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Universal function and its application to the 2*p*-3*s* transition in sodium

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The expansion of the universal function in terms of the momentum transfer squared, K^2, has been investigated. We find that in the region of $K^2 \ll 1$ a.u. both the Born approximation and the universal function yield a linear relationship between the generalized oscillator strength (GOS) and K^2, thus establishing the validity of the universal function for use in extrapolating the GOS through the unphysical region to the optical oscillator strength. As an illustration, the GOS for the inner-shell transition 2*p*-3*s* of sodium has been calculated using Hartree-Fock atomic orbitals and the universal function, and compared with measurement at 1000 eV. For $0.0 < K^2 < 0.01$ a.u. the universal function merges with the Born approximation, and shows a correct asymptotic behavior. At $0.1 < K^2 < 0.4$ a.u., the Born approximation fails to reproduce the measurement, while the universal function agrees excellently with the experimental data.

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I. INTRODUCTION

The region of small scattering angles is the most difficult region in the measurement of the electron differential cross sections (DCS's) for optically allowed transitions because the DCS increases dramatically with decreasing scattering angle, θ. This rapid variation of the DCS with θ as $\theta \rightarrow 0°$ introduces uncertainty in the measured DCS. Added to this problem is that experiments generally measure relative DCS which require normalization through various methods, including the limiting behavior of the generalized oscillator strength (GOS) as $K^2 \rightarrow 0$ [1–4]. For optically allowed transitions, Miller and Platzman [5] have recommended the examination of the GOS versus K^2 for useful information regarding the DCS and the integral cross sections. Unfortunately, for finite impact energy E, $K^2=0$ corresponds to unphysical scattering angles. Therefore, extrapolation of the GOS through the unphysical region to the optical oscillator strength (OOS) has to be effected [1,6,7]

The GOS and the DCS are related by

$$f^G = \frac{w}{2}\frac{k_i}{k_f}K^2\frac{d\sigma}{d\Omega} , \quad (1)$$

where f^G is the GOS; w is the excitation energy; k_i, k_f are, respectively, the incident and the scattered momenta; and K is the momentum transfer. Using Eq. (1) the experimental DCS data can be transformed to GOS. The total excitation cross section is then obtained by transforming the variable θ to K^2 and the integration over K^2. Recently, Msezane and Sakmar have developed an extrapolation formula for the GOS using rigorous bounds on K^2. This formula, they called the universal function [6,7], can be expressed as

$$f^G_{\rm uni} = -f^0\left[1+\frac{x^2-1}{1-xy}\right] , \quad (2)$$

where $x^2 = 1 - w/E$, w is the excitation energy, E is the energy of the incoming particle, $y=\cos\theta$, and f^0 is the OOS. The equation is applicable only to optically allowed transitions for small K^2 values.

In this paper we have compared expansions of the universal function and the Born approximation in terms of the momentum transfer squared, K^2, for any optically allowed transition in the region of small K^2. A linear relationship between the GOS and K^2 in the $K^2 \ll 1$ a.u. region indicates that the universal function always has the correct asymptotic behavior. Therefore, the universal function can be used in the calculation of the excitation cross sections and to guide experimental measurements and theoretical calculations. The Na 2*p*-3*s* inner-shell transition is used as an illustrative example. In Sec. II we present the theory. Sections III and IV present the results and the discussion and conclusion, respectively.

II. THEORY

The GOS and OOS can be calculated in the Born approximation as [9]

$$f^o = \frac{2\mu}{\hbar^2}(E_f - E_i)|\langle \phi_f|\mathbf{r}|\phi_i\rangle|^2 , \quad (3)$$

$$f^G=\frac{2\mu}{\hbar^2K^2}(E_f-E_i)|\langle\phi_f|e^{i\mathbf{K}\cdot\mathbf{r}}|\phi_i\rangle|^2 . \tag{4}$$

In the independent particle model, if $K^2 \ll 1$ a.u. the GOS can be expanded as

$$f^G \approx f^o\left[1-K^2\left[\frac{1}{3}\frac{\langle\phi_f|(r\cos\theta)^3|\phi_i\rangle}{\langle\phi_f|r\cos\theta|\phi_i\rangle}+\frac{1}{4}\frac{\langle\phi_f|(r\cos\theta)^2|\phi_i\rangle}{\langle\phi_f|r\cos\theta|\phi_i\rangle^2}\right]\right]$$

$$=f^0[1-cK^2] , \tag{5}$$

where c is a constant depending on the transition states, and ϕ_i and ϕ_f are the wave functions of the initial and final states. Equation (5) gives a linear relationship between the GOS and K^2 in the region $K^2 \ll 1$ a.u. provided that the Born approximation is valid. To calculate the constant c in Eq. (5) we need to know the wave functions for the transitions. However, these wave functions are not always readily available and if they are, the calculations become involved. Therefore, finding a reliable equation to extrapolate the GOS to the OOS has been the subject of investigation by atomic physicists for many years.

