THE PHYSICS OF IONIZED GASES

Edited by

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SPIG • 84

Institute of Physics Beograd, Yugoslavia

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Edited by

World Scientific

Published by

World Scientific Publishing Co Pte Ltd.
P. O. Box 128, Farrer Road, Singapore 9128
242, Cherry Street, Philadelphia PA 19106-1906, USA

ISBN 9971-50-001-9

Printed in Singapore by Kyodo-Shing Loong Printing Industries Pte Ltd.

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ACKNOWLEDGEMENTS

The XII Yugoslav Summer School and International Symposium on Physics of Ionized Gases was organized by

The Institute of Physics, Belgrade, Yugoslavia

under the auspieces of

- The Union of the Societies of Mathematicians, Physicists and Astronomers of Yugoslavia

and supported by

- The Council of Self-Managed Communities of Interest for Science of Socialist Republic of Yugoslavia

and

- The Committee for Physics of Self-Managed Community of Interest for Science of Socialist Republic of Serbia

PREFACE

This book contains 42 invited lectures and progress reports presented at the XII Yugoslav Summer School and International Symposium on Physics of Ionized Gases (XII SPIG '84), held in Šibenik, Yugoslavia, from September 3 to September 7, 1984. The invited programme covers all scientific topics of the Conference, concentrated on the Plasma Physics and Physics of Gas Discharges and on the supporting fields of Physics of Atomic Collisions and Physics of Particle Interaction with Solids.

The editors express their particular gratitude to the lecturers who kindly submitted their manuscripts in their final form for publication.

We beleive that this volume, containing contributions of many renown lecturers, will be a valuable source of information in the field both for graduate students and experts.

Editors

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WHAT FORMULAS ARE GOOD FOR REPRESENTING DIPOLE AND GENERALIZED OSCILLATOR-STRENGTH SPECTRA?*

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Introduction

The dipole oscillator-strength distribution $df/d\varepsilon$ for a single continuum excitation of an atom or molecule is a function of the kinetic energy ε of an outgoing electron. The distribution describes many optical phenomena such as absorption, refraction, and reflection; in particular, $df/d\varepsilon$ is equal to the cross section for ionization by a photon with energy $\varepsilon + I$, apart from a universal constant, where I is the ionization threshold for the relevant shell.[1] Furthermore, $df/d\varepsilon$ governs the ionization by glancing collisions of fast charged particles.[2] Recent years have seen considerable accumulation[3,4] of experimental data on $df/d\varepsilon$. Those data are indeed valuable for many applications in radiation physics, plasma physics, atmospheric physics, and astrophysics. In most of these applications, one needs a comprehensive set of data, i.e., numerical values of $df/d\varepsilon$ over a wide range of ε, say, from several eV to many keV; most often, one needs data at all ε at which $df/d\varepsilon$ is appreciable. However, it is unrealistic to expect for measurements to cover all the ε values. Consequently, one must find a method for systematizing the data so that one can extrapolate or interpolate them dependably.

It is from the above consideration that we started a series of studies[5-8] aimed at answering the question in the title. The present lecture is in effect a summary of those studies.

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*Work performed under the auspices of the U.S. Department of Energy.

Part 1 treats analytic properties of $df/d\varepsilon$ considered as a function of ε. To begin with, one distinguishes[9] two factors that together constitute $df/d\varepsilon$. The first factor is defined in terms of the dipole matrix element with respect to the final-state wavefunction whose amplitude near the origin is independent of ε. This factor is analytic at all finite ε, except for a universal singularity[5] at $\varepsilon = -I$, where I is the relevant threshold ionization energy. The other factor stems from the normalization of the final-state wavefunction on the energy scale. This factor[6] plays important roles in at least three respects. First, when the phase shift rapidly varies with real ε (a situation that we shall loosely call a resonance), the normalization factor exhibits a maximum, and its local behavior may be approximated by a Lorentzian form. Second, the same factor is crucial for consideration of the high-ε asymptotic behavior. Finally, the analytic continuation of the same factor to negative ε naturally leads to properties of bound states including the discrete oscillator-strength spectrum. Through several examples, we shall illustrate the use of all the analytic properties in the practical fitting of the $df/d\varepsilon$ data.

