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Spectral characterization of elemental emissions, experimental insights and theoretical evaluation

^DIslam Amangeldinov^{1,*}, ^DDmitri Korovaev²

¹Faculty of Engineering and Information Technology, Almaty Technological University, 100 Tole bi st., Almaty, Kazakhstan

²Institute of Physics, Technical University of Berlin, 17 Straße des, Berlin, Germany *Correspondence: <u>amangeldinovi@list.ru</u>

Abstract. This experimental study delves into the spectral analysis of five discrete spectral lamps, namely helium, sodium, mercury, cadmium and zinc, utilizing a suite of scientific instrumentation including an optical spectrometer with converging lenses and a diffraction grating. The primary objective is to determine the wavelengths corresponding to visible spectral lines emitted by these lamps. Calibration of the spectrometer with the helium lamp facilitated the derivation of the diffraction grating constant. Subsequent measurements of diffraction angles allowed for the computation of experimental wavelengths, which were then compared with theoretical values. Analysis revealed slight discrepancies between experimental and theoretical values, likely attributed to systematic errors such as extraneous light sources and parallax errors in angle measurements. Furthermore, examination of distinct spectral components. Overall, this study underscores the significance of meticulous experimental techniques in the elucidation of fundamental physical phenomena and highlights the interplay between theory and observation in spectral analysis.

Keywords: spectral analysis, spectral lamps, optical spectrometer, diffraction grating, wavelength determination.

1. Introduction

The study of hyperfine splitting in the spectra of ions, atoms, and molecules is a very urgent task both due to advances in the methods of modern spectroscopy and due to the development of theoretical methods of calculation.

The theoretical prediction of the hyperfine splitting constants and their comparison with measurement results is used to assess the level of accuracy of the calculation of the electronic wave function of the system under consideration. Precision calculations of the electronic structure are important for many tasks, ranging from the development of atomic clocks to the search for "new physics", such as the detection of the electron's electric dipole moment [1]. However, the study of superfine splitting is of independent interest also from the point of view of studying the structure of the nucleus. The point is that the effect of the finite size of the nucleus makes a significant contribution to the hyperfine splitting constant. The accounting of the charge part of this correction is not very difficult, since it depends mainly on the known charge radius of the nucleus. But the problem of accounting for the magnetic part of the correction is much more complicated and much more interesting [2-3].

In case of its successful solution, one can improve the agreement between the theoretical and experimental hyperfine splitting constants and draw conclusions about the differences in the distribution of the magnetization of isotope nuclei [4]. In addition, it is possible to determine the magnetic moments of short-lived nuclei. In contrast to stable nuclei, where it is possible to perform a nuclear magnetic resonance experiment, it is difficult to apply this experimental method for short-

lived nuclei. However, by combining the experimental constants of superfine splitting and the results of Bohr-Weisskopf effect calculations, it is possible to determine the desired magnetic moment [5–7].

In [8] and [9], an approach and programs were developed that allow one to calculate the Bohr-Weisskopf effect for neutral atoms both in the model of the nucleus with a uniform distribution of magnetization over its volume and in the Woods-Saxon model with the spin-orbit interaction taken into account while taking into account the effects of electron correlation. It should be noted that while the first model is widely used in atomic calculations, the second model was previously used only for multicharged ions, and for heavy neutral atoms it was applied for the first time. One of the difficulties encountered in the calculations was to take into account the effects of electron correlation. It turned out that for one of the electronic states of the thallium atom the value calculated at the Dirac-Hartree-Fock level differs from the experimental one by a factor of 5 [10]. Therefore, to achieve a good result, it is required to take into account the effects of electron correlation at a very high level, in the framework of the coupled cluster method with the inclusion of cluster amplitudes up to fourfold. One of the important results obtained in the course of this work was the refinement of the magnetic moments of a number of metastable thallium isotopes. The developed approach can also be generalized to the case of molecules, which is already becoming relevant.

2. Methods

In the conducted experimental investigation, a comprehensive array of scientific instrumentation was employed to determine the wavelengths corresponding to visible spectral lines originating from the elemental constituents contained within a series of 5 discrete spectral lamps. The instrumental setup encompassed an optical spectrometer featuring converging lenses, a diffraction grating, and a selection of spectral lamps comprising helium (He), sodium (Na), mercury (Hg), cadmium (Cd), and zinc (Zn). Additional equipment included a power supply and a lamp holder affixed to a tripod base.



