Chapter 9. Molecules

The purpose of this chapter is to analyse the quantum processes responsible for connection of atoms in molecules by electronic bonds.

Notes:

(1) Some aspects of the BSM concept about the chemical bonds may differ from the existing so far models. For this reason some new interpretations of the experimental data is provided.

(2) The derived vibrational curves may differ from the quantum mechanical vibrational curves especially in the limit region. The difference is due to the different models. From a point of view of BSM, the Quantum Mechanical (QM) models of the atoms and molecules appear as mathematical models. The QM models work in a space-time concept, which has a physical properties but is regarded as a void space. In such environments the interactions analysed by the Quantum Mechanical models does not provide information about the particle structure. The BSM models unveils this structures, but the calculation of the interaction energy is more complicated. For this reason only some simplified BSM models for diatomic molecules are derived. The advantage of these models is not in the accuracy of calculated energy levels but in the opportunity to determine the structural configuration of the simple molecule. In the same time they permits understanding the conditions for connection of atoms in molecules. This is not possible by the QM models.

9.1 Type of chemical bond

The BSM distinguishes the following types of chemical bonds

- ionic bond (IB)
- electronic bond (EB)
- IG field bond (IGB)
- Dipole induced bonds

9.1.1 Ionic bond

The BSM concept of the ions has been presented in §8.11. Let take example with NaCl, whose bond is considered as ionic. The compounds possessing ionic bonds exhibit two major features:

- The ionic compounds are usually dissolved in water. This means that the positive and the negative ions become separated. - The internuclear distances of the ionic bonds are usually much larger than the covalent bonds. This fact is in agreement with the BSM concept of the ionic bonded molecules.

Fig. 9.1 shows a NaCl molecule in which Na^+ and Cl^- are connected by ionic bond. The elements of the nuclei (protons and neutrons) and the possible quantum orbits are shown in one and a same scale. The zone of the bonded protons is drawn as ellipse. The interatomic distance in this molecule is experimentally determined.

A first harmonic quantum orbit is not possible to be used for diatomic molecules in which elements of Z > 10 are used. This rule is proved later in this chapter after a theoretical analysis of the derived Eq. (9.55) and its validation for simple diatomic molecules. It is apparent from Fig. 9.1 that the two ions could not be connected by a single quantum orbit, because the distance between the atoms is too big. It is defined by the size of the radii of the ions which are usually larger than the radii of the neutral atoms. The bonds of such molecules are based on the balance between the Column attraction forces and the properties of the proximity fields of the protons and neutrons, which was unveiled by the BSM. As a result, the molecules with ionic bond could not have a vibrational rotational spectra like other types of bonding in which quantum orbits are involved.



Fig. 9.1

Ionic bond in NaCl; The number in bracket shows the subharminic number of the quantum orbit. The closed loops 1 and 2 are magnetic lines formed by paired eight quantum orbits arranged symmetrically around the polar axis of CL⁻ ion. Every such orbit contains two electrons with opposite spins In summary, the main distinguishable features of simple molecular compound with ionic bonds are the following:

- The atoms connected by ionic bond does not possesses common electronic orbits. The binding energy is a result of attraction between the opposite charges of the ions.
- Due to the larger bond distance the IG forces are negligible in comparison to the electrical forces.
- Ionic bond compound can not exhibit a discrete optical spectrum

9.1.2 Electronic bond

According to BSM, the electronic bond (EB) between atoms connected in molecules are realised by one or more common quantum orbit. Under this category falls not only covalent bonds (between same elements) but bonds between different elements, as well. Most of the chemical bonds in the organic molecules are of EB type, others are of IG type. From the Atomic Atlas we see, that the spatial structure of the atomic nucleus of the different elements is determined by the proton and neutron spatial arrangement. For the chemical compounds the major role play the valence protons possessing some angular freedom mostly in the polar plane of the atomic nucleus. The atoms are possible to be connected in molecules by quantum orbits which operates in a same physical principles like the quantum orbits in the single atom. Additionally the IG forces between the atomic nuclei must be considered. It is evident, that the spatial structure of the molecule is determined by the spatial configuration of the atomic nuclei in which the valent protons are interconnected by quantum orbits. In some diatomic or multi-atomic molecules, not all valence protons are possible to be EB connection, due to the spatial restriction imposed by the atomic nuclei.

Electronic bonds are possible, not only between free valent protons (defining the principal valence of the element) but also of EB bonded protons. In some reactions the weak EB bonds could be broken and involved in internuclear EB bonds. For instance, the elements with Z number larger than 71, contain underlying proton shell with EB bonds (lantanide bonds), that are not converted to GBclp. In some strong chemical reagent (or catalyst) they can be broken and involved in internuclear EB bonds. Some compounds of Rn are of this type.

9.1.3 IG bond and dipole induced bond

The IG type of bond is a result of IG attraction. In the dipole induced bond the Wan der Walls forces. From a BSM point of view the IG correspond to some of the Wan der Walls forces. For this reason dipole induced bond usually could not be separated from IG bond. Compounds like ArHF and Ar2HF contain such type of bonds. Investigating vibrational states of Ar3HF molecule and comparing the results to the theoretical one J. Farrell et al. (1996) found about 11% difference. This difference, according to BSM is due to the IG forces, that are not considered in the QM model.

IG type of bonds exits in complex molecules especially from heavy elements. The IG type of bonds are usually weaker, than EB type.

9.2 Theoretical syntheses of chemical compounds

The knowledge about the nuclear configuration and the static and dynamical properties of the atoms provides the opportunity for theoretical structural modelling of chemical compounds. The modelling of simple dual or three atomic molecules is an straight forward procedure when using BSM atomic models. One useful verification for the BSM modelling is a comparison of the obtained structure with the VSEPR model of the molecules if it is known. The VSEPR model provides angles between the atoms in the molecules. This angles are determined experimentally by X-ray crystalography and other methods. The theoretical explanation of VSEPR model, however, is not so convincing than the BSM models. One argument in favour of this statement is in the observed different conformations of C₄H₄ molecule. This is due to the polar shape of carbon atomic nucleus, that is not apparent in the VSEPR model. In BSM model the angular freedom of the valence bonds are defined by the nuclear configuration. In summary:

• The angles between two atoms in a chemical compound with EB bond is determined by

the nuclear configuration, the angular freedom of protons involved in the internuclear EB bond and the IG forces between the nuclei

In Chapter 2 the quantum quasishrink effect has been discussed in connection to the photon wavetrain configuration. If considering this effect in two directions in respect to some equilibrium we may call it a **quantum quasi-scale change effect**.

The nuclear size of any element is completely determined by the size of the proton. It is not dependent of the quantum quasi-scale change effect. The quantum orbits, however, are dependable. The change factor depends of the nuclear mass and internuclear distance. For the Hydrogen molecule it may be small, but for heavier atoms is more significant. (This conclusion comes from the atomic spectra).

The Atomic Atlas provides the nuclear configuration by symbols for simplicity. In theoretical synthesis of molecules, however, Hippoped curves should be used for both, the proton and the quantum orbits with their dimensions. I this case, however, the twisting properties of the proton and some quantum orbits are not apparent. For simple inorganic molecules two or more view gives pretty adequate picture. The picture is more clear if only the central sections of the atoms are shown. For atoms with larger Z number the central nucleus contain one or more Argon nuclei that could be shown by oval. For drawing simplification there is not a need to show the protons and neutrons in this central part of the atomic nucleus. For more complicated organic molecules, however, the proton twisting affects their spatial configuration. In this case some special drawing program might be necessary.

The theoretical synthesis can be assisted by the following rules and considerations:

- Spatial configuration of the involved element (by Atomic Atlas)

- angular freedom of the free valence protons

- orbital pairing assuring the lower energy state

- EB type of bond is usually stronger than IG type

- considering the aggregate state

- vibrational properties of the synthesized molecule and molecule, inferred by the molecular and photoelectron spectra

- validation of the obtained molecular configuration by using data available by VSEPR model and crystalography

The equation of the quantum orbit trace length for free CL space was derived in §3.12.3 (Eq. (3.43.i)

$$L_{qo}(n) = \frac{2\pi a_o}{n} = \frac{\lambda_c}{\alpha n} \qquad [(3.43.i)]$$

where: n is the subharmonic number of the quantum orbit

We may use the subharmonic number of the electron motion for identification of the quantum orbit. So a quantum orbit with a subharmonic number of n, is a such orbit for which the electron moves with velocity corresponding to a quantum motion of subharmonic number of n (see Table 3.1 in Chapter 3). Then the ratio between the proton length and the length of the first subharmonic orbit is:

$$L_{pc}/L_{qo}(1) = 2.042685 \approx 2.$$
 (7.4)

In this relation, the proton and the quantum orbit, both are assumed to have a shape of a Hippoped curve with parameter $a = \sqrt{3}$. The shape of the proton, practically could be considered stable (at least for atoms with not very high Z number). The quantum orbit shape, however, may be distorted to some limit. In the equilibrium state of the molecule, although, we accept (and later it will be proved) that it is not distorted.

Initially we may consider that the size of the quantum orbit is affected by the distributed E-field inside the Bohr surface. This has been demonstrated by the Balmer model in Chapter 7. It is reasonable to accept that the volume enclosed by the Bohr surfaces of the individual atoms (connected by electronic bonds) in the molecule are united (or united Bohr quasispheres). In such way we may explain the lack of irradiative EM field while the electrons are orbiting. The concept of united Bohr quasisphere could be explained by a possible synchronization between the IG fields of RL(T) structures of the protons (deuterons) participating in the electronic bonds. So one question appears: Could the common orbit could be quasishrunk as in the case of Balmer model of BSM? (keeping in mind that the quasishrinkage is valid for the quantum CL space). In order to simplify the theoretical analysis in the beginning we may analyse in first the boundary orbits for which a possible quasishrinkage approaches zero. But **when it is necessary we may use a star notation "*" signifying, that the orbital parameter is quasishrunk**.

For drawing purposes, we may use the approximate relation (7.4), referring the dimensions of the quantum orbit to the dimensions of the proton. In such way we may select combinations of quantum orbits with different subharmonic numbers and serially combined orbits, as well. The selection option possibilities have been given in Table 7.1 (Chapter 7).

It is more connivent to operate with the length and width of the Hippoped curve instead of the orbital trace length. In such case, Eq. (7.4) and Table 7.1 (Chapter 7) could be used.

The proton length as a "length of a Hippoped curve " has been determined in Chapter 6 using Eq. 6.57. The same equation is valid for a quantum orbit with parameter $a = \sqrt{3}$. So we have:

 $L_p = 0.6277$ A - proton length

 $L_q(1) = 1.366$ A - length of the first subharmonic quantum orbit (in free CL space)

where: A (Angstrom) = 1×10^{-10} m

For drawing purposes, if using the approximate ratio of 2 (see Eq. 7.4), the fractional error is about 2%.