The universal function, recently developed [6,7], allows researchers to extrapolate easily the GOS to the OOS through the unphysical region and to ascertain the reliability of experimental measurements [8]. Equation (2) can be rewritten as

$$f^G_{\text{uni}}=-f^0\left[1-\frac{2}{[1+(K^2/2w)]}\right] . \tag{6}$$

Equation (6) has been found to be generally applicable for small K^2 and depends only on w. Equation (6) can be expanded as

$$f^G_{\text{uni}}=\left[1-\frac{K^2}{w}+\frac{K^4}{2w}+\cdots\right]f^o . \tag{7}$$

The leading term K^2 of Eq. (7) guarantees that Eq. (6) always has the correct asymptotic form. Although the coefficients of K^2 are different from those of the Born approximation, the main determinant of the behavior of the GOS when $K^2 \rightarrow 0$ is K^2 itself. Therefore, extrapolation curves of the GOS to the OOS using Eq. (6) will always merge with the curve of the Born approximation as $K^2 \rightarrow 0$.

Experimentally, Suzuki *et al.* [2] measured the electron differential cross sections and the GOS for the two optically allowed transitions $5p^6(^1S_0)\rightarrow 5p^5(^2P_{1/2})6s$ and $5p^5(^2P_{3/2})6s$ in Xe. Their GOS data were fitted with polynomials using the least-squares method and obtained the values for 400- and 500-eV impact energies,

$$f_{3/2}(K)=\left\{0.222-1.374\left[\frac{x}{(1+x)}\right]+1.484\left[\frac{x}{(1+x)}\right]^2+3.665\left[\frac{x}{(1+x)}\right]^3+\cdots\right\}\Big/(1+x)^6 , \tag{8}$$

$$f_{1/2}(K)=\left\{0.158-0.575\left[\frac{x}{(1+x)}\right]-1.227\left[\frac{x}{(1+x)}\right]^2+5.935\left[\frac{x}{(1+x)}\right]^3+\cdots\right\}\Big/(1+x)^6 . \tag{9}$$

For 100 eV the equations are expressed as

$$f_{3/2}(K)=\left\{0.222-1.204\left[\frac{x}{(1+x)}\right]-3.980\left[\frac{x}{(1+x)}\right]^2+30.49\left[\frac{x}{(1+x)}\right]^3+\cdots\right\}\Big/(1+x)^6 , \tag{10}$$

$$f_{1/2}(K)=\left\{0.158-0.404\left[\frac{x}{(1+x)}\right]-4.429\left[\frac{x}{(1+x)}\right]^2+11.84\left[\frac{x}{(1+x)}\right]^3+\cdots\right\}\Big/(1+x)^6 , \tag{11}$$

where x is equal to $(K/Y)^2$, and Y is equal to $\sqrt{2I}+\sqrt{2(I-w)}$. Here I and w are the ionization and excitation energies, respectively. In the resulting graphs of the GOS versus K^2, in the region of small K^2 ($K^2<0.1$ a.u.), the data points taken at 100, 400, and 500 eV lie on the same curve. Therefore, the Born approximation is applicable to their measurement so that curves of the GOS versus K^2 when $K^2 \ll 1$ a.u. should satisfy a linear asymptotic formula. Substituting the OOS and $x=(K/Y)^2$ into Eqs. (8) and (9) we have the asymptotic equations for 400 and 500 eV:

$$f_{3/2}=0.222(1-5.67K^2) , \tag{12}$$

$$f_{1/2}=0.158(1-5.07K^2) . \tag{13}$$

For the 100-eV impact we obtain the asymptotic equations

$$f_{3/2}=0.222(1-5.32K^2) , \tag{14}$$

$$f_{1/2}=0.158(1-4.50K^2) . \tag{15}$$

All these formulas have as the leading term K^2. Their success in the fitting of the experimental data also confirms our analysis.

Takayanagi *et al.* [3] measured the electron-impact excitation cross sections and the GOS for the transitions Kr $4p^6(^1S_0)\rightarrow 4p^5(^2P_{1/2,3/2})5s$ at 300 and 500 eV. Similar asymptotic equations can be obtained from their experimental data. The examination of the fitting polynomials of the other papers [1,4] also leads to the same desirable linear relationship. We have demonstrated that our theoretical analysis and the experimental practice imply the existence of a linear asymptotic relationship between the GOS and K^2 in the region of $K^2 \ll 1$ a.u. for the optically allowed transitions. As the universal function has a similar expansion, it will always behave correctly in the asymptotic region of the GOS, since it is determined mainly by K^2 itself for a given transition.

