ANALYTICAL PROPERTIES OF OSCILLATOR-STRENGTH DISTRIBUTIONS

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The optical oscillator strength distribution df/dE for ionization of an electron from an $n\ell$ subshell is a the sum of channel contributions.

That is

$$df/dE = dF_{\ell+1}/dE + df_{\ell-1}/dE. \quad (1)$$

In atomic units,

$$dF_{\ell+1}/dE = \alpha_{\ell+1}(E - E_{n\ell}) [R_{\ell+1}(E)]^2. \quad (2)$$

Here $\alpha_{\ell+1}$ is a numerical constant, $E = 1/2k^2$ is the kinetic energy of the ejected electron and $E_{n\ell}$ is its binding energy. The electric dipole matrix element $R_{\ell+1}$ is given by

$$R_{\ell+1}^2(E) = \left[\int P_{n\ell} r P_{E\ell+1} dr \right]^2 \quad (3)$$

$$= C_{\ell+1}^2(k) \left[\int P_{n\ell} r \bar{P}_{E\ell+1} dr \right]^2 = C_{\ell+1}^2(k) [\bar{R}_{\ell+1}(E)]^2 \quad (4)$$

where $P_{n\ell}$ is the initial (bound) state radial wave function and $\bar{R}_{\ell+1}$ is the reduced dipole matrix element. The normalization constant $C_{\ell+1}(k)$ is chosen so that the continuum state wave function $\bar{P}_{E\ell+1}$ is independent of E near $r = 0$.

It is always possible to fit Eq. (1) to a polynomial in E . In practice this rarely works over a wide range of ejected electron energies because in an

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analytical sense df/dE can be represented by a power series in E that converges only for small E . It is the purpose of this work to suggest new independent variables that can be used to fit optical oscillator strength distributions in an efficient manner. The wave functions $P_{n\ell}$ and $\bar{P}_{E\ell+1}$ were generated by the independent particle approximation employing Hartree-Slater potentials.

The partition in Eq. (3) is important in the present context because C and $\bar{R}$ have different analytical properties and may be discussed separately. The integrand in Eq. (4) is an integral function of E and from this it has been shown that the only singularity of $\bar{R}_\ell$ on the finite E plane resides at $E = E_{n\ell} = -I$. The presence of this singularity indicates that a power series representation of $\bar{R}_\ell$ in the variable E will show poor convergence. However, a new independent variable [J. Chem. Phys. 74, 6271 (1981)],

$$g_1 = E/(E + I) \quad (5)$$

maps a singularity free region in the E plane including the positive E axis into the unit circle of the g_1 plane. Therefore a series representation of $\bar{R}_{n\ell}$ in the variable g_1 converges for all physical values of E .

When $\ell = 0$ in Eq. (4) the dominant variation with E occurs in $\bar{R}_1(E)$. For this class of transition we may set $C_1 = 1$ and approximate df_1/dE by

$$df_1/dE = \sum_{n=1}^{n=N} a_n g_1^n \quad (6)$$

Fig. 1 shows an application of Eq. (6). The solid curve represents calculated values of df/dE for $\text{Na}(3s \rightarrow p)$. For convenience, the results have been

normalized to 1 at $g = E = 0$. The open circles represent a least square fit of the data to Eq. (6) with $N = 4$. The polynomial representation is quite good in view of the fact that this transition exhibits a Cooper minimum near $E = 1$ eV.

In the general case, it is necessary to also account for the properties of $C_{\ell\pm 1}^2(k)$ in Eq. (4). The function $C_{\ell\pm 1}^2(k)$ is known from an analysis of the closely related S matrix to possess poles in the k plane at $k = \pm i/\gamma_n$ ($n = 1, 2, \dots, \infty$) where γ_n are the bound state eigenvalues. Hence all the singularities of f including those of $\bar{R}_{\ell\pm 1}(k^2)$ are located on the imaginary axis of the k plane. The transformation

$$g_2 = \frac{k-\alpha}{k+\alpha} = \frac{\sqrt{2E} - \alpha}{\sqrt{2E} + \alpha} \quad (7)$$

maps the right half of the k plane into the unit circle of the g_2 plane. Thus in the more general case the differential oscillator strength may be represented by a polynomial approximant

$$df/dE = \sum_{n=1}^{n=N} a_n g_2^n \quad (8)$$

An application of Eq. (8) is shown in Fig. 2. The solid curve represents calculated values of differential oscillator strengths for $\text{Ne}(2p \rightarrow s, d)$. The data have been normalized to 1 at $E = 0$. The open circles were obtained by a least square fit of the data to a polynomial of degree 4 with $\alpha = 6I^{1/2}$. Again the fit is quite satisfactory.

The general approach illustrated by two examples above has been applied with success to oscillator strength distributions in several atoms including those exhibiting resonance structure.

Figure 1

Figure 2

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