Fig. 9.2 provides drawings of the basic atomic structures and set of available quantum orbits. The quantum orbits are shown by dashed line and annotated by their subharmonic number. Their lengths have been derived for a free CL space (without electrical field).



Fig. 9.2 Basic atomic structures and quantum orbits

The basic atomic structure annotation is : p - proton D - deuteron T - tritii He - helium The horizontal lines in the middle of D, T

and He are neutrons.

Fig.9.3 illustrates EB bondings between atoms in the simple molecules H_2 , HD and H_3 .



Fig. 9.3 EB bondings in some simple molecules

The H₃ molecule is not very stable at normal conditions. In space environments, however, its ion H_3^+ is observed. The atomic conditions providing stability of this ion are different than those described in Chapter 8 §8.11.1 about Na⁺ ion. The integrity of the molecule in H_3^+ is preserved despite the loss of one electron. A possible explanation about such configuration is that the other two electrons circle in common ring orbit, composed of serially connected quantum orbits (this option is not shown in the drawing). In absence of one electron the excess positive change of the H3+ may still provide integration of the individual Bohr quasishphere into a common Bohr quasiphere, so the two electron may circle in a common orbit composed of serially connected quantum loops.

The hydrogen molecule appears in two different states - Ortho and Para. The both states are distinguished by their molecular spectra and the molar heat capacity. The Para state has a larger molar heat capacity. According to BSM, the larger heat capacity should correspond to a larger IG field, or the protons should be closer. The Ortho state may have two substates: Otho-I type and Ortho-II type. The Ortho-II may appear only in very low temperatures. The possible configurations of the Ortho-I and Ortho-II states of H_2 are illustrated in Fig. 9.4 a. and b.



Fig. 9.4. Ortho-I and Ortho-II state of H₂ molecule

Fig. 9.5 shows the possible configuration of H_2 - para state.



Para state of H₂ molecule

In both ortho states the both electrons share one orbits. So they have opposite QM spin. In Ortho-I, the orbit trace length corresponds to one quantum loop of first harmonic. In Ortho-II the orbit trace length is a sum of two first harmonic quantum loops (serially connected quantum loops). The Ortho-II state may appear only in low temperatures. The optical spectrum usually shows the signature of both ortho states and a para state as well. The conversion between ortho and para state is also more probable at lower temperature, and can be conserved in a room temperature for quite longer time. At normal temperature, the mixture ratio between ortho-I and para state is about 3:1.

9.3 Concept of integrated Bohr surfaces

The integration of the Bohr surfaces between the different protons within atomic nuclei was discussed in Chapter 7. In the chemical EB bonds, a similar conditions are created between the Bohr surfaces of the involved valence protons. Then conditions for quantum orbits are created for the EB bonding electrons. Fig. 9.6 illustrates the shape of the covalent Cl_2 molecule, where the two valence Bohr surfaces are integrated into one.

The Cl₂ molecule is drawn in scale. The internuclear distance is known by experimental data. Some of the atomic weak EB are not exactly in the drawing plane. Two of four GBclp are also shown. The covalent bond is a EB type. If not considering a quantum quasishrink effect (that we will see later practically does affect the internuclear distance), its length corresponds to a third subharmonic quantum orbit (electron energy of 1.51 eV). In the right down corner of the same figure, the Bohr surface of the valence proton, when not involved in a chemical bond is shown. It is evident, that the two Bohr surfaces of the valence protons from different atoms might integrate into one surface. In this case the shape of the individual Bohr surface could be modified but the definition condition given by Eq. (7.3.a) (Chapter 7) is still valid. In such case the orbital conditions becomes similar as in the Balmer series model, with the exception that the distance between the two cores are not fixed.



Fig. 9.7 Cl₂ molecule

9.4 Molecular spectra as a signature of molecular oscillations

9.4.1 Difference between QM model and BSM model of the molecular spectra

Initial note: In order to distinguish the single electron from multi electron system, in the atoms, we will use the following terminology in this chapter:

- electron (electron system according to BSM, consisting of electron shell, internal positron and central core)

- electron system (multiple electrons for atoms with Z > 1

The oscillating properties of the physical models of atoms connected in molecules by electronic bonds should provide a molecular spectra with discrete lines. The molecular spectra is the most authentic signature of the molecule. The theory of the molecular spectra is based on the Quantum Mechanical (QM) model of the atom. From the point of view of BSM (QM) is quite good mathematical model providing almost excellent spectral data. It is carefully adjusted by using number of constants, most of which are experimentally tuned. Although, as in the case of the atomic structure, we could not make equivalence between the mathematical model and the physical one.

The goal of BSM is not to replace or correct the QM model of molecular spectra, but to find out what are the real oscillating properties of the atoms connected in molecule.

Under oscillating motion we mean not simple but a complex type of motion. Let to see, what are the parameters, making the QM model different from the physical one.

- The atoms participates in a molecule as a QM atomic model

- The QM orbital arrangement is different, than the BSM orbitals, but the angles between orbital planes in some cases might be a similar

- The CL space environment in not considered in QM models

- The bonding orbital shape is different for QM and BSM models

- The quasishrink factor with its dependence of internuclear distance is not taken into account in QM model

- The IG forces controlling the quasishrink space are not apparent in QM model

The QM model of the molecular spectra is initially based on the concept of rotated reduced mass whose radius is changeable. While the CL space and IG forces are not apparent, number of additional rules are involved in the QM model, obtaining in such way quite good corrections for the missing factors. The big success of the QM model is based on the effect of energy conservation principle, when working in quantum units and orbital plane configurations (by s, p, d .. type of orbits). This approach allows to simulate the real processes by energy balances only. In QM model, the energy oscillations are described by wave equations in which hamiltonian operators are used. Proper selection of the solutions of these equation known as wavefunctions with number of selection rules and constants provide molecular spectra matching quite well the observed spectra.

The QM model of the molecular spectra is based on the Bohr type of atomic model. It also deals preliminary with the electron configurations, described by selected wavefunctions, corresponding to f, p, d, s type of orbits, spin orbits couplings, and number of additional factors describing the arrangement of the orbits. In fact the orbits are presented as electron clouds, due to the uncertainty principle used as an basic postulate in the QM. While in the Bohr model all orbits above ground state have a trace length larger than $2\pi a_a$, in BSM model, all their possible trace lengths are smaller than $2\pi a_o$. In other words, they can be considered as enclosed inside the Bohr surface. Fortunately the QM model uses the basic parameters h, q, e_o and m_o, that are defined for the external CL space. This approach matches to the Bohr atomic model, where the orbits are larger than $2\pi a_{a}$. This fact removes the problem of the possible corrections of this parameters in the quantum quasishrink space, inside the Bohr surface. But from the other side: In the QM concept of molecular spectra, the quasishrink effect and the IG field are both dismissed by the adopted concept of **Born-Operheimer approximation.**

The Born-Operhimer approximation is introduced in QM in order to neglect the nuclear contribution. In fact if considering only the Newtonian masses their contribution is negligible. In such case the equation solutions get considerable simplification. In result of this, however, the quasishrink effect and the IG field parameters become hidden. Later some additional corrections are involved as a particular rules, in order to correct the spectra, but the above mentioned parameters are left hidden. Therefore, the obtained final solutions in fact describes the energy related with oscillating motion of the electron systems of connected atoms. The potential energy between the IG field of the atoms and their influence on the molecular oscillations are not apparent in the QM model.

According to BSM, there are two different oscillating systems:

- the bonding system

- the atoms with their electron systems.

The bonding system includes the valent protons (Deuterons) and the bonding electrons. There is comparatively weak connection between the bonding electrons and the atomic nuclear electrons by their variety of magnetic couplings and QM spin.

The oscillation can be understood only if considering the energy balance in the very basic level of the prisms interaction. This is the balance between the IG (CP) forces and IG(TP) forces. It is more convenient to work with energy balances of IG fields. The system involved in such balance should include not only the atomic nuclei and bonding system, but the CL space as well. The BSM provides a 3 dimensional real model of the molecular structure, in which the both system, mentioned above are quite distinguishable. One major advantage is the knowledge of the dimensions of the proton, neutron, the atomic nuclei and the size and shape of the quantum orbits. Later in this Chapter it will be shown, how both interacting fields IG(CP) and IG(CP) are determined and involved in the molecular oscillation process leading to a photon emission (or absorption).

The QM model, after applying the Born-Operheimer approximation, deals primary with the adopted configuration of the electron system (s, p, d, ..), described by wavefunctions in which some orbits are considered as common for both nuclei. The model involves number of constants, whose value are determined from the experimentally observed spectra. The adjusted in such way mathematical model provides vibrational rotational spectra that matches quite well the observed spectra of the molecules.

We see, that the BSM model has a quite different approach than the QM model. This leads to the following discrepancy between the both models:

(a) The "fundamental" frequency or band, according to QM terminology, in fact is a signature of the binding electron system. It does not provide the full picture of the nuclear motion in the molecule.

(**b**) The real resonance frequency between the two nuclei is much lower, than the "fundamental" frequency.

(c) the process of molecular vibration and rotation described by QM model, whose signature is the "vibrational-rotational" spectrum, appears quite different by BSM model.

(d) The QM model makes distinction between pure rotational and rotational vibrational spectra, but the physical process is not quite apparent

The proof of the above statements will be presented in the next few paragraphs.

The adopted QM therm "vibrational-rotational" spectra comes from the accepted initial model of a "rigid rotor".

The molecular oscillating motion, according to BSM is quite different, than the QM concept, but it provides the same type of spectra. It is quite more logical for explanation and does not need the use of the Heisenberg uncertainty principle. The relativistic effects can also be clearly identified and separated. So they could be analysed separately. In such aspect, the BSM model is able to provide analysis by a classical means.

The QM mechanical model, tuned by number of experimentally determined constants, provides pretty accurate molecular spectra. In many cases we can use them as a reference, with a purpose to unveil the real molecular motion.

9.5 Molecular oscillating model of BSM

9.5.1 General considerations and features

9.5.1.1 Complexity of oscillations

The complexity of the molecular oscillations increases with the number of valent protons, the atomic Z number and the number of atoms in the molecule. Let make some categorization about oscillation complexity:

(1) homonuclear diatomic molecules with single valence

(2) not homonuclear diatomic molecules with single valence

(3) covalent diatomic molecules with valence larger than one

(4) linear three atomic molecules as HCN

(5) diatomic and poliatomic molecules with consumed valences

(6) poliatomic molecules with not consumed valences

9.5.1.2 Fundamental proper frequencies of the nuclear system and the bonding electron system

All the atoms exhibit high order helicity defined by the twisted proton shape. So their motion in CL space possesses translational and rotational components. The same is valid for the molecules, but simultaneously with rotational motion they vibrate. The dynamics of the molecules could be analysed easier if separating them virtually into a bonding system and nuclear molecular system. This separation is valid only for molecules from atoms with Z number larger than two.

