WEB OF SYNERGY:

International Interdisciplinary Research Journal

Volume 2 Issue 2, Year 2023 ISSN: 2835-3013

https://univerpubl.com/index.php/synergy

Factors Affecting the Half-Width of Contours of Spectral Lines

Rayimov Nurbek

1st year Master's student of Karshi State University, Faculty of Physics

Article Information

Received: December 26, 2022

Accepted: January 27, 2023

Published: February 28, 2023

Keywords: *spectral line, contour, energy level, half width.*

ABSTRACT

In this article, we consider the factors affecting the half-width of contours of spectral lines.

Introduction:

We know that the transitions between discrete energy states are monochromatic, and the frequency of the absorbed or emitted photon is given by:

$$\nu_{ij} = \frac{E_i - E_j}{h} \quad (1)$$

In fact, any energy state has a certain width, so the transitions between these energy states are not strictly monochromatic, occupying a certain frequency range in the spectrum (Figure. 1).

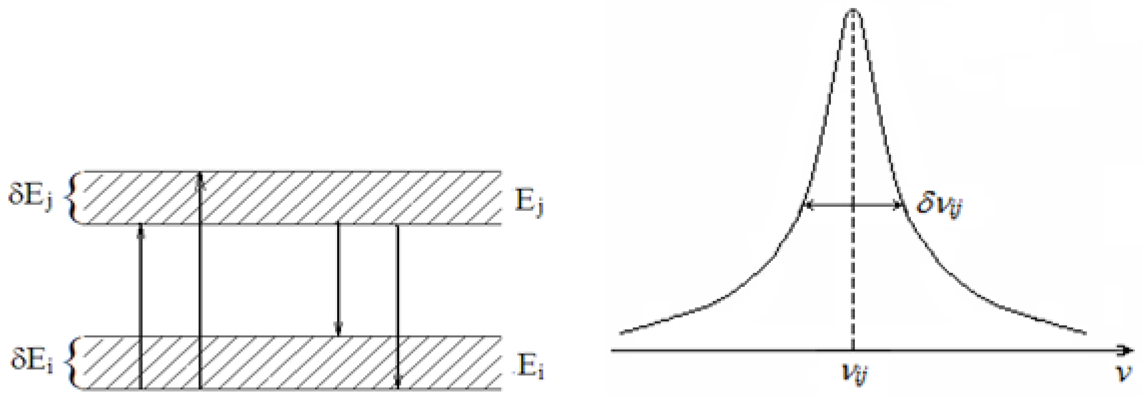

Figure 1. Transitions between energy levels with a certain width.

In this case, the energy and frequency width in the transition between energy levels is as follows.

$$\delta E_{ij} = \delta E_i + \delta E_j \quad (2)$$

$$\delta\nu_{ij} = \frac{\delta E_{ij}}{h} \quad (3)$$

1.Natural latitude

The width of the stationary states corresponding to a system of quiescent particles, or the width of the contour, is called the natural width. There is a connection between the energy width of the stationary states and the residence time of the particles in the wake state, i.e. from the uncertainty principle in quantum mechanics of energy and time as follows

$$\delta E \cdot \delta t \sim \hbar = \frac{h}{2\pi} \quad (4)$$

It can be seen from (4) $\delta t \longrightarrow \infty$ that the energy state is very narrow when aspiration occurs, i.e

$$\left.\begin{array}{l} \delta t \to \infty \\ \delta E \to 0 \end{array}\right\} \quad (5)$$

In the ground energy state (5) can be observed, that is, the particle has a lot of ground state or lives a lot. The natural contour is the narrowest contour compared to other contours. If we substitute taking into account the residence time, we get the following for each case:

$$\delta E_i = \frac{\hbar}{\tau_{e_i}} = \frac{h}{2\pi\tau_{e_j}} \quad (6)$$

δE_{ij} -for a combination of stationary states can be written to $(i \to j)$ transition

$$\delta\nu_{ij} \sim \frac{1}{2\pi}\left(\frac{1}{\tau_{e_i}} + \frac{1}{\tau_{e_j}}\right) \quad (7)$$

τ_{e_i}, τ_{e_j}, - s i and j average survival of cases.

τ_{e_i} and τ_{e_j} are determined by the values of a A_i nd A_j, and the probability of spontaneous transition.