As an example, we have calculated the GOS for the inner-shell transition $2p$-$3s$ in sodium. We used the Clementi and Roetti [10] wave functions for the $2p$ and $3s$

states of sodium. In calculating the GOS and the OOS, it is convenient to quantize along the **K** axis. Then the 2*p*-3*s*, $m=\pm 1$ amplitude vanishes, and the dominant amplitude is the 2*p*-3*s*, $m=0$. Inserting all the constants in Eq. (3), the optical oscillator strength (dimensionless units) for the 2*p*-3*s* transition of sodium becomes

$$f^o = 0.049\,952 \tag{16}$$

which compares very well with the accepted value of 0.05.

The GOS in Eq. (4) can be expanded as

$$f^G = \frac{2\mu w f^o}{\hbar^2 K^2}\left[\frac{4\pi}{3}\right]^2 \left| I_{11} + \sum_{j=2}^{5} I_{1j} + \sum_{i=2}^{8} I_{i1} + \sum_{i=2}^{8}\sum_{j=2}^{5} I_{ij} \right|^2 , \tag{17}$$

where I_{ij} are integrals containing the 3*s* and 2*p* exponents. If the momentum transfer squared, K^2 is smaller than the exponential coefficients of the 2*p* and 3*s* wave functions, then f^G for the transition 2*p*-3*s* in sodium reduces to

$$f^G = f^o[1 - 1.517K^2 + 1.132K^4] \; . \tag{18}$$

As can be seen, the calculation gives a linear relationship between the GOS and K^2, if $K^2 \ll 1$ a.u. This supports the analysis leading to Eq. (5). The GOS's in the full Born approximation and the Born approximation keeping up to K^2 and K^4 terms have been calculated in this paper and compared with the universal function result.

III. RESULTS

In Fig. 1 we have contrasted the GOS from various levels of the Born approximation, the universal function, Eq. (6) (solid line) and the data of Bielschowsky *et. al.* [11] measured at 1000-eV impact energy (solid circle). Born approximations dotted line, to order K^2; dashed line, to order K^4; and dashed-dotted line, full. As can be seen, our various levels of the Born approximation merge as $K^2 \to 0$ but with different slopes. In Fig. 1 the GOS is not decided generally by K^2 alone. The behavior of the K^2

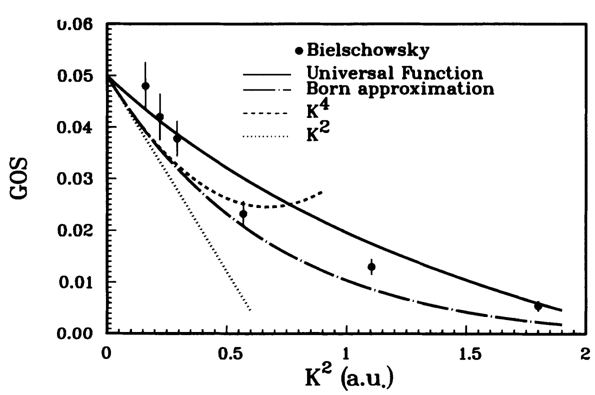

FIG. 1. Relationship between GOS and K^2 for the transition of sodium 2*p*-3*s*. Solid circle, the measurement of Bielschowsky; dashed-dotted lines, calculation of the full Born approximation; dotted and dashed lines, Born approximation kept up to K^2 and K^4; solid line, universal function.

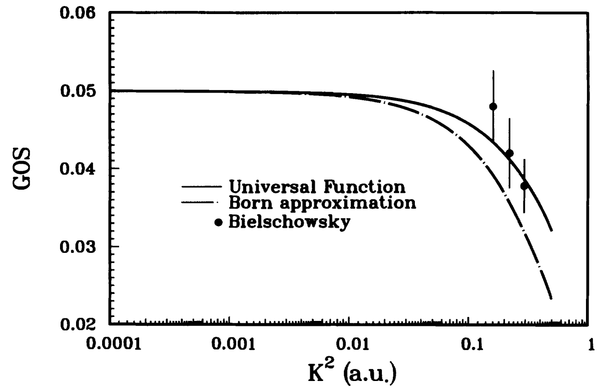

FIG. 2. Comparison of the GOS when K^2 is small. Dashed-dotted line, full Born approximation; solid line, universal function; solid circle, the measurement of Bielschowsky.

and K^4 curves relative to the full Born approximation is interesting; the K^4 curve is the better approximation to the full Born approximation. Regardless of the order of the approximation, the Born approximation fails to reproduce the measurement when $0.1 < K^2 < 0.4$ a.u. even though the Na 2*p*-3*s* transition is almost in the Born approximation regime viz. when $E = 1000$ eV, $x \equiv \sqrt{1-(w/E)} = 0.9843$ (true Born corresponds to $x = 1.0$). The universal function approaches the OOS and agrees well with the measurement.