- The bonding system involves those valence protons that are connected by quantum orbits and their electrons.

- the bonding systems are in the middle between the atoms, while the atomic nuclei are in the periphery

- The nuclear molecular system involves the atomic nuclei participating in the molecule together with their electrons. So the connected valence protons with their electrons are not part of this system. The above separation allows also to distinct the integrated Bohr surfaces of the bonding system from the Bohr surfaces of the individual atoms.

- The SPM vectors of the volume enclosed of the bonding system (characterized by integrated

Bohr surfaces) and those of the nuclei may not be synchronized

Differences between the bond system and molecular nuclear system

Now let emphasize some differences between formulated above two systems of the molecular complex.

No one of the both systems possesses a single proper frequency. There are few reasons for this:

- such type of system could not be considered as a rigid body system

- the quantum interactions with CL space are different for the electrons and protons (and neutrons). The parameters involved in the quantum interactions are their magnetic moments. The magnetic moments of the proton and neutron are quite different than the magnetic moment of the electron.

- a small change of internuclear distance involves a large IG energy imbalance in comparison to the electromagnetic energy

- the IG field controls the E-field inside the Bohr surface of the bond system (this will be demonstrated by the analysis of H_2 molecule oscillations)

In result of these considerations, the both systems exhibit not a single proper frequency but set of proper frequencies. For simplification of the analysis, we may consider, that each system posses own **equivalent fundamental frequency.** Such frequency is a centre of mass of the proper frequency set with specific distribution.

In case of simple molecules H2 ortho-I and D2 ortho -I, the both systems, generally valid for atoms, degenerate into one system (equivalent to a bond system) with one equivalent fundamental frequency. Due to the quantum interactions it appears as a set of frequency in the far IR range of the spectrum, known as rotational spectrum.

Equivalent molecular fundamental frequency

The equivalent **molecular fundamental frequency** according to the quantum mechanical considerations for diatomic molecule could be described by the classical equation

$$f_n = \frac{1}{2\pi} \sqrt{\frac{k_n}{M}} \tag{9.A.1}$$

where: k_n is a force constant expressing the inertial and quantum properties of the atom

M - is a reduced Newtonian given by the combination of the two nuclear masses ma1 and m2.

$$M = \frac{m_1 m_2}{m_1 + m_2} \tag{9.A.2}$$

It is more convenient to express the frequency in wavenumbers, \bar{v} in units of cm⁻¹, because this is the most common used parameter in the IR spectroscopy.

$$\bar{v} = \frac{10^{-2}}{2\pi c} \sqrt{\frac{k_n}{M}} \quad [\text{cm}^{-1}]$$
 (9.A.3)

The Eq. (9.3) is in agreement with Bohr atomic model, where, the nucleus is very small in comparison to the orbit radius. This means than the influence of the nucleus on the spatial position of the orbit plane could not be defined.

In the BSM model of Hydrogen, the spatial position of any orbital plane (or quasiplane) is well defined by the spatial position of the proton quasiplane. Consequently the large magnetic moment of the electron will influence the inertial properties of the neutral Hydrogen. The same conclusion should be valid for the bond system in any molecule (with electronic bond).

The above considerations require correction of the inertial mass M. participating in the classical Eq. 9.3. For H_2 -ortho-I molecule the equation take a form

$$\bar{v} = \frac{10^{-2}}{2\pi c} \sqrt{\frac{k_p \,\mu_p}{m_p \mu_e}}$$
 (9.A.4)

where: k_p - is a strength (force constant) of the proton pair bond, m_p is a proton mass, μ_p/μ_e - is a magnetic moment ratio

In many molecules bonding pairs of deuterons instead of protons are mostly involved. Their strength constant is different and could be denoted as k_d . The Eq. (9.4) could be generalise to any diatomic molecule or group. For a homonuclear molecule it takes a form:

$$\bar{v} = \frac{10^{-2}}{2\pi c} \sqrt{\frac{bk}{M^*}}$$
 $M^* = Zm_p \frac{\mu_p}{\mu_e} + Nm_n \frac{\mu_n}{\mu_e}$ (9.A.5)

where: k is a strength of proton or deuteron bonding pair, b - is the number of bonding pairs, Z - is an atomic number, N - is the number of neutrons in the atomic nuclei, μ_n is the neutron magnetic moment.

Some aspects about the BSM considerations:

The hadrons (proton, neutron) have larger inertial mass than the electrons, but smaller magnetic moments. The electrons have smaller inertial mass, but larger magnetic moments. The nuclear electron system is carried by the nuclear hadron structure, whose IG field simultaneously defines the electrical charge and E-filed configuration inside the integrated Bohr surface. (Note: the integrated Bohr surface may have a shape of manifold). In the same time the large magnetic moment means a large interaction with a CL space. So the nuclear electron system may influence the motion of the nuclear hadronic system.

The above BSM considerations are not taken into account in the Quantum Mechanical model of the molecule based on a the Bohr planetary atomic model, were the nucleus is comparatively quite small.

The strength of the molecular bond depends of the internuclear distance. The latter may take different quantum values from the allowed set of quantum orbits. In any single value of this set there are additional quantum conditions due to the quantum quasi-scale change effect that affect the orbital conditions. The kinetic energy is a factor dependable of the quantum orbit parameters. In result of this dependence, the fundamental molecular oscillations exhibit not one, but **set of molecular proper frequencies**.

The set of the molecular proper frequencies could be considered as a proper resonance frequency modified by the quantum orbit conditions and internuclear distance.

Optical signature:

The molecular proper frequencies are comparatively lower than the bonding system frequencies discussed in the next paragraph. In the vibrational level with higher energy their contribution to a CL space pumping is quite small in comparison to the contribution of the bonding system. For this reason their optical signature may be identified in the lowest vibrational level. The lowest level according to BSM corresponds to the internuclear distance at equilibrium. The optical signature of the molecular proper frequencies appears at this level and is known as "pure rotational" spectrum.

The definitions "vibrational-rotational" and "pure rotational" comes from the Quantum mechanical model. According to BSM real physical model, however, the oscillations are of mixed type. The rotated molecule vibrates simultaneously with the equivalent fundamental molecular frequency. This vibration in fact is involved in the CL space pumping and photon emission, while the rotation energy is constant during the process with optimal angular velocity dependable of the molecular kinetic energy.

While the optical contribution of the molecular frequencies in other vibrational levels are not apparent, it does not mean that the corresponding oscillations are absent. In the oscillating process providing "vibrational rotational" spectra they are persistent.

Equivalent proper frequency of the bonding system

The bonding electron system is connected strongly to the bonding protons and weakly to the nuclear electrons by the QM spin and orbital magnetic coupling. These interactions take place in the volume enclosed by integrated Bohr surfaces. This system is also not a rigid system so it exhibits multiple proper frequencies. Their optical signature is a set of spectral lines with more complex arrangement in P R and Q branches (the Q branch is additionally dependable of the of the bonding type and may be absent in some configurations). The line distribution and the envelop of these branches depends of number of factors, that will be discussed in the following paragraphs. The spectrum of the bonding system is also centred around one average frequency, that could be accepted as an equivalent proper frequency of the bonding system. In the Quantum mechanical model of rigid rotor this frequency is known as a "fundamental frequency".

Basic differences between optical spectra generated by the bonding and nuclear systems

The vibrational motion of the both systems are mutually dependable, because they have lot of

common parameters. The optical spectra, however show some basic differences.

(a). The optical spectra of molecular proper frequencies ("pure rotational spectra" according to QM model) is in the longer wavelength range (FAR IR) approaching the radio frequency range.

(b) the line width of the optical spectra generated by the binding system frequencies are much narrower, in comparison to those of the molecular proper frequencies (given by the pure rotational spectrum)

About (a): The bonding strength parameter k_n is dependent mostly of the number of connected valences and the possible orbit from the quantum orbit set. So its variation with Z number is restricted to a finite sets of values. The *M* parameter, however, does not have such restrictions. Therefore, the equivalent molecular fundamental frequency tends to increases with the atomic number. This means a tendency of their optical signatures towards longer wavelength range.

About (b):

In the molecular proper frequencies, all electrons of the nuclei are involved in a CL space pumping. The pumping efficiency, however is small, because the nuclear orbits have fixed but different plane orientations. The integrated Bohr surface for any nuclei may have a shape of manifold. In such case the pumping and radiation efficiency of the system are a partly deteriorated. In result of this the emitted light is not so monochromatic, i. e. the line width is broader.

For the bonding system, the CL pumping and radiation conditions are different. A single bond of pair valence protons (deuterons) possesses a common quantum orbit, occupied by two electrons (for a neutral molecule). This provides an optimized conditions for CL space pumping and photon radiation, so the line widths are much narrower.

Summary:

- A vibrating homonuclear diatomic molecule is characterised by two different equivalent fundamental frequencies: one for the nuclei and a second - for the bonding electron system
- The two equivalent frequencies are dependable of the internuclear distance and quantum

orbit conditions. In result if this they appear as sets, denoted as proper frequency sets.

- The both frequency sets put own signature on the vibrational motion of the atoms and CL space pumping capability of the system.
- The direct optical signature of the molecular frequency set is the "pure rotational" spectrum at the equilibrium distance between the nuclei.
- The H₂ and D₂ molecule are excluded from the general concept of molecular separation into a two system, because their nuclei are directly involved in the bonding system. However their analysis is quite useful for determination of the features of the two systems.

9.5.2 CL space pumping and radiation (absorption) capability of the bonding electron system

The bonding electron system includes the bonding electrons connected to the bonding valence protons. The vibrational motion between the atoms affects directly the bonding quantum orbits, characterised with their quantum energy in conditions of a quantum quasi-scale change (for length) CL space. Every bonding pair of protons possesses own quantum orbits with electrons, with relatively high freedom for CL space pumping and radiation (or absorption). The process, however is synchronised to some extend with other bonding pairs and the molecular oscillations.

The main distinctions in the optical spectra related to the proper frequencies of the bonding and molecular nuclear system are the following:

- the signature of the fundamental frequency of the bonding electron system is a series of lines, spaced much closer, than the frequency set of the fundamental molecular frequency.

- the lines series follows a specific progression

- the lines are much narrower in comparison to the lines generated by the proper molecular frequencies.

Notice: We must point out some difference in the terms "fundamental frequency" used in the BSM model and QM model.

The term "fundamental vibrational frequency" used in the QM model, is relevant to the fundamental frequency of the bonding electron system used by BSM model. In QM model, the Srodinger equation for harmonic oscillator (see D. A. McQuarrie, p.p 162, (1983) does not contain IG forces. Solving this equation for H_2 molecule a frequency called a "Fundamental Vibrational Frequency" is obtained. Then looking at IR spectra of diatomic molecules these frequency are identified and the force constants are calculated for them. The estimated in a such way frequencies for different molecules are shown in Table 9.1. According tot BSM interpretation, however, they correspond to the equivalent fundamental frequencies of the bonding systems of the shown molecules.