As we know $\tau_e = \frac{1}{A_{ij}}$;, to get around this $i \to j$, we can write the following

$$\delta\nu_{ij} = \frac{1}{2\pi}\left(A_i + A_j\right) \quad (8)$$

The distribution of intensity in the natural contour (during absorption) is based on the following law

$$\frac{dW_{ю}}{dt} = \frac{e^2}{m} \cdot \frac{\gamma\omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + 4\gamma^2\omega^2}\varepsilon_0^2 \quad (9)$$

ε_0^2 - Light wave amplitude

$e = 1{,}602191 \cdot 10^{-19} k$ - electron charge

$m_e = 9{,}10955 \cdot 10^{-31} kg$ - mass

$\frac{e}{m} = 1{,}7588 \cdot 10^{11} kg^{-1} \cdot k$

$\nu = \nu_0 = \frac{\omega_0}{2\pi}$ the intensity has a maximum value at this point and the intensity decreases equally on both sides. The wider the contour, the greater the fade.

$\omega_0 = \frac{k}{m}$ is called the natural oscillation frequency of the oscillator. k- is the quasielastic constant.

It can be seen from the 9th formula that the absorption depends on the frequency. A similar formula can be written for the radiation spectrum, that is, the intensity distribution function in the radiation spectra

$$\varphi_{tabiiy}(\nu) = \frac{W^{н}(\nu)}{W^{н}(\nu_0)} = \left(\frac{\gamma_0}{2}\right)^2 \cdot \frac{1}{4\pi^2(\nu - \nu_0)^2 + \left(\frac{\gamma_0}{2}\right)^2} \qquad (10)$$

γ_0 -extinction coefficient (sec^{-1})

The contour whose intensity distribution obeys the 10th formula is called dispersion or Lorentz contour. The contour of natural expansion follows the same distribution as its half-width

$$\delta\nu_{\frac{1}{2}tabiiy} = \frac{\gamma_0}{2\pi} \qquad (11)$$

The Lorentz contour will look like this.

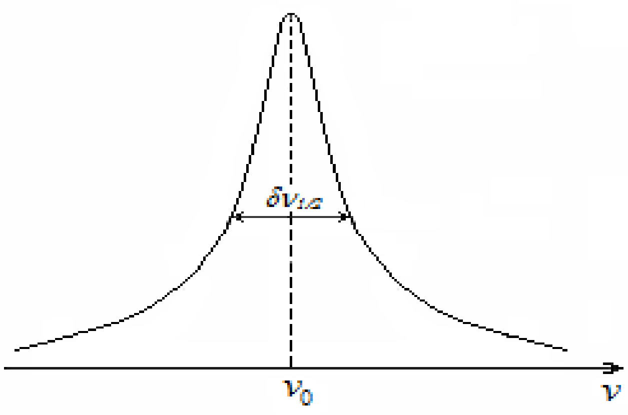

Figure 2. Dispersion (Lorentzian) distribution of spectral line contour.

In gases, it is usually the half-width of the natural expansion contour equal to $\delta\nu_{\frac{1}{2}tabiiy} = 10^{-4} A^{\circ}$

2. Doppler broadening

The essence of this phenomenon is that the frequency of absorbed or emitted quantum changes due to the speed of movement of the molecule. Let's assume that the light is propagating along the z-axis. Let the molecule form an angle θ with respect to the z axis and move with speed (Fig. 3).

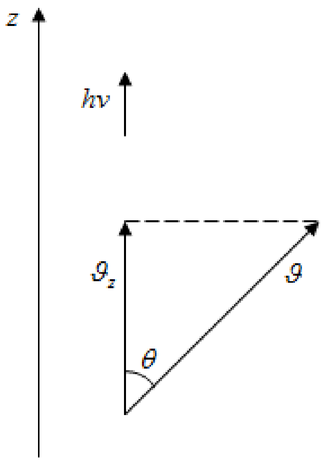

Figure 3. Emission of a light quantum by a molecule in motion

At that time, the frequency of the spectral line changes due to the Doppler effect

$$\nu - \nu_0 = \nu_0 \frac{\vartheta}{c} \cos\theta = \nu_0 \frac{\vartheta_z}{c} \qquad (12)$$

c - is the speed of light

ν_0 - absorption or radiation frequency of the particle

ϑ_z - the projection of the speed relative to the z axis.

One of the main properties of Doppler broadening is that if the molecule is moving perpendicularly to the light quantum (12) according to the formula, the broadening is zero (change in frequency is 0). If it is perpendicular, it will be equal $\cos 90^0 = 0$. The best effect is either or.