Figure 2 compares the GOS in the full Born approximation (dashed-dotted) line, the universal function (solid line), and the measurement (solid circle) at small K^2. Clearly, the universal curve gives excellent agreement with the measurement, except for the last experimental point which we believe has not been measured with sufficient accuracy, the reason being that all data points must lie on or below the universal curve [7]. Interestingly, for this particular transition, contrary to the expected behavior [7], the Born approximation at $0.1 < K^2 < 0.4$ a.u. underestimates the experimental data, thus exhibiting inconsistent prediction. At $0.0 < K^2 < 0.01$ a.u. both the universal function and Born approximation approach the OOS linearly. It is well known that the Born approximation is suitable in the region $K^2 \to 0$. As the universal function merges with the Born approximation in this region it demonstrates that it has the correct asymptotic behavior to extrapolate the GOS to the OOS. At $0.1 < K^2 < 0.4$ a.u. the Born approximation fails to reproduce the experimental data. Consequently, normalization of the measured relative DCS to the Born curve as is the normal practice, would lead to incorrect absolute cross sections. However, the universal function still agrees with the measurement very well. This demonstrates the reliability of the universal function to guide measurement.

IV. DISCUSSION AND CONCLUSION

In this paper we have studied the asymptotic behavior of the universal function in the region of small K^2 and compared it with the Born approximation. In this region of small K^2 the well-known experimental fitting polynomials such as those employed by Suzuki *et al.* and others have been shown to have as the leading term K^2, just as the Born approximation and the universal function, demonstrating that the GOS versus K^2 satisfies a linear asymptotic formula. This ensures that the universal function will always behave correctly in the asymptotic region of the GOS since it is determined only by K^2 for a given transition. The merging of the Born approximation and the universal function GOS in the region $K^2 \rightarrow 0$ demonstrates that the latter is suitable for extrapolating the GOS through the unphysical region to the OOS.

Using the Na $2p$-$3s$ inner-shell transition as an example, we have demonstrated that in the region of validity of the Born approximation the universal function indeed merges with the Born approximation and has the correct asymptotic behavior to extrapolate the GOS through the unphysical region to $K^2=0$. When K^2 increases the Born approximation fails to reproduce the experimental data as it is only suitable for the high energy and small scattering angle (or $K^2 \ll 1$ a.u.). The region of K^2 where the universal function can be applicable is dependent on $K^2/2w$. The range is larger when w is large. In electron-xenon scattering [8] we found that it gives excellent agreement for $K^2<0.05$ a.u. The excitation energy (36.1 eV) of the $2p$-$3s$ in sodium is larger than the $5p^5(^2P_{3/2})6s$ excitation (8.4 eV) in xenon. Therefore we expect that the universal function will still fit the experimental data very well as shown in Fig. 2 when the Born approximation fails. The universal function also has the advantage of simplicity. It can be used exactly as given in Eq. (6). What now remains is its improvement to include the treatment of dipole forbidden transitions as $K^2 \rightarrow 0$ and its use to correct many existing small-angle DCS for optically allowed transitions.

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[1] E. N. Lassettre and A. Skerbele, J. Chem. Phys. **60**, 2464 (1974).
[2] T. Y. Suzuki, Y. Sakai, B. S. Min, T. Takayanagi, K. Wakiya, and H. Suzuki, Phys. Rev A **43**, 5867 (1991).
[3] T. Takayanagi, G. P. Li, K. Wakiya, and H. Suzuki, Phys. Rev. A **41**, 5948 (1990).
[4] G. P. Li, T. Takayanagi, K. Wakiya, and H. Suzuki, Phys. Rev. A **38**, 1240 (1988).
[5] W. F. Miller and R. L. Platzman, Proc. R. Soc. London Ser. A **70**, 299 (1957).
[6] A. Z. Msezane and I. A. Sakmar, Phys. Rev. A **49**, 2405 (1994).
[7] A. Z. Msezane and Z. Chen (unpublished).
[8] A. Z. Msezane and Z. Chen, Phys. Rev. A **49**, 3083 (1994).
[9] Harald Friedrich, *Theoretical Atomic Physics* (Springer-Verlag, New York, 1990), p. 220.
[10] E. Clementi and C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974).
[11] C. E. Bielschowsky, C. A. Lucas, and G. G. B. de Souza, Phys. Rev. A **43**, 5975 (1991).