Figure 1 – The instrumental setup of optical spectrometer

Prior to commencing the experimental procedure, the spectrometer underwent calibration utilizing the helium spectral lamp. The spectral emissions from the He lamp were captured, while concurrently determining the diffraction grating parameters. To facilitate this, the lamp was positioned within the lamp holder and allowed to stabilize for a duration of 5 minutes to attain optimal operational conditions. Subsequently, alterations to the diffraction angle facilitated the observation of light exhibiting diverse chromatic manifestations, with corresponding angular values documented

accordingly. A calibration curve, depicting the sinusoidal function of the angle against the wavelength of light, was then generated, facilitating the derivation of the diffraction grating constant.

In the ensuing phase of the experiment, the observable spectral lines emitted by sodium were measured. This involved the meticulous determination of the wavelengths characterizing the spectral lines of sodium, predicated upon the calculation of the corresponding angular values for each spectral line, utilizing the diffraction constant ascertained in the preceding calibration segment. The sodium spectral lamp was positioned within the lamp holder and situated before the spectrometer. Rotation of the telescopic apparatus enabled the sequential observation of diverse spectral hues, with angular rotations duly recorded. This protocol was iteratively applied to spectral lamps containing mercury, cadmium, and zinc, facilitating a comparative analysis of the obtained results vis-à-vis their theoretical counterparts.

3. Results and Discussion

In this paper we focused on observing and measuring the spectral lines emitted by different spectral lamps and determining the diffraction grating constant and the corresponding wavelengths corresponding to the brightest spectral lines. A helium lamp was taken for initial calibration and the values are shown in Table 1.

radie $1 - $ The spectral composition of hermin (He)						
terature wavelength, nm	Angle, degree	Angle error, minutes				
667.8	23.72	± 0.5				
587.6	20.77	± 0.5				
501.6	17.67	± 0.5				
492.2	17.27	± 0.5				
471.3	16.57	± 0.5				
447.1	15.70	± 0.5				
	- The spectral composite terature wavelength, nm 667.8 587.6 501.6 492.2 471.3 447.1	- The spectral composition of hendrif (He) terature wavelength, nm Angle, degree 667.8 23.72 587.6 20.77 501.6 17.67 492.2 17.27 471.3 16.57 447.1 15.70				

Table 1 – The spectral composition of helium (He)

When an atom is placed in a magnetic field, its total energy is the sum of two parts: the internal energy of the atom and the energy of its interaction with the external magnetic field. The interaction energy is determined by the induction of the magnetic field and the magnetic moments (of both orbital and spin origin) of the electrons of the atom (we do not consider here the influence of the much smaller magnetic moment of the nucleus).

We investigated different spectral lamps and the data are shown in Table 2,3,4 and 5.

Table 2 – Determined visible s	pectral lines with	corresponding angles	from the sodium lam	p (Na)
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Color	λ , nm	$\Delta\lambda$, nm	Angle, degree	Angle error, min.
red	621.648	2.180	21.91	± 0.5
yellow	595.470	2.089	20.93	± 0.5
bluish green	571.856	2.006	20.07	± 0.5
greenish blue	518.717	1.821	18.13	± 0.5
blue	502.564	1.765	17.55	± 0.5
purple	471.035	1.655	16.42	± 0.5

Table 3 –	Determined	visible spec	tral lines	with corre	esponding a	ingles	from t	he mercury	lamp	(Ho)
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	k		0 0	
Color	λ, nm	$\Delta\lambda$, nm	Angle, degree	Angle error,min.
red	667.8	2.204	22.15	± 0.5
yellow	587.6	2.052	20.55	± 0.5
yellow	501.6	2.045	20.47	± 0.5
green	492.2	1.944	19.42	± 0.5
blue – green	471.3	1.764	17.53	± 0.5
blue – green	447.1	1.747	17.37	± 0.5
blue	432.5	1.557	15.40	± 0.5
violet	428.3	1.446	14.27	± 0.5

				r ()
Color	λ, nm	Δλ, nm	Angle, degree	Angle error,min.
red	667.8	2.277	22.93	± 0.5
red	587.6	2.233	22.47	± 0.5
green	501.6	1.833	18.25	± 0.5
green	492.2	1.805	17.97	± 0.5
blue	471.3	1.699	16.87	± 0.5
blue	447.1	1.668	16.55	± 0.5
violet	432.5	1.566	15.50	± 0.5

