} \langle \eta | \mu | \xi \rangle$$

$$\times \left\langle \left\langle \eta \xi \left| \left(\frac{i\lambda_0^2 \{ \omega - [H_n(f) - H_{n'}(f)] / \hbar \} + \Phi_{nn'}}{2\pi c F_0} \right)^{-1} \right| \epsilon' \eta' \right\rangle \right\rangle$$

$$\times \langle \eta' | \mu | \xi' \rangle, \quad (2)$$

where the symbols have their usual meaning. The Hooper⁴ distribution functions are used to describe the static ion field $W_r(f)$.

In the following we have characterized the previous calculations as Griem *et al.* (GKSI),⁵ Bacon and Edwards (GKSII),⁶ Shen and Cooper (SC),⁷ and Kepple and Griem (KG),⁸ which is indicative of the particular treatment of close collisions used in the various calculations rather than of the calculations themselves. This method of comparison was chosen because previous calculations have utilized different cutoff procedures at large impact parameters (in this report $\rho_{\max} = \rho_D$) and some have ne-

TABLE I. Values of K [Eq. (1)] determined by the present calculations as a function of temperature. Also shown are the values of K used by KG as a function of temperature. In addition, we show the values of K determined using the formalism of Shen and Cooper, as applied to the two-state case. In the GKSI formalism $K=0$, while in the GKSII formalism, on which the calculations of BE are based, $K=-1$.

Spherical quantum numbers specifying upper (n) and lower (n') states					Temperature ($^{\circ}\text{K}$)							
$n_1 m_1$	$n' l_2 m_2$	$n' l_4 m_4$	$n_3 m_3$	$\frac{2Q}{3}$ (a. u.) $K(\text{SC})$	10^4	2×10^4	3×10^4	4×10^4	5×10^4	6×10^4	10^5	1.2×10^5
300	200	200	300	126.0	0.132	0.29	0.30	0.33	0.35	0.38	0.40	
310	200	200	310	99.0	-0.055	0.09	0.11	0.13	0.16	0.18	0.21	
311	200	200	311	99.0	-0.055	0.09	0.11	0.13	0.16	0.18	0.21	
320	200	200	320	45.0	-0.676	-0.90	-0.88	-0.85	-0.81	-0.77	-0.73	
321	200	200	321	45.0	-0.676	-0.90	-0.88	-0.85	-0.81	-0.77	-0.73	
300	200	210	310	-29.4	0.983	0.84	0.84	0.85	0.86	0.87	0.89	
310	200	210	300	-29.4	0.983	0.70	0.71	0.73	0.75	0.77	0.80	
310	200	210	320	-20.8	0.221	0.70	0.70	0.71	0.71	0.72	0.73	
311	200	210	321	-18.0	0.221	0.70	0.70	0.71	0.71	0.72	0.73	
320	200	210	310	-20.8	0.221	0.54	0.55	0.56	0.57	0.58	0.60	
321	200	210	311	-18.0	0.221	0.54	0.55	0.56	0.57	0.58	0.60	
311	200	211	300	-29.4	0.983	0.69	0.70	0.72	0.74	0.77	0.79	
311	200	211	320	10.4	0.221	0.70	0.70	0.71	0.71	0.72	0.73	
321	200	211	310	-18.0	0.221	0.54	0.55	0.56	0.57	0.58	0.60	
300	210	210	300	114.0	0.018	0.15	0.18	0.21	0.23	0.26	0.29	
310	210	210	310	87.0	-0.307	0.09	0.09	0.11	0.12	0.15	0.17	
311	210	210	311	87.0	-0.346	-0.09	-0.07	-0.04	-0.01	0.02	0.05	
320	210	210	320	33.0	-0.668	-1.38	-1.35	-1.32	-1.27	-1.22	-1.18	
321	210	210	321	33.0	-0.724	-1.41	-1.38	-1.35	-1.30	-1.25	-1.20	
300	211	211	300	114.0	0.018	0.15	0.18	0.21	0.23	0.26	0.29	
310	211	211	310	87.0	-0.346	-0.09	-0.07	-0.04	-0.01	0.02	0.05	
311	211	211	311	87.0	-0.327	-0.02	-0.01	0.02	0.04	0.07	0.10	
320	211	211	320	33.0	-0.836	-1.48	-1.46	-1.42	-1.37	-1.33	-1.28	
321	211	211	321	33.0	-0.808	-1.38	-1.35	-1.32	-1.27	-1.22	-1.18	
322	211	211	322	33.0	-0.724	-1.24	-1.22	-1.18	-1.14	-1.09	-1.05	
$K(\text{KG}) = 0.78 + 8kT/3E_H$ (independent of matrix element)					-0.95	-1.12	-1.29	-1.46	-1.63	-1.80		

