Generalized oscillator strength for the $3s$-$3p$ transition in sodium

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Solutions of the close-coupling equations are obtained for sodium in a four-state approximation ($3s,3p,4s,3d$) at energies of 22.1, 54, and 150 eV. Generalized oscillator strengths (GOS) deduced from the resulting differential cross sections for the $3s$-$3p$ transition are plotted as a function of momentum transfer squared (K^2). The resulting GOS do not tend to the exact value of the optical oscillator strength as K^2 goes to 0, thus violating Lassettre's hypothesis. While Lassettre's theorem is not satisfied exactly, the concepts underlying this hypothesis are still useful at sufficiently high energies.

I. INTRODUCTION

The generalized oscillator strength (GOS) is a useful tool for studying the behavior of electron-atom excitation cross sections at small momentum transfer. The initial idea of expressing the differential cross section for excitation in terms of the GOS was first put forward by Bethe.[1] However, this concept remained essentially dormant until its revival by Lassettre[2] when it was exploited to determine optical oscillator strengths for atomic transitions. Since then, the usefulness of the GOS has been demonstrated in a number of applications. Two of the more notable applications have been the normalization of relative differential cross section data and the measurement of photoabsorption and photoionization cross sections[3] for atoms and molecules. The Bethe-Born expression for the GOS is

$$g_{if}^{B}(K^2)=\frac{E_{if}}{K^2}\,|\langle f\,|\,e^{i\mathbf{K}\cdot\mathbf{r}}\,|\,i\rangle\,|^2\,, \tag{1}$$

which can be related to the first Born differential cross section by

$$\left.\frac{d\sigma}{d\Omega}\right|_B=\frac{2k_f}{E_{if}k_iK^2}g_{if}^{B}(K^2)\,. \tag{2}$$

The concept of the GOS is not confined to just the first Born approximation (FBA). When one has a differential cross section obtained by some other means (e.g., experimental data or a close-coupling calculation) one can invert Eq. (2) and define the apparent GOS by

$$g_{if}^{A}(K^2)=\frac{E_{if}k_i}{2k_f}K^2\frac{d\sigma}{d\Omega}\,. \tag{3}$$

In the above equations, k_i and k_f are the electron momenta before and after collision, $\mathbf{K}$ is the momentum transfer vector, and E_{if} is the excitation energy of the transition. The usefulness of the GOS lies in the fact that as the energy of the incident electron increases, the limiting value of the GOS (for inelastic collisions) as the momentum transfer goes to zero is just the optical oscillator strength (OOS). This result has often been utilized to put relative cross sections on an absolute scale.[4-6] The conditions for the applicability of the GOS limit theorem were generalized by Lassettre *et al.*[7] who deduced that the GOS converges to the OOS as $K^2\rightarrow 0$ regardless of energy and irrespective of the applicability of the first Born approximation.

The validity of Lassettre's theorem has recently been questioned by Bonham and Goruganthu[8] and by Msezane and Henry.[9-11] Bonham and Goruganthu[8] demonstrated that the validity of the limit theorem depends on how the extrapolation from the minimum K ($\sim E/2k_i$) to $K=0$ is performed. It was shown that Lassettre's theorem corresponds to an off-the-energy-shell extrapolation to $K^2=0$. The on-the-energy-shell extrapolation was shown to yield a small correction to the Lassettre's theorem result. The limiting behavior of the GOS at small K values has also been studied by Huo.[12] The evidence of Msezane and Henry was of a calculational nature. After converting the differential cross sections that resulted from multistate close-coupling calculations into GOS, Msezane and Henry found that the apparent GOS for the resonance transitions in Mg^+, Zn^+, and Cu did not converge to the optical oscillator strength as $K^2\rightarrow 0$. On the contrary, the GOS seemed to reach a maxima at some particular value of K^2 and would afterward decrease as K^2 tended to zero. This effect was most noticeable at the highest energies. In this paper we intend to look at the limiting behavior of the GOS for the resonance transition ($3s$-$3p$) in sodium in order to determine how accurately Lassettre's theorem is obeyed for this particular transition. Furthermore, we will investigate whether the maxima at small but nonzero K^2 in the GOS reported by Msezane and Henry also occurs for the resonance transition in sodium.

II. RESULTS

We have chosen to study the sodium system since the differential cross sections were already in existence from a previous study[13] of electron-impact processes in sodium. Some experimental GOS results also exist.[4,14] We do not show a detailed comparison with experiment in this paper

since the experimental data are put on an absolute scale by assuming the validity of Lassettre's theorem and the errors in the individual data points are too large for any definite conclusions to be drawn. The small excitation energy for the $3s$-$3p$ transition makes it particularly suitable for probing the GOS at very small values of momentum transfer. Details of the four-state ($3s$,$3p$,$4s$,$3d$) calculations are as follows. The on-shell T-matrix elements are obtained by solving the set of coupled Lippmann-Schwinger (LS) equations using (24-point) Gaussian quadratures to discretize the kernel in momentum space. The coupled LS equations are solved for total angular momentum (J) between 0 and 24. The contribution of exchange interactions to the kernel is included for $J=0$ to 16. At high energies and small angles a very large number of partial waves contribute to the differential cross section. Consequently, great care should be taken with the calculation of the partial-wave T-matrix elements, and also with the calculations that produce the differential cross section. Since the differences between the full solution of the coupled equations and the unitarized Born approximation (UBA) are very small for $J \geq 24$, the UBA is used to compute the T-matrix elements for J between 25 and 80. Rather than computing the three-dimensional T-matrix element using the partial-wave sum directly, the (symbolic) form