"Fundamental Vibrational Frequency" according to QM model of harmonic oscillator, coresponding to equivalent proper frequency of the bonding system according to BSM model

Molecule	\overline{v} (cm ⁻¹)	Molecule	\overline{v} (cm ⁻¹)	
H ³⁵ Cl H ⁷⁹ Br H ¹²⁷ I ³⁵ Cl ³⁵ Cl ⁷⁹ Br ⁷⁹ Br	2886 2559 2230 556 321	¹²⁷ I ¹²⁷ I ¹⁶ O ¹⁶ O ¹⁴ N ¹⁴ N ¹² C ¹⁶ O ¹⁴ N ¹⁶ O ²³ Na ²³ Na ³⁹ K ³⁵ Cl	213 1556 2331 2143 1876 158 278	

The frequency position of $H^{35}Cl$, for example, is quite accurate, and appears in the middle between P and R branches of the vibrationalrotational spectrum. The synthetic spectrum of $H^{35}Cl$, together with $D^{37}Cl$ is shown in Fig. 9.8.



Fig. 9.8 Spectra of H³⁵Cl and D³⁷Cl

The synthetic spectra show the position and intensity of the lines without their linewidths. The shown vibrational rotational spectrum of HCl, according to QM model is known as spectrum corresponding to the fundamental frequency of HCL molecule, given in Table 9.1. The two branches P and R are really centred around the value of 2886 cm⁻¹. According to BSM model this is the equivalent fundamental frequency of the HCl molecule.

The shown spectrum contains only P and R branch. Later we will see, for which type of molecules and bonding systems this type of spectrum is a typical one. The P and R branches exhibit the following general features.

- The line frequency of the R branch are higher, than the P branch.

- The energy distribution of the lines in the branches follows a nonlinear orders reference often as progressions. They have different span coefficients for P and R branch.

- R branch lines are more intensive, than P branch lines

From the spectrum in Fig. 9.8 we see, that the $D^{37}Cl$ set of lines is slightly shifted from the $H^{35}Cl$ set in the direction of lower frequencies. The equivalent molecular fundamental frequency should have a frequency shift in the same direction according to Eq. (9.1) if only *M* is changed, while k_n is a same. The k_n parameter corresponds to the strength of the bonding system. The strength of the bonding system is determined by the connected pairs of valence protons (or deuterons) and the subharmonic number of the quantum orbit. It varies within a limited range for molecules of different atoms. In the same time *M* may vary in larger range. This leads to the following conclusion:

Molecules of heavier atoms will exhibit lower equivalent molecular fundamental frequency.

The above made conclusion could be verified by examining rotational spectra of different molecules.

9.5.3 Characteristic features of the molecular oscillations

Relying on the discussed so far considerations we may provide some conclusions about the characteristic features of the molecular oscillations. Their proof will be presented in the following analysis, provided in this chapter.

- The Bonding electron system, possesses much higher equivalent fundamental frequency, than the molecular one. Its motion, generally follows, the motion of the nuclei
- The IG field of both nuclei will influence their vibrational motion and internuclear distance
- The bonding electron system, interacts strongly with a CL space and weakly with other electrons of the atomic nuclei.
- The bonding electron system affects the smoothness of the vibrational motion, due to the stronger quantum interaction with CL space.
- The bonding electron system is sensitive to external factors, as photons, electrons, electrical filed, magnetic field, and collision of the molecule with another molecule or atom. In result of such interactions, the fundamental molecular oscillation, may be perturbed.
- The perturbation of the molecular oscillations provides rich combinational conditions for transitions between different vibrational levels (including additional levels of orbit distortion, discussed later).

9.5.4 BSM concept of oscillations for molecules with EB type bonds

Balance of forces and its diversity of oscillations

Let use the example of diatomic molecule consisting of light atoms.

In the Balmer model we have seen, that the electron motion is governed by the balance of the three type of forces: IG forces, Internal Coulomb forces and inertial forces. The Newtonian gravitational force between the electron and proton was neglected. The inertial mass expressed by the centripetal acceleration, is comparatively small, but still plays a role in the force balance.

9.5.4.1 Diversity of molecular oscillations and their categorization.

In the molecular model, the internuclear distance is in the order of quantum orbit length. A simple test shows, that the Newtonian gravitational energy is much smaller than the bonding energy and transition energies. Therefore, its contribution could be ignored.

The problem with the inertial mass is different. The inertial mass participates in the centrifugal forces. For one and same molecule these forces are dependent of the molecular velocity (due to the helical interaction with CL space). For different type of molecules, these forces are dependent of the mass distribution in the molecule and the rotational symmetry. This two factors could be defined by the moment of inertia around the axis, passing through the centre of mass point. From this point of view, the molecular oscillations could be divided into two different types:

- I-st type oscillations - for molecules (or fractions of molecules) with low moment of inertia

- II-nd type oscillations - for molecule (or fractions of molecules) with higher moment of inertia

It is clear, that the centrifugal forces will obtain a definite value when the angular frequency corresponds to the equivalent fundamental molecular frequency given by Eq. (9.A.5).

In §9.7.5.D it will be shown, that due to the quantum quasishrink effect the change of the internuclear distance estimated by the external CL space length unit is negligible.

The above statement provides one very important conclusion:

(A). The radial component of the vibrating nuclei estimated in CL space unit length is negligible. Consequently the work for displacement of the CL space node by the FOHSs of the both nuclei should be contributed only for the rotational motion. In fact this is the inertial interaction of the protons and neutrons with the CL space.

The conclusion (A) gives a possibility to estimate the rotational energy by a classical way.

 $E_{rot} = 0.5I\omega_{rot}^2 = 2\pi^2 I v_{rot}^2$ where I - is the moment of inertia and ω_{rot} is the angular rotational frequency

The moment of inertia for diatomic homonuclear molecule is

$$I = m(0.5r_n)^2 = 2m_n \frac{r_n^2}{4} = m_p A \frac{r_n^2}{2}$$
(9.A.6)

The rotational frequency v_{rot} could be estimated by vibrational frequency v_{vib} defined as an equivalent fundamental frequency of the molecule. For H₂-ortho-I molecule it is shown in §9.9.2 (Table 9.4) that the ratio between both frequencies is

 $v_{vib}/v_{rot} = 2:1$

At such ratio the symmetry of the inertial interactions with CL space is preserved for a complete rotational cycle. For other homonuclear diatomic molecules such condition could be satisfied only for even ratio between the both frequencies.

The vibrational frequency, that in fact is the molecular equivalent fundamental frequency, could be estimated by the maximum of the envelope of the "pure rotational" spectrum. The latter is presented as set of lines whose distribution is given by the QM equation:

$$P_J = (2J+1) \frac{\exp(-(hcBJ(J+1)/kT))}{q_r} \qquad (9.A.7)$$

 $q_r = \Sigma(2J+1)\exp(-(hcBJ(J+1)/kT))$ - is a partition function

The plot of Eq. (9.A.6) for CO molecule with constant $B = 1.9225 \text{ cm}^{-1}$ at T = 298 K is shown in Fig. 9.9



Fig. 9.9 Distribution of population among the rotational states of CO at room temperature

The temperature affects the shape of the curve by a horizontal span factor. The shape of the population curve for different diatomic groups is similar, but with different span coefficients. The shape is also similar to the theoretically obtained curve of the momentary velocity distribution of the oscillating CL space node, discussed in Chapter 2 §2.9.6.A. It is shown again in Fig. 9.9.A.



Fig. 9.9.A

The both curves have a shape close to Maxwel distribution of the velocity. This velocity is dependent of the molecular kinetic energy. Having in mind the helicity of the atomic and molecular structures it is evident that the rotational frequency should be correlated with the equivalent molecular fundamental frequency. Consequently the latter depends of the absolute temperature of the gas substance.

The pure rotational spectrum is usually given in units of cm⁻¹. So it is convenient to estimate the vibrational and rotational frequency in a same units. The rotational frequency is: $\omega_{rot} = 2\pi v_{rot} = 2\pi c \bar{v}_{rot} (cm^{-1}) 10^2$.

Then the rotational energy of diatomic homonuclear molecule in (eV) is

$$E_{rot} = \frac{1}{q} \pi^2 m_p c^2 A r_n^2 \bar{v}_{rot}^2 (cm^{-1}) 10^4 \quad \text{eV}$$
 (9.3)

where: m_p - is the proton mass, A is the atomic mass, r_n - is the internuclear distance and \bar{v}_{rot} is the rotational frequency in cm⁻¹

In Eq. (9.3) m_p is used instead of average value between the proton and neutron mass, because the difference between them is quite small.

The rotational energy, calculated by Eq. (9.3) should be compared to the bonding energy for the equilibrium point of the vibration, that from its side is defined by the IG field and the number of involved valence protons and bonding electrons. For the IG field it has to be kept in mind its different participation between the protons (deuterons) involved in the bond system (synchronized IG field)

and between nuclear systems (not synchronized IG field).

If E_{rot} is much smaller than the bonding energy at the equilibrium, the molecular oscillation is of I-st type, otherwise it is of II-nd type.

For the molecules with I-st type oscillations the inertial moment is ignored. This simplifies the analysis of some light molecules. For molecules with II type oscillations, the inertial moment could not be neglected. Some complex molecules may have the both type of oscillations. Some light molecules, also may have large moment of inertia, because it is dependable not only of the Newtonian mass, but the configuration of the bonding orbit as well.

The BSM model of vibrational motion for molecule of I-st type is different, than the Quantum Mechanical model of harmonic oscillator and its anharmonic corrections.

Type of spatial motion

We may distinguish the following spatial type of motion:

- linear vibrations (along one axis)

- quasirotational vibrations

The linear vibrations are typical for molecules with single valence bond. The H_2 ortho states serve as a typical examples. However, linear vibrations may occur also for molecules with larger number of connected valences but with symmetrical positions of the atomic nuclei.

Molecules involved in linear vibrations posses only P and R branches in their optical spectrum

The quasirotational type of vibrations are possible only for molecules, possessing more than one bonding quantum orbit. The most simple example of such motion is demonstrated by the Oxygen diatomic molecule O_2 . The configuration of O_2 molecule in one of its state is shown in Fig. 9.10.



Fig. 9.10

 O_2 molecule in one of its states

(2) - quantum orbit of second subharmonic

The Oxygen atoms, has been discussed in Chapter 8 The external proton shell includes two pairs of protons GBclp bonded in the equatorial region and two valence protons. Such configuration provides a large freedom of the angular position of the two valence protons and offer a possibility for different states of the homonuclear oxygen molecules. In any particular state, however, the angular position is fixed by a proper quantum orbit. The quantum orbit in the state shown in the figure correspond to the second subharmonic or energy level of 3.4 eV.