Distribution of intensity in the Doppler contour

$\varphi(\nu)_{дon} = \frac{I(\nu)}{I(\nu_0)} = e^{-\left[\beta(\nu-\nu_0)^2\right]}$ (13) It can be seen from (13) that the intensity distribution changes according to the exponential law.

$$\beta = \frac{m_\mu c^2}{2\kappa T} \cdot \frac{1}{\nu_0^2} \qquad (14)$$

m_μ -the mass of the molecule

c - speed of light

k - Bolsmann's constant

T - absolute temperature

The higher the temperature, the stronger the Doppler effect.

Thus, Doppler broadening depends on the mass and temperature of molecules.

From (12) and (14) we can write the following.

$$\delta\nu_{\frac{1}{2}dop} = 2\nu_0\sqrt{\left(2\kappa T / m_\mu c^2\right)\ell n 2} \quad (15)$$

Due to the Doppler effect, the half-width of the spectral line contour can be extended up to $10^{-2}\overset{0}{A}$

$$\delta\nu_{\frac{1}{2}dop} = 10^{-2}\overset{\circ}{A} \qquad (16)$$

The Doppler contour obeys the Gaussian function.

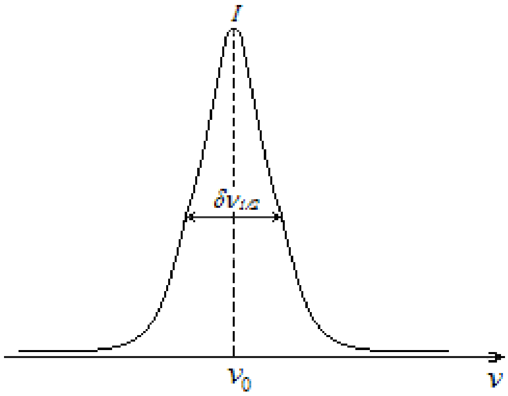

Figure 4. Doppler contour of the spectral band

3. Expansion due to collisions

One of the main reasons for the expansion of the contour of spectral lines in gases is the collision of molecules. When molecules collide with each other, they can move between stationary states due to the energy they gain due to the collision. Therefore, the composition of the resulting spectrum changes. The intensity distribution in the contour formed by the collision is as follows:

$$\varphi(\nu)_{to'q} = \frac{I(\nu)}{I_0(\nu_0)} = \frac{1}{\left(\frac{4\pi}{j_{to'q}}\right)^2(\nu-\nu_0)^2+1} \qquad (17)$$

$j_{to'q}$ —is the extinction coefficient associated with collisions.

The collision of identical molecules is based on the kinetic theory of gases

$$I_{to'q} = \frac{1}{\tau_{to'q}} = N\vartheta\delta \qquad (18)$$

$\tau_{to'q}$ - average time between collisions

N - is the number of molecules per unit volume

δ - the cross-sectional surface of the particle

ϑ – average speed

$$\delta\nu_{\frac{1}{2}to'q} = \frac{1}{2\pi\tau_{to'q}} = \frac{N\vartheta\delta}{2\pi} \qquad (19)$$

It can be seen from (17) that the intensity distribution in the collision contour is Lorentzian.

Usually

$$\delta\nu_{1/2_{to'q}} = (0,2 \div 0,5)\overset{0}{A} \quad (20)$$

Summary:

There are several factors that affect the half-width of the contour. In general, the total half-width of the contour

$$\delta\nu_{um} = \delta\nu_{1/2_{tabiiy}} + \delta\nu_{1/2_{dop}} \delta\nu_{1/2_{to'q}} + \delta\nu_{1/2_{boshqasabablar}}$$

Experiments show that the contour of the real spectral band in gases consists of the sum of the Doppler and collision contours, i.e. superposition. The central part of the band is due to the Doppler contour, and the wing part is due to collisional broadening. For example, at low pressure and high temperature, the contour of light molecules is Doppler-like because the speed of molecules is higher. Due to the large number of collisions between molecules at high pressures, the expansion can be explained mainly by collisions.

References:

1. Еляшевич М.А. Атомная и молекулярная спектроскопия. М.- 1962 г.
2. Герцберг Г. Спектры и строение двухатомных молекул. М.- 1949 г.
3. Герцберг Г. Колебателные и врашателные спектр многоатомных молекул. М.- 1979 г.
4. Маер Г.Г. Электронные спектры многоатомных молекул. Л.- 1969 г.
5. Чулановский В.М. Введение молекулярного спектралного анализа. М-Л.- 1951 г.