$$T = V + \sum_l (T_l - V_l) \tag{4}$$

is used. In the above expression T_l and V_l are the partial-wave T- and V-matrix elements, respectively, and T and V are the three-dimensional forms. The advantage of this formulation is that any numerical inaccuracies inherent in computing the partial-wave sum are minimized and that using the three-dimensional V-matrix (i.e., first Born) element enables an infinite number of partial waves to be included. The differential cross section is computed by squaring the T matrix and including the appropriate angular momentum and kinematic factors. Differential cross sections of the $3s$-$3p$ transitions were obtained at energies of 22.1, 54.4, and 150 eV. The numerical accuracy of these differential cross sections is about 1% or 2%.

The GOS resulting from the close-coupling (CC) differential cross sections are shown in Fig. 1. Also shown in Fig. 1 is the GOS that is predicted by the FBA which goes to the optical oscillator strength $K^2=0$. At the smallest values of momentum transfer the GOS derived from the CC calculations do not tend toward the exact value of the OOS. Instead, they approach a limit which is slightly smaller than the OOS. At the highest energy (150 eV), the minimum value of momentum transfer squared ($\sim 10^{-4}$ a.u.) was extremely small, and for all practical purposes may be regarded as the physical realization of the limit. Even here, there is a small deviation from the OOS. However, in one respect these curves indicate that the concepts underlying the GOS are still quite useful. While Lassettre's theorem may not be satisfied exactly, the deviations of the apparent GOS extrapolated to $K^2=0$ from the OOS are quite small for $E \geq 54.4$ eV.

In this respect our calculations are consistent with the conclusions of Bonham and Goruganthu.[7] The comparison with the work of Msezane and Henry[9-11] is not nearly so clear cut. In one respect our results are consistent with the calculations of Msezane and Henry, we find that Lassettre's generalization is not valid. However, in another respect our calculations are not consistent with those of Msezane and Henry, i.e., we find no evidence of a maxima in the GOS at a small (nonzero) value of the momentum transfer. While this does not invalidate their results, since their calculations were for different systems, it demonstrates that the irregularities in the GOS curves for dipole transitions produced by Msezane and Henry are not universal features that occur for all atomic and ionic systems. However, of the calculations carried out by Msezane and Henry,[9-11] only one[10] was on an uncharged species. While one might expect the small-angle behavior (for inelastic transitions) of differential cross sections for charged targets to be similar to those for neutrals, there are very few rigorous analytic results for inelastic transitions in a Coulomb field and so even a comparison of the Born and Coulomb-Born cross sections would be quite valuable as a guide to whether the Coulomb boundary conditions induce any unique effects in the differential cross sections.

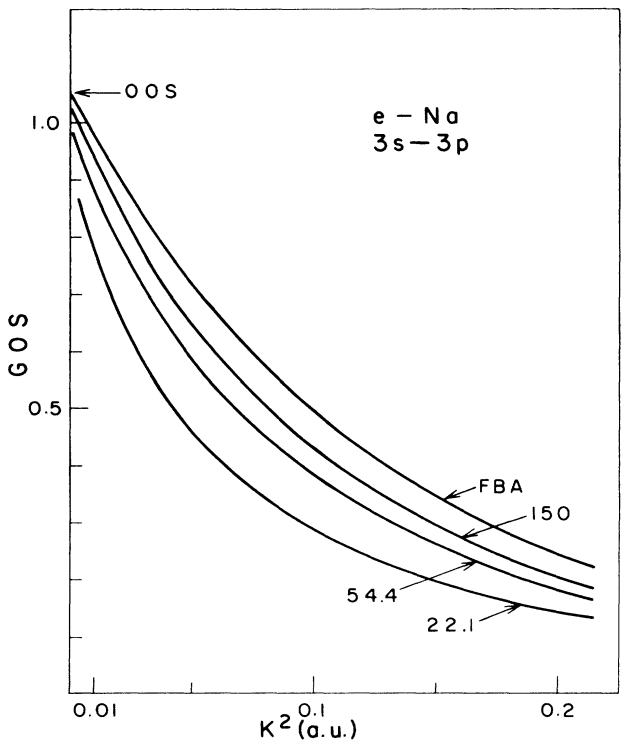

FIG. 1. Comparison of apparent GOS obtained from Eq. (3) using differential cross sections coming from four-state close-coupling calculations at energies at 22.1, 54.4, and 150 eV. Also shown is the GOS obtained using the Bethe-Born expression (labeled FBA). The value of the OOS in the Hartree-Fock (length) approximation is denoted by the arrow.

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