From Fig. 9.10 we see that the points O and O' in the centre of the bonds are completely symmetrical in respect to the polar molecular axis. Let consider a vibration as a rotational motion with centre O with limited amplitude. Then the other bond makes motion in a limited arc, that could be approximated by a linear type of motion. For one and same molecule, the centre of such motion can be alternatively change between O and O'. Such kind of osculations are like rotational motion with limited amplitude and alternatively changed centre of rotation. For this reason it is called a quasirotational motion (vibration). It is evident, that such type of motion is possible also between molecules with three symmetrical bonds (N $_2$ molecule for example). Such type of motion is possible in many complex molecules. One specific feature of this motion is their signature in the optical spectrum.

Molecules involved in quasirotational vibrations possess Q branches together with P and R branches in their optical spectra.

Detailed discussion of the above statement will be presented in §9.5.7.4.1.

9.5.4.2 Statistical cycle

In order to analyse the molecular oscillations, from the classical point of view, a concept of **statistical vibrational cycle** containing large number of vibration periods is used. It is called statistical, because one molecule, is barely able to complete such whole cycle. Any absorption, excitation, quenching or emission is able to distort severely the statistical vibrational cycle. The statistical cycle is idealised, because: - it does not show the simultaneous rotational motion

- the emission and absorption processes are ignored so the statistical cycle could be regarded as amplitude modulated vibrational frequency

- it can be regarded as statistically averaged from many molecules

- the cycle is shown by the equivalent fundamental molecular frequency

- the vibrations of statistical cycles are performed in conditions of IG field, i. e. non linear environments.

The shape of the statistical cycle is shown in Fig. 9.11. In the same figure the analogical electrical equivalent circuit is presented



Fig. 9.11. Idealised statistical cycle and equivalent circuit diagram

In the left side of the diagram the trend of different fields and energies are shown, denoted as:

 E_{IG} - is an IG field potential

 E_{IP} - is an Ionization potential

 E_{DIS} - is a dissociation limit

E - is a momentary system energy

If referred to a single molecule the cycle is not realistic, because it could be distorted either from absorption or emission of photons.

Note: In §9.7.5.D it will be shown, that the internuclear distance estimated by the CL node unit length is so small, that it is negligible even in

comparison to the proton core thickness. What is change is the quantum quasishrink space. But in our analysis we may still consider some finite amplitude of vibrations, having in mind, that they work against a tremendous IG forces.

There is one specific feature of the shown oscillations: The amplitudes are asymmetrical. In a first gland this may look confusing. However it is possible due to the following features, some of which has been already mentioned:

- the quantum quasishrink effect of E-field inside the Bohr surface

- the quantum conditions of the bonding orbit

- the inverse cubic dependence of IG forces from distance

The quantum quasishrink effect has been discussed in the Balmer model. The case of molecular bonding orbit, however is distinguishable by the following:

(a) In the Balmer series the conditions of orbital length defined by the protons dimensions are constant.

(b) in the molecular bonding orbit the conditions of the orbital length are defined by the internuclear distance that is dependent of the total energy balance

(c) the internuclear distance for the bonding orbit is self adjustable, so we may accept initially that the orbit will intercept the proton quasiplane in the locus point (this will be later proven)

As a result of the above mentioned distinctions, the quantum quasishrink effect at Balmer series could be identified as a static, while this in the molecular bond, as a dynamic **self adjustable quasi-change effect (for distance).** The latter exhibit different pumping capability.

In the equivalent circuit diagram, the proper cycle is determined by the inductance L and capacitor C. The Diode D_1 , proper shunted with resistor R_2 causes the nonlinearity of the amplitude. The resistor R causes the attenuation of the oscillations. If a short pulse A is supplied in the input an oscillating cycle, corresponding to phase t_3 could be observed by the Oscilloscope O.

The presented model of statistical cycle contains three phases:

 t_1 - phase of absorption t^2 - radiation lifetime

 t_3 - phase of radiation

They are discussed in the next paragraph.

9.5.4.3 Phases of the molecular oscillations

The phases, indicated as t_1 , t_2 , and t_3 , cover the full normal cycle of the molecule, including the absorption, radiation lifetime and emission. The normal cycle excludes any possible perturbations, mentioned in the previous paragraph. In analogy with atoms, such cycle corresponds to optical pumping and spontaneous emission of photons.

The phase t_I is an absorption phase, during which the molecule absorbs photons, whose wavelengths match to the spectral features of the molecule. In this process, mostly the electron system is involved, because it has much richer spectral features, than the nuclear capability of photon absorption. The duration of the phase t_I is not a constant, because the energy may be pumped by single line, by few lines and by multiple spectral lines.

The phase t_3 is an emission phase. The main distinguished feature from the phase t_1 is that its time duration is strictly defined by the molecule configuration, and appears as a constant. This is valid for a case of spontaneous emission (but not for a stimulated emission used in the lasers where the lifetime is shortened).

The phase denoted by t_2 is a radiation lifetime of the exited molecule. The duration of this phase may depend not only of the pure vibrational motion but also of the possibility the bonding electrons to juggle some energy with other electrons in the atom. This automatically involves interaction between all electronic orbits and the distributed Efield, controlled by the atomic local IG field.

The rotational motion exists, but the system appears fixed to a some proper vibrational level. The duration of this phase is very dependable of the Z number of the bonded atoms and molecular configuration. In case of H₂ molecule it might be intrinsically short. For molecules comprised of atoms with larger number of electrons the juggling energy capability increases significantly and so the radiation lifetime. In some particular cases, like $O_2(a^1\Delta_g)$ in the night Earth atmosphere above 80 km, the radiation lifetime is about 58 min.

The lack of radiation during the phase t_2 could be explained by the the capability of the IG

forces to modulate the proximity electrical field around the protons involved in the electronic bond. Additionally the bonding electron system may interact with the underlying electron shells, around the GBclp, that posses highly spatial oriented orbits in a strong IG field. Having in mind the orbit tilt, the QM spin, and the electron spin momentum of the whole complex, it is possible a temporally stable energy to circulate in a form of running waves in the internal volume of the atoms. All these considerations may provide stable conditions for vibration in the time interval t_2 without loss of energy.

9.5.5. Molecules with I-st type oscillations

9.5.5.1. H_2 ortho-I state as a simplest diatomic molecule

For initial proof of the presented concept of vibrational oscillation of diatomic molecule, we will analyse the simple H_2 molecule - ortho state. The configuration of this molecule with bonding quantum orbit of first harmonic is, illustrated in Fig. 9.12



Fig. 9.12 Vibrational scheme of H_2 - ortho-I state

The quantum orbit quasiplane plane does not coincide with the quasiplanes of the protons. It passes through the locuses of the proton clubs. The following notations are used:

 L_p - is a proton length

- $L_q^{(1)}$ is a long side of first harmonic quantum orbit
- r_n is the distance between the Hydrogen atoms r_o is the distance at equilibrium
- r distance between the electron and the proton core in the circular section of the orbit

Now let add one real feature to the vibrational motion of I-st type oscillations: the quantum levels. The quantum levels are caused by the finite dimensions, that the bonding quantum orbit could occupy in the space of integrated Bohr surfaces. It is more convenient to express the quantum levels by the energy instead of internuclear distance. In this case the energy levels inside the Bohr surface could be regarded as an energy levels in external CL space. Such equivalence of the energy has been found in the Balmer model, (Chapter 7).

Fig. 9.13 shows the vibrational intervals of the H2 molecule as a typical vibrational curve of diatomic molecule according to QM model. In the right part of the figure the Photoelectron (PE) spectrum of this molecules is shown. Its reflection by straight line at angle larger than 45° means that the space intervals of the PE spectrum are proportional to the vibrational levels but stretched. This spectrum, discussed later in 9.6.1 is shown in Fig. 9.19. This stretched PE spectrum is likely caused by the lost energy for recoiling of the atomic nuclei during ionization. The largest peak of the PE spectrum corresponds to the largely populated vibrational level.



Quantum levels of H2 ortho-I state as a liner diatomic molecule and its Photoelectron spectrum.

The parameters shown in Fig. 9.13 are: E_B - binding energy (known also as ionization energy), E_{dis} - dissociation energy level, rn - internuclear distance, E_k - electron spectrum (expressing the PE spectrum); levels 0, 1, 2 - vibrational levels with intervals 1/2, 3/2, 5/2 ...)

The QM vibrational curve is drawn in coordinates of energy level towards radius vector r of anharmonic oscillator. This option is not suitable for BSM analysis, in which the mentioned effect of quantum quasi-scale change exists. In order to find the signature of this effect it is more convenient to express the energy levels, shown in Fig. 9.13 as a direct function of the quantum number of the level. The shape of the obtained vibrational curve is shown in Fig. 9.13A.



Fig. 9.13A Vibrational levels in function of vibrational quantum numbers

We may call the shape of the curve shown in Fig. 9.13A - vibrational ladder. The E parameter referenced to the bonding (ionization energy EB in the further analysis can be regarded as a momentary energy of the system. We see that this energy directly connected to the vibrational levels is quantized. The quantum levels are shown by horizontal blue lines. The steps of the vibrational ladder, correspond to different quantum orbits, obtained as a result of the quantum quasispace change effect. Referenced to the equilibrium point of level 0 this affect appears as quasishrink for the right side from level 0. While in the Balmer model this effect is a quasishrink and referenced to a fixed distance (because the proton core dimensions defining the quantum orbit is fixed), for the electron bonding orbit this distance is defined by the internuclear distance between the two atomic nuclei. The latter parameter in this case is self adjustable from the total energy balance of the system in which the IG field plays a very important role.

Summary:

• The BSM model and QM model, both provide the same type of vibrational level transitions, but BSM model shows the real physical process in which the IG field and its enormous energy become apparent.

9.5.6 Approximate calculation of the system energy in the equilibrium state

Let calculate the system energy for H_2 ortho-I state. For this purpose we will take into account the following logical considerations:

The orbiting electrons between two protons are able to neutralize their charges. We may assume that every orbiting electron is able to neutralize one charge, by interconnecting its E-filed lines to the proton E-field inside the Bohr surface. Let considering the moment, when one of the electrons is in the locus of the left proton and the other one in the locus of the right proton. Their velocity in this case are normal to the direction of the vibration and does not contribute to the momentum energy of the system. This energy, then can be estimated, by considering two unit charges at distance r_n. Now let assume, that the left proton and the right electron are both missing. The system energy in this case is $q/4\pi\varepsilon_o r_n$ [eV]. The same results is for the other symmetrical case. Adding the two symmetrical cases we should get the full system energy. $\frac{2q}{4\pi\epsilon_0[L_q(1) + 0.6455L_p)]}$ = 16.06 eV(9.4) $E_{SYS} =$

The obtained value matches very well to the parameter Vertical Ionization Potential, used in the QM model and determined by the Photoelectron spectrum (discussed later and shown in Fig. 9.19).

$$E_{VIP} = 15.967 \text{ eV}$$
 (9.5)

The parameter EVIP corresponds to the largest peak of the PE spectrum, so it is easily identifiable. It is a signature of the most populated vibrational energy level. Consequently, we may consider this energy to be equal to the system energy, calculated by Eq. (9.4) From the data about molecular orbital constants for H2 we also have a value of average kinetic energy equal to 15.98 eV. (http://physics.nist.gov/cgi-bin/Ionization/ta-

ble.pl?ionization=h2). All this gives us a confidence for using of the theoretical Eq. (9.4) in the further analysis.