Part 2 deals with the generalized oscillator strength, which is the only non-trivial factor in the differential cross section for the inelastic scattering of a charged particle by an atom or molecule, evaluated within the first Born approximation.[2] The distribution $df(K,\varepsilon)/d\varepsilon$ of the generalized oscillator strength for ionization is a function of both ε and momentum transfer K. The K-dependence of this function at a fixed ε is best elucidated through an analysis from the point of view of the theory of functions of a complex variable (which may be either K or K^2). This point of view was first advanced by Lassettre,[10] who specifically treated the generalized oscillator

strength for the excitation to a bound excited state. Our recent work[8] is an extension of the work of Lassettre. Results of our analysis lead to practical methods for fitting the data specifically for ionization.

Part 1. Dipole Oscillator-Strength Distribution

1.1. The reduced matrix element and the normalization factor

The essential ingredient of $df/d\varepsilon$ is the single-electron radial dipole matrix element. For a transition from an initial bound orbital $r^{-1}P_{n_0\ell_0}(r)$ to a final continuum orbital $r^{-1}P_{\varepsilon\ell}(r)$ of an atom, the radial matrix element $R_\ell(\varepsilon)$ is defined by

$$R_\ell(\varepsilon) = \int_0^\infty P_{\varepsilon\ell}(r) r P_{n_0\ell_0}(r) dr, \tag{1}$$

where $\ell = \ell_0 \pm 1$. It is convenient to distinguish two causes for the ε-dependence of $P_{\varepsilon\ell}(r)$, and hence of $R_\ell(\varepsilon)$. First, $P_{\varepsilon\ell}(r)$ obeys the Schrödinger equation

$$[d^2/dr^2 - 2V(r) - \ell(\ell+1)r^{-2} + 2\varepsilon]P_{\varepsilon\ell}(r) = 0, \tag{2}$$

where and in what follows we use the atomic-unit system (in which $e = \hbar = m = 1$). Suppose that $\bar{P}_{\varepsilon\ell}(r)$ is the solution of Eq. (2) whose amplitude near the origin is independent of ε, i.e.,

$$\bar{P}_{\varepsilon\ell}(r) = r^{\ell+1} \qquad \text{near } r = 0. \tag{3}$$

However, $P_{\varepsilon\ell}(r)$ appropriate for Eq. (1) must satisfy the normalization condition

$$\int_0^\infty P_{\varepsilon\ell}(r)\, P_{\varepsilon'\ell}(r) dr = \delta(\varepsilon - \varepsilon'), \tag{4}$$

and it differs from $\bar{P}_{\varepsilon\ell}(r)$ by a factor $C_\ell(\varepsilon)$. That is to say,

$$P_{\varepsilon\ell}(r) = C_\ell(\varepsilon)\, \bar{P}_{\varepsilon\ell}(r). \tag{5}$$

Thus we may write

$$R_\ell(\varepsilon) = C_\ell(\varepsilon)\, \bar{R}_\ell(\varepsilon), \tag{6}$$

where $\bar{R}_\ell(\varepsilon)$ is the matrix element with respect to $\bar{P}_{\varepsilon\ell}(r)$, and it may be called the reduced matrix element. For real ε (i.e., for physical

values of ε), the functions $P_{\varepsilon\ell}(r)$ and $\bar{P}_{\varepsilon\ell}(r)$ may be taken as real, without loss of generality. Therefore, $C_\ell(\varepsilon)$, $\bar{R}_\ell(\varepsilon)$, and $R_\ell(\varepsilon)$ are all real-valued for real ε.

