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Investigation of the radiation parameters of an oscillating charge in an ion system

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Abstract. A solution to the problem of determining the frequency spectrum and intensity of electromagnetic radiation generated by an oscillating charge in a dipole-quadrupole system has been obtained. The analysis of the obtained dependences for the oscillation frequencies reveals that knowing the maximum and minimum frequencies of the oscillating charge radiation spectrum allows for the calculation of molecular parameters. This analysis can be applied to study the electromagnetic radiation spectra of atoms and molecules in an excited state, as well as the parameters of the crystal lattice.

1 Introduction

To increase the efficiency of technological processes and improve the quality of products, there is a need for fast, accurate, reliable, informative methods for analyzing the composition and structure of chemical compounds.

The development and implementation of express methods for analyzing the composition and structure of molecules based on spectroscopy can increase the efficiency of using raw materials and energy resources, improve the quality of finished products.

The purpose and practical significance of the presented work are determined by the need to study the factors affecting the accuracy and reliability of spectroscopic radiation analysis, depending on the features of the molecular structure. Vibrational spectroscopy allows us to obtain information about the chemical composition, chemical structure of molecules, the presence and mutual position of individual atoms and chemical groups. The application of vibrational spectroscopy methods in chemistry and chemical technology requires fundamental knowledge in the field of spectral radiation theory. In the present work, relations are obtained for determining the intensity of electromagnetic radiation generated by an oscillating charge in an ionic system, depending on the geometry of the location of ions in molecules and on the direction of oscillation of the generating charge [1].

2 Materials and methods

The radiation parameters of an oscillating charge are analyzed using the equations of motion for an oscillating charge in an electric field. The radiation reaction force is included to

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account for the energy loss due to radiation. The equations are solved to obtain the frequency spectrum and intensity of the radiation.

The radiation parameters are measured using spectroscopic techniques. The frequency spectrum and intensity of the radiation are recorded and analyzed to determine the molecular parameters.

The data is analyzed using the obtained relations for determining the intensity of electromagnetic radiation generated by an oscillating charge in an ionic system. The analysis includes calculating the molecular parameters from the radiation spectrum parameters.

3 Results and discussion

First we will study a system of seven charges: negative charges $Q_1 = Q_2 = Q_3 = Q_4 = Q_-$ are located at the vertices of a rectangle with sides *2a* and *2b*, positive charges $Q_5 = Q_6 = Q_+$ are located in the center of sides *2b* of the rectangle, oscillating negative charge q is located in the center of the rectangle (Figure 1).

Let us consider two cases: 1 – charge oscillations in a straight line parallel to the sides *2b* of the rectangle (Figure 1); 2 – in a straight line parallel to the sides *2a* (Figure 2). The equation of charge motion in both the first and second cases has the form [2]

$$m\frac{\partial^2 z}{\partial t^2} = \left(\sum_{i=1}^{6} \vec{F}_i\right)_z, \tag{1}$$

where *m* – is the mass of the charge q, $\left(\vec{F}_i\right)_z$ – *z* is the projection of the force acting from the side of the charge Q_i onto the charge q.

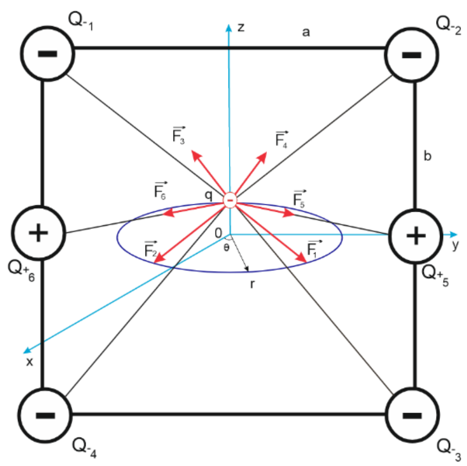

Fig. 1. The arrangement of charges and interaction forces in vertical oscillations.

In the first case, the *z* axis of the cylindrical coordinate system is parallel to the sides *2b*, in the second – *2a* of the rectangle. The forces of interaction between charges are determined by the equation:

$$F_i = \frac{1}{4\pi\varepsilon_0}\frac{Q_i q}{r_i^{\,2}}, \tag{2}$$

where $\varepsilon_0 = 8.85 \cdot 10^{-12} F/m$ is the electric constant, r_i is the distance between the i-charge and the charge q when it is displaced from the equilibrium position $z << a, b$. Taking into account the smallness of the parameters $z/a, z/b << 1$, the equation of charge motion q parallel to the sides *2b* (Figure 1) will take the form [3]:

$$m\frac{d^2z}{dt^2} = -\frac{2q}{4\pi\varepsilon_0}\left[\frac{4Q_-b^2}{d^5} + \frac{Q_+}{a^3}\right]z, \tag{3}$$

where $d^2 = a^2 + b^2$.

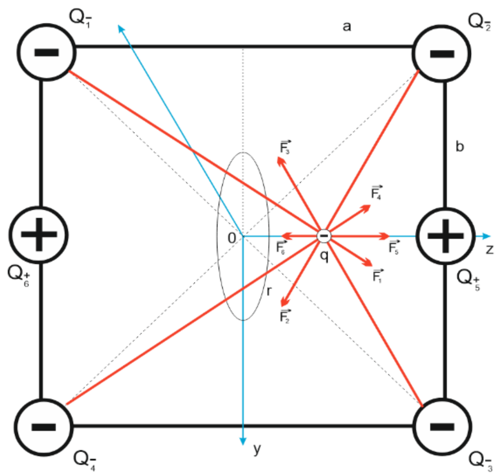

Fig. 2. Diagram of the arrangement of charges and interaction forces in horizontal oscillations.