Consequently, for practical purposes we may accept, that

$$E_{SYS} \approx E_{VIP} \tag{9.6}$$

9.5.7 Experimental evidence about the BSM concept of molecular vibrations

9.5.7.1 Cross analysis

The presented concept of molecular vibrations in CL space can be proved by analysis of two phenomena of simple diatomic molecule: the molecular spectra and the photoelectron spectra.

Number of methods for obtaining of Photoelectron spectra exist. For our purpose, the most informative method is the He I photoelectron spectroscopy. In this method, the photoelectron spectrum is obtained, when molecules of the investigated gas in vacuum conditions are irradiated by He I resonance line at 584 A, possessing an energy of 21.23 eV. The bound electrons are usually with energy below 20 eV and the photoionization provides free photoelectrons. Their kinetic energy is measured by electron energy analyser. The energy spectra is the rate of detected electrons in function of their kinetic energy.

9.5.7.2 Difference between the ionization mechanism for atoms, and molecules

The photoelectron (PE) spectrum is informative for the internuclear bonds and vibrational levels of molecules. If neglecting the motion of the atom of the molecule (referencing to laboratory frame) the energy balance equation is:

$$E_K = hv - E_{IP} \tag{9.7}$$

where: E_K is the kinetic energy of the bound electron; hv - is the photon energy of the ionization source; E_{IP} - is an "Ionization Potential" or "Ionization Energy", term adopted due to the QM model.

If applying a photoelectron spectrum for atoms Eq. (9.7) is valid for the whole range of obtained PE spectra. This equation, however, could not be applied directly for a photoelectron spectrum in molecules because of the following differences:

- All the quantum orbits in the atom are confined to the fixed distance, defined by the proton dimensions, estimated in absolute scale.

- The quantum orbits of the molecular bonding electrons are confined to distance that is dependent of the self adjustable internuclear distance. The above differences affect especially the estimated energy of the bound electron by the measured kinetic energy of the photoelectron.

According to PE theory for molecules, the energy balance is given by Eq. (9.8).

$$E_{K} = hv - E_{IP} - (\Delta E_{vib} - \Delta R_{rot})$$
(9.8)

where: E_K is the measured energy of the photoelectron.

The terms in the bracket, denoted as vibrational and rotational energy, provides correction for E_K in order to reflect the internal energy of this electron. In BSM interpretation of PE spectrum this correction is referred to the IG field between the atomic nuclei and the electronic bonds.

Important feature of the PH spectra is that the range of the energy bands is shrunk. This is apparent from the analysis of H2 molecule (provided later) when comparing with the corresponding optical ban of same vibrational levels. The reason for such effect is the energy loss of extracted photoelectron. Losing a electron the molecule becomes a positive ion. The interaction between this ion and the negative electron causes a partial loss of its energy for recoiling of the ion.

9.5.7.3 Signature of the vibrational bands in the Optical and Photoelectron spectrum

 E_{VIP} is easily identified by the PE spectrum of the simple molecule like H₂ ortho-I. Even the corresponding vibrational bands, could be identified from the optical spectrum, and the feature of E_{VIP} parameter as well. (This will be shown later in Fig. 9.19). But while, the energy range of the PE spectrum is shrunk, the energy range for the optical spectrum is not.

The relation between the vibrational levels of H2 ortho-I and the optical and PE spectrum is illustrated in Fig. 9.15. The following notations are used:

E - is a momentary energy scale

E_{SYS} - system energy

 E_{IP} is a ionization potential (known also as binding energy)

 r_n - is an internuclear distance at equilibrium point

 Δr_n - is the range of change of r_{ne} are the ranges of displacement



Vibrational levels of H_2 ortho-I and their relations to the optical and photoelectron spectra

 E_{DIS} - is known as a dissociation energy (although it may not lead to dissociation of transitions are between the energy levels and the metastable state see J. H. Black and A. Dalgarno, 1976)

 E_A and E_B energies defining the position of the metastable state).

 E_{K} - is a PE spectrum parameter ("electron kinetic energy")

1,2 3 - vibrational bands

The vibrational curve is shown as function of vibrational quantum numbers. They are referenced to the change of internuclear distance r_n . It will be shown later that the range of this change is intrinsically small due to the strong contribution of the IG field.

The vibrational curve is idealized in the range of the dissociation limit but in the following later analysis we will use vibrational levels with small number.

The optical vibrational bands shown in the left side corresponds to transitions between the vibrational levels and the metastable state. The PE spectrum is shown below the vibrational ladder. The PE levels are reflected by a line with angle larger than 45 deg (multiplication factor < 1) in order to show the stretched PE levels in respect to those of optical spectrum.

From the Fig. 9.15, the functional relation between the Optical and PE spectrum becomes apparent. One and a same shape of the quantum vibrational curve defines two different shapes of the Optical and PE spectrum. Working only by the energy levels, we see that, if applying a proper offset and multiplication factor to the PE spectrum, we will obtains the optical spectrum and vice versa. Consequently, the inverse task - obtaining the vibrational levels from the Optical and PE spectrum is also possible. In the same time we may get the relation between the vibrational levels and the momentary internuclear distance. This is done in the following later paragraphs.

The BSM analysis suggests one reasonable explanation of the metastable state of H_2 . The quantum orbits for this state may have exactly the same trace length and shape as Lq(1) but it can be formed of the trace length of two quantum loops of second subharmonics connected in serial. Then the distance between the two protons, if not considering any deformation of the orbital shape is unchanged. Keeping in mind that the IG field is able to control the spatial configuration of the proximity electrical field we may attribute this to a common synchronization of the IG energy of the two protons and the two electrons. Such effect, however, may work up to a limited distance between the protons. In this range Eq. [(9.18)] is valid. The IG field may be propagated beyond this distance (up to some limit) but the two protons fields are not any more commonly synchronized.

Summary:

- The Vibrational oscillation of homonuclear diatomic molecule exhibit unique Optical and PE spectrum.
- The vibrational quantum motion could be analysed by using a proper set of the vibrational transitions and the corresponding PE spectrum.
- The PE spectrum exhibit different energy offset and energy scale factor.

9.5.7.4 Fine structure of the optical molecular spectra

9.5.7.4.1 Effect of the variation of bonding length and tilt on the quantum orbits.

The electron system of the atoms follows the nuclear motion, but they are not rigidly connected to the nuclei. They have also different resonance frequencies. The contributors for this difference are not only the inertial factors but the different magnetic moments as well (different magnetic moment of electron in comparison to the proton and neutron). The bonding electrons, possessing own spin momentum and QM spin (orbital momentum), interact with the nuclear atomic electrons, via magnetic interactions inside the integrated Bohr surface. We may consider, that the bonding electrons are elastically connected to the nuclei. In result of such connection, the following effects might be possible:

(a) the quantum orbit shape is unchanged but could not follow exactly the vibrational motion

(b) the quantum orbit size is unchanged, but the shape is distorted

(c) the quantum orbit size and shape are the same but phase delay occurs between the dynamical quantum quasishrink effect and the phases of the two electron proper frequencies (electron shellpositron) and (positron- core.

According to the definition of the quantum loop, it is the orbital trace length that defines the quantum orbit. The shape of the orbit could be modified, without disturbing this condition. The shape is defined by the E-field configuration and the classical electron spin momentum. The change of the shape, however affects the strength of the quantum effect and efficiency of the CL space pumping. The strength is maximum, when the spinning electron intercept the magnetic lines of the proton at angle close to 90 deg.

In later analysis (not shown) it has been found that a quantum orbit with shape of Hippoped curve and parameter $a = \sqrt{3}$ matches very well to the experimental data. Therefore, We may consider, that, the quantum orbit is free of distortion at parameter $a = \sqrt{3}$

The possible distortions of the bonding orbit are two:

- symmetrical distortion

- asymmetrical distortion

The both types of distortion are shown respectively in Fig. 9.16, a. and b.



Shape distortions of the bonding quantum orbit, a. - symmetrical, b. - asymmetrical

The case of symmetrical distortions is valid when the bonding length is changed but the long proton axes are aligned. The asymmetrical distortion appears, when the bonding length is a same but the proton axes get tilting.

The bonding orbits of the molecules with linear type of vibrations exhibit symmetrical type of distortion. Such type of distortion is valid also for the bonding orbits of the quasirotational vibration that exhibit quasilinear motion in arc.

The symmetrical orbit distortion may cause a small change of the internuclear distance that could provide some displacement from the defined vibrational level. The asymmetrical effect for displacement from the vibrational level, however is much smaller.

9.5.7.4.2 Oscillations providing vibrationalrotational spectra with P and R branches only

The equivalent proper frequency of the bonding system is higher, than the equivalent proper frequency of the molecule. So it is the first one that could put its signature in the vibrational cycle. It appears as a set of proper frequencies providing own levels above or below the given level of the vibrational ladder. The symmetrical distortion of the bonding orbit allow appearance of this levels as P and R branch.

Now one basic question may arise:

Why the frequency set appears above and below the vibrational level and with a spacing asymmetry?

For light diatomic molecules, the rotational energy is much smaller, than the bonding energy at equilibrium. Then the inertial interaction of the nuclei could be neglected in the vibrational motion, considering an energy balance only of the quantum quasishrink effect. Such energy balance is between IG(CP) and IG(TP) of CL space (Chapter 2) discussed later in §9.7.5.B, C. The motion of the bonding system is subjected to this balance. The change of IG(TP) defines the proton electrical field inside the Bohr surface, while IG(CP) - the charge unity. It is reasonable to expect, that the motion of the bonding system could not follow exactly the phase of the IG field oscillations. Some phase difference could be be expected. The assumption of a phase difference comes from the fact, that the electron has a finite inertial mass and axial spin momentum. The obtained phase difference may cause overshooting of the vibrational motion of the bonding system in respect to the vibrational level defined by the IG field oscillation. In result of all these considerations, the vibrational motion of the bonding system provides a set of quantum levels, around the vibrational level.

The formation of R and P branches from the frequency set of the bonding system is illustrated later by the analysis of H_2 and D_2 molecules. They both could be considered as basic units involved in any EB bonding system in the molecules.

The process of P and R branches formation is illustrated by Fig. 9.17, where a section of vibrational curve is shown with three consecutive vibrational levels.