Analytic properties of $\bar{R}_\ell(\varepsilon)$, now considered as a function of complex variable ε, is simple.[5] It is analytic for all finite ε except at a universal singularity at $\varepsilon = -I$. The cause for this singularity is elementary. First, consider contributions to $\bar{R}_\ell(\varepsilon)$ from finite r. From the general theory of differential equations, one knows that $\bar{P}_\ell(\varepsilon)$ is analytic for all finite ε, because ε appears in Eq. (2) as a constant coefficient. Therefore, the contribution to $\bar{R}_\ell(\varepsilon)$ from finite r is a function analytic for all finite ε. Next, consider the contribution to $\bar{R}_\ell(\varepsilon)$ from large r at which the asymptotic behavior of the wavefunctions prevails. There the dominant factor of $P_{n_0\ell_0}(r)$ is $\exp[-(2I)^{1/2}r]$, and the dominant factor of $\bar{P}_{\varepsilon\ell}(r)$ is $\exp(\pm ikr)$. The product of the two exponentials gives $\exp[\pm ik - (2I)^{1/2}]r$. Thus $\bar{R}_\ell(\varepsilon)$ diverges at $\pm ik = (2I)^{1/2}$, i.e., at $\varepsilon = -I$. (More generally for $\mathrm{Re}[\pm ik - (2I)^{1/2}] > 0$, the integral diverges, but its analytic continuation is definable there. Thus $\bar{R}_\ell(\varepsilon)$ is singular at the point $\pm ik = (2I)^{1/2}$ only.) Although the location of the singularity is physically inaccessible, it is nevertheless important to recognize its presence. In other words, it is appropriate to represent $\bar{R}_{\varepsilon\ell}(\varepsilon)$ in terms of a variable that incorporates the singularity.

An example of such a variable is

$$g = \varepsilon/(\varepsilon + I). \tag{7}$$

To see its significance, one may view Eq. (7) as a conformal mapping from the complex ε plane onto the complex g plane. The half plane on the right of the vertical line $\mathrm{Re}\ \varepsilon = -I/2$ (the shaded region in Fig. 1) is mapped onto the interior of the unit circle. The singularity $\varepsilon = -I$ is mapped to $g \to \infty$. Physical data for the oscillator-strength pertain

to real positive ε (forming the continuum), and to discrete negative values ε_1, ε_2, ... of ε (forming the discrete spectrum); we may call the set of all those ε values the physical domain. By Eq. (7), the physical domain (indicated by the heavy line and dots in Fig. 1) is mapped onto a segment of the real axis on the g plane, and this segment is entirely within the interior of the unit circle. Because $\bar{R}_\ell(\varepsilon)$ has no singularity other than ε = −I, it is analytic in g certainly within the unit circle, and thus may be expressed by an absolutely convergent series in powers of g. In many examples,[5-7] the use of a polynomial in g of a modest degree is sufficient for effective representation of data on df/dε.

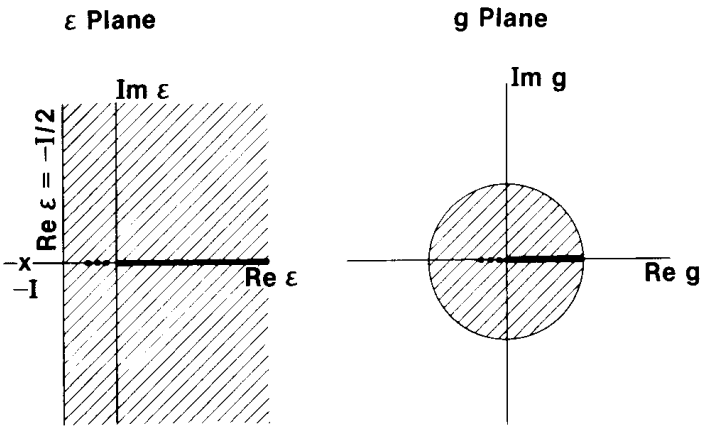

Fig. 1. Conformal mapping g = ε/(ε + I).

The quantity $C_\ell(\varepsilon)$ may be called the normalization factor or the enhancement factor,[9] and is closely related to what the solid-state theorist calls the density of states. General properties of $C_\ell(\varepsilon)$ have been studied both analytically and numerically.[6] When the phase shift $\delta_\ell(\varepsilon)$ changes rapidly with ε, $C_\ell(\varepsilon)$ shows a maximum. We may call this situation a resonance; in this case, the fitting of df/dε requires some parameterization of $C_\ell(\varepsilon)$, the use of a new variable, or both.[6] Further discussion on this topics is seen in Section 1.3.