The equation of motion of the charge q in the direction parallel to the sides *2a* can be represented as

$$m\frac{d^2z}{dt^2} = -\frac{2q}{4\pi\varepsilon_0}\left[\frac{4Q_-a^2}{d^5} - \frac{2Q_+}{a^3}\right]z. \tag{4}$$

It follows from equations (3), (4) that in the first case electromagnetic radiation with a frequency is generated

$$\omega_1 = \sqrt{\frac{2q}{4\pi\varepsilon_0 m}\left[\frac{4Q_-b^2}{d^5} + \frac{Q_+}{a^3}\right]}, \tag{5}$$

and then

$$\omega_2 = \sqrt{\frac{2q}{4\pi\varepsilon_0 m}\left[\frac{4Q_-a^2}{d^5} - \frac{2Q_+}{a^3}\right]}. \tag{6}$$

It follows from equation (6) that the oscillation of the charge q in the direction parallel to the sides *2a* will be stable if the condition is met.

$$\frac{2Q_-a^2}{d^5} > \frac{Q_+}{a^3} \text{ or } \frac{Q_-}{Q_+} > \frac{d^5}{2a^5}. \tag{7}$$

For example, for a=b, this ratio has the form $Q_-/Q_+ > 2^{3/2}$. It can be seen from equations (5) and (6) that the oscillation frequency of ω_1 exceeds ω_2, while the frequency ratio is determined by the geometry of the location and the magnitude of the charges causing oscillations of the generating charge q:

$$\frac{\omega_1}{\omega_2} = \left[\frac{\frac{4a^3b^2}{d^5} + \frac{Q_+}{Q_-}}{\frac{2a^5}{d^5} - \frac{Q_+}{Q_-}}\right]^{1/2} \tag{8}$$

Charge oscillations q generate electromagnetic radiation in a cylindrical coordinate system: the z axis is directed vertically for ω_1 and horizontally for ω_2. In the plane $z = 0$, under the condition $\frac{\partial}{\partial\theta} = 0, \frac{\partial}{\partial z} = 0$, it follows from Maxwell's equations [2]

$$\left(rot\vec{B}\right)_z = \frac{1}{r}\frac{\partial}{\partial r}rB_\theta = \mu\mu_0 j_z + \mu\mu_0\left(\frac{\partial\vec{D}}{\partial t}\right)_z, \tag{9}$$

$$\left(rot\vec{E}\right)_\theta = -\frac{\partial E_z}{\partial r} = -\frac{\partial B_\theta}{\partial t}. \tag{10}$$

that E_z and B_θ components of electromagnetic radiation are excited. In equations (9), (10): j_z is the current density created by an oscillating charge; $\mu_0 = 4\pi \cdot 10^{-7} H/m$ is the magnetic constant; μ is the relative magnetic permeability of the medium; $\vec{D}$ is the vector of electrical induction [4].

To calculate the intensity of electromagnetic radiation, it is necessary to know the amplitude of oscillation of the oscillating charge q. If the charge q is an ion in a molecular crystal lattice, then the oscillation amplitude can be estimated from the ratio [5].

$$\frac{A^2 m\omega^2}{2} = kT, \tag{11}$$

where $k = 1.38 \cdot 10^{-23} J/K$ is the Boltzmann constant, T is the absolute temperature, ω is the circular oscillation frequency, m is the mass of the charge q [6, 7].

$$A = \sqrt{\frac{2kT}{m\omega^2}} = \frac{1}{\omega}\sqrt{\frac{3kT}{m}}. \tag{12}$$

Knowing the amplitude of the oscillation of the generating charge, we determine the average intensity of electromagnetic radiation:

$$I = \frac{q^2 w^2}{6\pi\varepsilon_0 c^3}, \tag{13}$$

where $w = A\omega^2$ is the amplitude of the oscillating charge acceleration q, $c = 3 \cdot 10^8 m/s$ is the velocity of electromagnetic waves in vacuum. Taking into account the ratio (12), the expression for the radiation intensity takes the form:

$$I_{1,2} = \frac{kTq^2\omega_{1,2}^2}{2\pi\varepsilon_0 mc^3}. \tag{14}$$

The last equation shows that the radiation intensity of "vertical" vibrations with a frequency of ω_1 significantly exceeds the intensity of horizontal vibrations with a frequency of ω_2. In addition, it should be noted that equation (14) is similar to the Rayleigh-Jeans law for thermal radiation.

4 Conclusion

From the above analysis of the electromagnetic radiation of an oscillating charge, it follows that a wide range of electromagnetic waves of different polarization and intensity is generated in the dipole-quadrupole system. By determining the intensity of radiation, the frequency spectrum and the ratio of the maximum frequency to the minimum, it is possible to determine the parameters of the location of charges, as well as the geometric parameters of the crystal lattice.

The obtained research results can be used in applied physico-chemical research, in particular, in spectroscopy, as well as in the presentation of physics and chemistry courses at technical universities.

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