The provided concept of overshooting with the shown phase is in agreement with the analysis of P and R branch formation for H_2 and D_2 molecules (ortho-I state) given later in this chapter in §9.9.3. The correctness of accepted sign of the phase delay might be a topic of discussion. However it is possible to be verified by study of P and R branches for some linear diatomic homonuclear molecules for which enough optical and PE spectra exist.



Section of three consecutive levels of the vibrational ladder with fine structure levels from the bonding system frequency set. In the right side the corresponding optical spectrum from transition between these levels and the lowest level is shown

The practical realization of the overshooting process is possible due to the symmetrical distortion of the bonding orbit. We may reference the obtained set of levels as "**orbit distortion levels**" in order to preserve the clearness of the physical concept. They corresponds to the J levels of the QM model. For the BSM model the J numbering does not need to start from 0 and from 1 for R and P branches respectively.

In the QM model these levels are considered rotational, due to the accepted initial theoretical concept of "rigid rotor" and they are denoted by J levels.

We will continue to use J notation for the orbital distortion levels. They are directly related to the spectral lines contained in the P and R branches of the molecular spectra.

From the BSM model, the following rules could be formulated:

(1) When the transition is between one vibrational level and the lowest (zero) level, the photon energy of the lines is equal to the difference between the instant system energy and the optical boundary energy (see §9.5.7.4 and Fig 9.15). The PE spectrum has a shape corresponding to a set of such type of transitions.

(2) The line strength corresponds to the populated degree of the vibrational level

(3) There is no line in the middle between P and R branches because, the probability of exact matching the proper frequency set of the bonding system with the vibrational level determined by IG field balance is quite low.

(4) When estimated by external CL space units, R branch corresponds to a symmetrical stretching of the quantum orbit, while P branch to a symmetrical shrinking (assuming the parameter $a = \sqrt{3}$ is preserved). R branch is from the side of larger internuclear distance, while P branch is from the shorter one. Their different line spacing is a result of the IG field balance (Note: This consideration needs to be additionally verified).

(5) Both P and R branches have nonlinear line spacing counted from lower to higher J numbers. This non linearity is a result of two nonlinear factors: IG field and the reaction of the bonding electron to the orbital distortion.

(6) The P and R branches in the molecule of heavier atoms should be less spread around the middle point of equivalent transitions

(7) For one and a same molecule the P and R branches, estimated by energy levels, are more compact for $(v_i - v_{i+1})$ transitions, than $(v_i - 0)$ transitions

(8) The optical signature does not show line shape deterioration due to a level jittering, despite the fact that the electron system is elastically connected to the nuclear hadron structure. This may lead to two conclusions:

-The vibrational motion is quite small, while the energy is juggled by the quantum quasishrink effect

-The IG field balance leading to a photon emission (absorption) is a quite fast process.

Some of the first J numbers due to the orbit distortion are even apparent in some PE spectra with high resolution. The PE spectrum observed by J. E. Pollard et al., J. Chem. Phys, 77, 34-45, (1982) and given in Fig. 9.19, shows signature of low J numbers.

From the way the PE spectra is usually obtained it is clear, that the first PE peak is accumu-

electrons from vibrational bands lated by possessing a lower number (see Fig. 9.15). If the band 1 only is scanned with high resolution, then the obtained PE spectrum will carry the signature of the orbit distortion levels, corresponding to J levels of the optical spectrum. Such experiments is performed by G. K. Cook and M. Ogawa (1965). They obtain absorption spectrum of N2 in the far UV range. Their method is different than the method which uses He resonance line. They scan a monochromatic line, observing simultaneously the optical spectrum and the ionization current. In such approach the photoelectron energy range shrink effect does not exists. The obtained PE spectrum is shown in Fig. 9.18.



Photoionization yield-curve and absorption spectrum for N_2 gas (courtesy of G. K. Cook and M. Ogawa (1965).

9.5.7.4.3 Oscillations providing vibrationalrotational spectra with P, R and Q branches

The concept of the quasirotational motion has been discussed in §9.5.4.2. A specific feature of this motion is that one electrical bond serves as a centre of the motion, while the other vibrates by stretching and shrinking, and they interchange alternatively. The quantum orbit of the bond with vibrational motion exhibits symmetrical orbit distortions. So this motion contributes to P and R branches, as described in the previous paragraph. The quantum orbit of the other bond, that is a centre of such motion exhibit asymmetrical distortion, due to change of the angle between the bound protons. The change of the angle causes some change of the spatial configurational of the E-field around the clubs of the bound protons. This causes a distortion of the Hippoped shape of the quantum orbit. In a first approximation we may consider, that the distance between the pair bonds serving as a centre of rotation and the nuclei is not changed. This approximation is more valid for molecule from heavier atoms. This means that, the IG field in this point is a same. Then the pumped CL space by the electron of the bond serving as a point of quasirotation will have an energy staying in the middle of the P and R branches that are contributed by the other bond. Consequently this type of oscillations contributes to the Q branch of the optical spectrum. The asymmetrical distortion in fact may displace slightly the orbital position from the equilibrium, corresponding to P R branches. So the Q branch contains more than one line, additionally spread in small spectral range. The heavier diatomic molecules with pair bonds exhibit smaller spread of the Q branch, in comparison to the lighter molecules (for example H₂ para molecule). This indicates that the Q branch line spacing is sensitive to the displacement from the equilibrium distance. In heavier molecules, the bonding electrons interact with larger number of atomic electrons from the internal shells. The latter are much more stronger connected to the protons, providing in such way more stable reference point. For this reason the Q branches of the heavier molecules are less spread.

In many molecules the Q branches appear as more than one set. This is a result of the QM spin orbit interaction between the bonding and other electrons of the atom.

Summary:

- Molecules with linear vibrations exhibit "vibrational-rotational" spectrum with P and R branches only
- Molecules with quasirotational vibrations vibrations exhibit spectrum with P, R and Q branches.
- The P and R branches of the molecules with quasirotational vibration are from the quasilinear vibrating bond, while the Q branches

are from the bond, that is a centre of the quasirotational motion.

9.5.8 A possible mechanism of the Ramman scattering and rotational Ramman spectra according to BSM

Ramman spectra are features only of molecules. The atoms can not posses such kind of spectra. Ramman spectra are obtained when the molecule is exited by strong monochromatic radiation. Such excitation in the optical range is very efficient when the radiation energy is from a laser.

Now let see what happens when the molecule is irradiated by strong monochromatic radiation. We have seen that the molecular system is very sensitive to a change of the momentary energy balance. The strong monochromatic radiation (additionally coherent for irradiation by laser) inputs some amount of energy into the volume of the Bohr surface. The obtained energy disturbs the energy momentary balance of the system, so the system undergoes fast transition from one internuclear distance to another. This corresponds to transition from one vibrational level to another directly without following the vibrational curve. So the system jump to another energy level, but the input energy usually is different than the obtained energy between the levels. So the excess energy is released right away as photon. The matched level may be not only vibrational but also some "vibrational - rotational" level. The process is so fast, that it seems as a scattering. It does not require a finite CL pumping time as in the spontaneous emission.

The Ramman scattering may be referenced not only to the vibrational and vibrational-rotational levels, but also to the quantum levels of the electrons in the nuclei. When the irradiating energy is proper selected and the molecules are in the ground state (lowest vibrational energy) a "rotational" Ramman spectra could be obtained.

"Rotational" Ramman spectra

The "pure rotational" spectrum is a signature of the proper frequency set. The energy difference between the bottom level and its neighbour is larger than between neighbouring levels with higher vibrational number. The line spacing for this vibrational level resulted from a quantum shape change is also large. Therefore, when the molecule possesses a lowest vibrational energy some signature of pure rotational spectrum might be well separated at the) vibrational level. Such experiments are provided.

Ramman scattering

Now let suppose, that molecule in lowest vibrational state are irradiated by proper quantum energy in order to reach some higher vibrational level pretty accurately. Then the small energy with a proper frequency signature will be translated to higher vibrational level. If the irradiated quantum energy is proper selected the condition for photon energy difference will appear exactly in the vibrational level between P and R branches. So by scanning the irradiation photon energy the levels are possible for resolving.

In fact the condition for photon energy difference are fulfilled for two symmetrical levels from both sides of the vibrational curve. Their energy is one and a same, but the internuclear distances are different. It is evident, that the emitted spectral lines will have the same signature as the "pure rotational" spectrum, partly modified from the different internuclear distance. The Stoks component corresponds to the longer distance and Antistoks - to the shorter one.

The "vibrational-rotational" spectrum is a signature of the proper frequency set of the bonding system. The "rotational" Ramman spectrum is a signature of the molecular proper frequencies set. The fact that they are quite distinct leads to a conclusion that:

• The molecular and the bonding system equivalent fundamental frequencies are different.

The Ramman effect is characterized with one specific feature: the photons are emitted right away after the activation (no apparent lifetime of activated state as in the atomic and molecular spectra). For this reason the Ramman effect is known as a Ramman scattering. The BSM concept is in full agreement with this feature. Its explanation is discussed later in §9.7.5-D.

9.6 Vibrational bands of H₂ ortho-I state.

9.6.1 Photoelectron spectrum

The H_2 ortho molecule exhibits a typical molecular oscillations of I-st type. This is evident from the shape of its PE spectrum



Fig. 9.19

PE spectrum of H_2 molecule (courtesy of J. E. Pollard et al. (1982)

The spectrum is obtained by using a He I resonance line (21.23 eV). The energy scale is referenced to E_k .

From the PE spectrum in Fig. 9.19 we see, that the largest peak is at 5.26 eV. So

 E_{VIP} = 21.23 – 5.26 = 15.97 eV. , and according to Eq. (9.9), this is also $\rm E_{SYS}$ at point B (see Fig. 9.15).

9.6.2 Identification of the vibrational levels by the Optical spectrum

The optical spectrum for the same state, corresponds to the system $(B^{1}\Sigma_{u}^{+} - X^{1}\Sigma_{g}^{+})$, known also as a Lyman system. The optical bands of this system have only P and R branches, but not Q branches. This is in agreement with the considerations discussed in §9.5.7.4. Good experimental measurements of this system are provided by I. Dabrowsky (1984). Using these data, we may identify the optical transitions between the vibrational levels, by using the following criteria:

- The photon energy and line abundance should follow the similar trend as the vector, obtained by the PE spectrum

- The third optical band should be the most populated one

There are two sets of strongly populated optical bands, whose levels and trends are very close. The first one is from transitions: (0-1), (0-2), (0-3) and so on, denoted by BSM as (0-v) set. The second one is from transitions: (1-1), (1-2), (1-3) and so on, denoted by BSM as (1-v) set. In both sets, the third consecutive optical bands are the most populated and their population corresponds to the PE energy level trend. We accept, that the difference between the both sets corresponds to the Quantum Mechanical electron spin (in BSM model two electrons circulate in opposite directions, while the proton twisting serves as a reference). The signatures of the two optical sets appear also in the PE spectrum shown in Fig. 91.17. If comparing the energy difference between the two set with the energy difference of the fine line splitting in atomic Hydrogen, it looks larger. But we do not have to forget the shift effect involving directly the IG energy, that may contribute to the larger energy separation between the two sets of optical bands and PE peaks. From the cross validation between the energy level trends of both type of spectra we conclude, that the PE spectrum of Fig. 9.16 corresponds to both sets.