glected various terms of \mathcal{R} (in this report the complete \mathcal{R} matrix is used), and hence an absolute comparison would tend to hide the essential results of the present investigation.

The values of K were determined in the same way as was done in Ref. 1 and are given in Table I as a function of temperature. These values of K are estimated to be accurate to ± 0.05 . Shown for comparison are the values based on the SC and KG developments. In addition, we have $K = 0$ according to the GKSI formalism and $K = -1$ for the GKSII formalism on which the calculations of BE are based.

In order to compute the H_α line profile, the Φ_{mn} matrix elements using the K 's of the present calculation (given in Table I) were first transformed to the parabolic system. The profile $S(\alpha)$ was then calculated in the usual way using Eq. (2). Profiles based on previous calculations were calculated in similar fashion using the relevant K 's. The resulting profiles for an electron density of $10^{17} e/cm^3$ and a temperature of 2×10^4 °K are shown in Fig. 1 (renormalized to a peak intensity of 1). The SC curve lies almost exactly on top of the KG curve and therefore is not shown. The BE(GKSII) curve is slightly narrower than the KG curve, but not suf-

ficiently so as to be distinguishable on the scale used. The profile calculated using the present values of K is seen to be approximately 5% broader than that of KG. This relative behavior is a function of temperature for a given density and is illustrated in Fig. 2 where we have plotted the ratio of the half-width using the present K 's to the half-width using the K 's of KG as a function of temperature for an electron density of $10^{17} e/cm^3$. The ratio was calculated at the temperatures 10^4 , 2×10^4 , 4×10^4 , and 6×10^4 and a smooth curve drawn through the theoretical points (denoted by the small circles). From this figure we see that the present calculations are $\sim 11\%$ broader at 10^4 °K and $\sim 5\%$ narrower at 6×10^4 °K. Similar curves may be plotted for different electron densities.

In the present calculations, Φ_{mn} has an imaginary part [Eq. (1)]. The values of \mathcal{I} are given in Table II as a function of temperature. Including the imaginary part of the Φ_{mn} matrix elements in the H_α profile calculation results in a shift to the red with no apparent asymmetry about the peak intensity. At 2×10^4 °K and a density of $10^{17} e/cm^3$ the shift is approximately $+0.3 \text{ \AA}$, while at the same temperature but at a density of $10^{18} e/cm^3$ the shift is approximately $+1.9 \text{ \AA}$.

TABLE II. \mathcal{I} [Eq. (1)] as a function of temperature.