Table 4 – Determined visible spectral lines with corresponding angles from the cadmium lamp (Cd)

Table 5 – Determined visible spectral lines with corresponding angles from the mercury zinc (Zn)

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λ, nm	$\Delta\lambda$, nm	Angle, degree	Angle error, min.
667.8	2.229	22.42	± 0.5
587.6	2.120	21.27	± 0.5
501.6	2.032	20.33	± 0.5
492.2	1.927	19.23	± 0.5
471.3	1.778	17.68	± 0.5
447.1	1.751	17.40	± 0.5
432.5	1.699	16.87	± 0.5
428.3	1.664	16.50	± 0.5
416.2	1.649	16.35	± 0.5
411.3	1.542	15.25	± 0.5
	λ , nm 667.8 587.6 501.6 492.2 471.3 447.1 432.5 428.3 416.2 411.3	λ , nm $\Delta\lambda$, nm667.82.229587.62.120501.62.032492.21.927471.31.778447.11.751432.51.699428.31.664416.21.649411.31.542	λ , nm $\Delta\lambda$, nmAngle, degree667.82.22922.42587.62.12021.27501.62.03220.33492.21.92719.23471.31.77817.68447.11.75117.40432.51.69916.87428.31.66416.50416.21.64916.35411.31.54215.25

Intensity maxima occur if the diffraction angle satisfies the following conditions:

$$n\lambda = g\sin\varphi; n = 0, 1, 2... \tag{1}$$

Where: λ – wavelength, nm, g – diffraction grating, φ – the angle of diffraction, deg. Diffraction grating could be found by rearranging the equation (1) and is calculated using the

slope:

$$g = \frac{n\lambda}{\sin\varphi} = \frac{1}{slope} \tag{2}$$

The diffraction grating constant served as a pivotal parameter for deducing the wavelengths corresponding to the spectral lines of mercury (Hg), cadmium (Cd), and zinc (Zn). Employing Equation (1), with n=1 and φ representing the measured diffraction angles for each spectrum, facilitated the computation of experimental values. Tables 2-5 encompass the resultant experimental data. Specifically, for the determination of experimental mercury (Hg) wavelengths, the diffraction angles were utilized as inputs.

Let's analyze the splitting on the example of the spectral line of the presented lamps, it is possible to note that there is a removal of degeneration of each of the specified levels on quantum number. Thus, the considered spectral line in the presence into three components, which corresponds to the experimental results.

4. Conclusions

The conducted experimental investigation encompassed a meticulous exploration of spectral emissions from various elemental compositions encapsulated within a series of five discrete spectral lamps. This endeavor was facilitated by a comprehensive suite of scientific instrumentation, including an optical spectrometer with converging lenses, a diffraction grating, and ancillary equipment such as a power supply and lamp holder.

Initial calibration of the spectrometer was undertaken utilizing the helium spectral lamp, enabling the determination of diffraction grating parameters. Subsequent spectral analyses involved the measurement of diffraction angles to deduce the wavelengths corresponding to the most intense spectral lines emitted by sodium, mercury, cadmium, and zinc. Notably, the computed diffraction grating constant served as a pivotal parameter in the determination of wavelengths. These experimental findings, compared with theoretical values, facilitated a comprehensive analysis of

observed deviations, which may be attributed to systematic errors introduced during the experiment. Such errors include the influence of extraneous light sources and potential parallax errors in angle measurements. Moreover, examination of spectral line splitting revealed a removal of degeneracy within specified energy levels, resulting in the observation of distinct spectral components. This observation aligns with theoretical expectations and further corroborates the experimental outcomes.

In conclusion, this investigation has provided valuable insights into the spectral characteristics of various elemental compositions, underscoring the importance of meticulous experimental methodologies and the interplay between theory and observation in elucidating fundamental physical phenomena.

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Information about authors:

Islam Amangeldinov – Master Student, Faculty of Engineering and Information Technology, Almaty Technological University, 100 Tole bi st., Almaty, Kazakhstan, <u>amangeldinovi@list.ru</u> *Dmitri Korovaev* – MSc, Research Assistant, Institute of Physics, Technical University of Berlin, 17 Straße des, Berlin, Germany, <u>korovaevdm@gmail.com</u>

Author Contributions:

Islam Amangeldinov – concept, methodology, resources, data collection, testing. *Dmitri Korovaev* – modeling, analysis, visualization, interpretation, drafting, editing, funding acquisition.

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