Spherical quantum numbers specifying upper (n) and lower (n') states				Temperature (°K)					
$n'l_1m_1$	$n'l_2m_2$	$n'l_4m_4$	$n'l_3m_3$	10^4	2×10^4	3×10^4	4×10^4	5×10^4	6×10^4
300	200	200	300	-8.77	-12.36	-15.19	-17.66	-19.91	-22.03
310	200	200	310	-5.91	-8.74	-11.10	-13.20	-15.14	-16.95
311	200	200	311	-5.91	-8.74	-11.10	-13.20	-15.14	-16.95
320	200	200	320	-2.81	-4.04	-5.11	-6.12	-7.11	-8.08
321	200	200	321	-2.81	-4.04	-5.11	-6.12	-7.11	-8.08
300	200	210	310	-0.10	-0.32	-0.54	-0.73	-0.89	-1.02
310	200	210	300	-0.38	-0.68	-0.91	-1.11	-1.26	-1.39
310	200	210	320	-0.23	-0.34	-0.44	-0.52	-0.59	-0.65
311	200	210	321	-0.20	-0.30	-0.38	-0.45	-0.51	-0.56
320	200	210	310	-0.23	-0.34	-0.43	-0.50	-0.57	-0.62
321	200	210	311	-0.20	-0.30	-0.37	-0.43	-0.49	-0.54
311	200	211	300	-0.38	-0.68	-0.91	-1.11	-1.26	-1.39
311	200	211	320	0.12	0.17	0.22	0.26	0.29	0.32
321	200	211	310	-0.20	-0.30	-0.37	-0.43	-0.49	-0.54
300	210	210	300	-9.28	-13.35	-16.62	-19.49	-22.11	-24.55
310	210	210	310	-7.54	-10.97	-13.78	-16.26	-18.51	-20.61
311	210	210	311	-6.87	-10.21	-12.99	-15.47	-17.74	-19.85
320	210	210	320	-4.19	-6.01	-7.52	-8.91	-10.21	-11.48
321	210	210	321	-4.17	-5.96	-7.46	-8.83	-10.12	-11.38
300	211	211	300	-9.28	-13.35	-16.62	-19.49	-22.11	-24.55
310	211	211	310	-6.88	-10.22	-13.00	-15.48	-17.75	-19.86
311	211	211	311	-7.25	-10.69	-13.53	-16.04	-18.32	-20.44
320	211	211	320	-4.14	-5.88	-7.34	-8.67	-9.94	-11.18
321	211	211	321	-4.04	-5.82	-7.31	-8.68	-9.98	-11.24
322	211	211	322	-3.96	-5.79	-7.35	-8.77	-10.12	-11.41

In conclusion it should be pointed out that the use of the classical-path approximation down to \hbar is rather extreme and quantum effects are possibly significant in this region. Nevertheless the present treatment of strong collisions should be an improvement over previous treatments.

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Entropy, the Wigner Distribution Function, and the Approach to Equilibrium of a System of Coupled Harmonic Oscillators*

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The entropy is determined of a quantum-mechanical system whose statistical state is characterized by a Wigner distribution function that is Gaussian in form. It is found to depend only on the variance of the distribution function. This enables us to study quantum mechanically the approach to equilibrium of coupled harmonic-oscillator chains, a system for which a classical treatment has been given recently by Robertson and Huerta.

In this paper we calculate the entropy of a quantum-mechanical system that is in a state characterized by a Wigner distribution function^{1,2} which is Gaussian in form. We then study the approach to equilibrium of a system of an infinite harmonically bound weakly coupled *quantum-mechanical* harmonic-oscillator chain. The approach to equilibrium of this system, when each harmonic oscillator is replaced by a classical harmonic oscillator, has been recently studied in great detail by Robertson and Huerta.^{3,4} We find that the reduced N -particle Wigner distribution function is the same as the classical one that was calculated by Robertson and Huerta [Ref. 3(a), Eq. (9)]. We also find that in the limit as $t \rightarrow \infty$ the entropy is the same as the equilibrium entropy for a system of N -independent quantum oscillators.

Let the quantum-mechanical system be in a state characterized by a Wigner distribution function of

the form

$$f^{(W)}(q, p) = [(2\pi)^2(\alpha\beta - \gamma^2)]^{-1/2} \times \exp\left(-\frac{1}{2} \frac{\alpha q^2 + \beta p^2 - 2\gamma qp}{\alpha\beta - \gamma^2}\right). \quad (1)$$

The parameters α , β , and γ may be shown to be related to the average values of the operators \hat{q}^2 , \hat{p}^2 , and $\hat{q}\hat{p}$ by the following relations:

$$\alpha = \langle \hat{p}^2 \rangle, \quad \beta = \langle \hat{q}^2 \rangle, \quad \gamma = \frac{1}{2} \langle \hat{q}\hat{p} + \hat{p}\hat{q} \rangle. \quad (2)$$

We shall show that such a Wigner distribution function occurs in the problem mentioned above. It also occurs in other problems such as parametric amplification^{5(a)} and Brownian motion.^{5(b)}

The entropy of a quantum-mechanical system in a state characterized by the density operator $\hat{\rho}$ is given by