9.6.3 Identification of the common nonlinear trend between the Optical set and PE spectrum, and estimation of E_I parameter.

Firstly we will accept, that the shape of optical set and the PE spectrum are both part of parabolas, but with different coefficients. This assumption will be confirmed later. Then we may apply the rule, that the difference between two parabolic functions is also a parabola. Using the level number as an argument (according to BSM numbering), we may identify the common trends of the energy levels by the following procedure.

- digitizing the PE spectrum of Fig. 9.19 into a vector E_{PE} (E_{PE} instead of E_K is used in order to avoid a possible confusion in a later analysis)

- form a vector of (0-v) set, denoted as E_0 .

- form a vector of (1-v) set, denoted as E_1 .

- make a vector difference $\Delta E_0 = E_0 - E_{PE}$ and $\Delta E_1 = E_1 - E_{PE}$

- fit to a simple nonlinear equation (first try a second order polynomial)

- plot the curves

- find the interception point between E_{PE} and $(E_0 - E_{PE})$ and $(E_1 - E_{PE})$.

From the fine structure model presented in §9.5.7.4. it follows, that the most accurate quantum

Table 9.3

energy value of the vibrational bands should be in the middle between the first J lines of the P and R branches.

	H ₂ ortho-I vibrational quantum levels identified by (0-v) set and PE spectrum Table 9.2							
Vib. level	transition by QM	Ist R line (eV)	Ist P line (eV)	E ₀ (eV)	E _{PE} (eV)	ΔE_0 (eV)		
0	(0-1)	10.76	10.65	10.66	5.79	4.87		
1	(0-2)	10.186	10.168	10.177	5.52	4.65		
2	(0-3)	9.728	9.71	9.719	5.27	4.45		
3	(0-4)	9.298	9.281	9.289	5.025	4.264		
4	(0-5)	8.896	8.88	8.888	4.8	4.088		
5	(0-6)	8.522	8.507	8.5145	4.58	3.934		
6	(0-7)	8.177	8.163	8.17	4.38	3.79		
7	(0-8)	7.8626	7.8482	7.855	4.2	3.655		

Table 9.2 provides data for (0-v) set with related parameters E_{PE} and $(E_0 - E_{PE})$ vectors and Table 9.3 - for (1-v) with the similar related parameters.

 H_2 ortho-I vibrational quantum levels identified by (1-v) set and PE spectrum

Vib. level	transition by QM	Ist R line (eV)	Ist P lin (eV)	e E ₁ (eV)	E _{PE} (eV)	ΔE_1 (eV)
1	(1-1)	10.873	10.817	10.826	5.79	5.036
2	(1-2)	10.35	10.33	10.34	5.52	4.82
3	(1-3)	9.891	9.8739	9.882	5.27	4.612
4	(1-4)	9.461	9.444	9.4525	5.025	4.4275
5	(1-5)	9.057	9.043	9.05	4.8	4.25
6	(1-6)	8.685	8.67	8.677	4.58	4.097
7	(1-7)	8.34	8.326	8.333	4.38	3.953
8	(1-8)	8.0252	8.0117	8.0184	4.2	3.8184
9	(1-9)	7.7409	7.7282	7.7345	4.0375	5 3.697
10	(1-10)	7.4896	7.4778	7.4834	3.88	3.603

From the Tables 9.2 and 9.3, vectors of E_0 , ΔE_0 and E_I , ΔE_1 in function of band levels are formed, and fitted to a polynomial of second order $y = a + bx + cx^2$. The vector E_{PE} is also fitted to a same polynomial. The chosen polynomial fits quite well for all vectors with std in order of 0.0038. The fitting coefficients are respectively:

for E₀: a=11.174884 b=-0.52778274 c= 0.01408631 for ΔE_0 : a=5.1015982 b=-0.2386875 c=0.007276785 for E₁: for ΔE_1 : for E_{PE}: a=6.0749265 b=-0.29214977 c=0.0072671569

Fig. 9.21 shows the plot of E_0 , E_{PE} and ΔE_0 in function of the vibrational level. The extrapolat-

ed curve regions are marked by dashed lines (Note: the curves may not look smooth due to drawing and printing capabilities).



Fig. 9.21 Vibrational levels by the optical band set (0-v)and PE spectrum for H₂ ortho-I. The solid line shows the observed data, the dashed lines show the extrapolated data from the optical spectrum

From interpolated curves one finds that EPE and ΔE_0 intercepts at 18.147. The first derivative of all three plots at this point are close to zero. At the PE spectrum, the band (level) number 18 (by BSM numbering) appears still distinguishable by amplitude and energy difference. If E₀ and E_{PE} were not correlated properly, the interception of E₀ and ΔE_0 would not coincide at band 18. So we accept the band 18 as the last one before the boundary limit convergence. For this band from the fitted curve for E₀ we obtain the experimental value of E_B. $E_B = 6.239 \text{ eV}$ (9.9)

 $E_B' = 3.163$ ev - shrunk value of E_B estimated by PE spectrum

Therefore we may accept the last band to be 18 (this will be confirmed later) and denote it as v_m .

$$D_m = 18$$
 (9.10)

The parameter E_B determined by this approach is approximate. But it helps to identify one real physical parameter and to find its relation the energy levels shown in Fig. 9.15.

9.7. Theoretical analysis of H₂ ortho-I molecule oscillations

9.7.1 Estimation of rotational energy

The analysis of the H_2 otho-I properties will help to understand the electronic bondings in the molecules. For this reason we will investigate the momentary system energy of H₂. Firstly we will check what type is the molecular oscillation, by comparing E_{rot} and E₁ energy. Using the value of rotational constant, provided by Dieke and Blue (1935) and Dieke, (1958): $B_e = 27.30 \text{ cm}^{-1}$ and applying Eq. (9.A.6) we see that the maximum of the population curve appears for J=2 at temperature 77K and between 2 and 3, but closer to 2 for 298K. Accepting J=2, corresponding to an equivalent molecular frequency of 54.6 cm-1 we may use it for estimation of the rotational energy by Eq. (9.3).

Note: The experimental value from different experiment shows a variation. The correct choice and some experimental considerations according to BSM are discussed in §9.9.2 and § 9.11.

Another needed value is the internuclear distance at the equilibrium point. In the following analysis we will see, that the deviation from the internuclear distance estimated by the free space CL node scale is negligible. So we may use the internuclear distance for point B (dissociation limit) given by the equation: $r_n = L_q(1) + 0.6455L_p = 1.795$ A

Then rotational energy by Eq. 9.3 is:

$$E_{rot} = 0.02 \text{ eV}$$

We see, that $E_{rot} \ll E_B$ (9.11)

The condition (9.11) indicates that the energy of the vibrational motion could not exceed the metastable state. Consequently this is a molecule with a first type oscillations, according to the criterion, defined in §9.5.4.1. Additional check of this condition could be made by the shape of its PE spectrum. The bottom edge of the peaks set is not elevated. This is observed even for HD and D₂ molecule, so for H₂ it is strongly valid. (The PE spectrum of H₂ and HD are pretty close, see J. E. Pollard et al., (1982)),

Consequently:

• the centrifugal forces in H₂ ortho-I state are negligible in comparison to the bonding forces.

The above conclusion indicates that H_2 ortho-I state could be considered as a typical case of I-st type molecular vibrations, discussed in §. 9.5.4.1.

9.7.2 Considerations for energy balance involving IG field potentials

The condition (9.11) allows to simplify the energy balance of the oscillation motion, by neglecting the negligible rotational energy of H_2 ortho-I.

The energy balance should be considered for the whole system, comprised of:

- two protons with their internal RL(T) structures and IG field potentials

- two electron of opposite QM spin, sharing a common orbit of first harmonic

- the internal E-field enclosed in the integrated Bohr surfaces of both protons

- the CL space enclosed by the integrated Bohr surfaces

All these energetic components are included in a total general energy balance between two potential fields: IG field and E-field. The magnetic filed from the orbiting electrons is locked inside the Bohr surface and does not appear in the external CL space. So we may consider that its energy is included in the Bohr surface volume energy estimated by the external CL space parameters. This means, that E-field should participate in the balance with its full static value, that is the unit charge. From the other side, we know, that the E-field (charge) is contributed and controlled by the IG field. Now we are very close to the possibility to obtain a relation between some characteristic parameter of IG field and the controlled E-field. We may formulate this relation in a following way:

- The electrical field energy of a helical structure in CL space is adjusted to the energy of unit charge by the balance of IG forces.
- The unit charge energy is equal to the Intrinsic Gravitational potential of the structure referenced to a free CL space

It is difficult to obtain the relation parameters for a single particle like a proton or even for the Hydrogen atom. However, we may obtain the relation by analysis of the motion behaviour of pair of similar charge particle. Such particles are pair protons forming a H_2 molecule together with two electrons. The H_2 ortho-I molecule, shown in Fig. 9.12 is quite suitable for such analysis.

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9.7.3 Definition of C_{IG} factor and using it as a characteristic parameter of the IG potentials

The IG potential between two particles can be determined in a classical way, by separating them from their initial distance to infinity. Mathematically this is expressed by integration of the acting between them IG forces from the initial distance to infinity. Let determine the IG(CP) potential (CP denotes the IG vectors of the central part of the prisms) between two hadron structures. Because we accepted that the energy of the electrical charge is a part of the IG energy we should not take the charge into account. The IG law varies with inverse cubic power of the distance.

Having in mind all this considerations, the IG(CP) potential (Energy) between the two protons or neutrons) can be estimated by the expression.

$$E_{IG}(CP) = -2\int_{r_{ne}}^{\infty} \frac{G_o m_{po}^2}{r^3} dr = \frac{C_{IG}}{\left(L_q(1) + 0.6455L_p\right)^2} \quad (9.13)$$

where: m_{po} is the Intrinsic mass of the proton, G_0 is the intrinsic gravitational constant

 $C_{IG} = G_o m_{po}^2$ - IG factor

Note: The factor 2 in front of the integral comes from the two arm branches (along *abcd* axes) of the CL space cell unit. They both are included in the xyz cell unit to which all the CL space parameters are referenced. All equations using C_{IG} factor in the following analysis confirms the need of factor 2.

 C_{IG} factor for IG forces between two intrinsic masses is similar as Gm_p^2 factor for Newtonian gravitational forces between two Newtonian masses of proton. Despite the unknown value of G_o , the determination of the C_{IG} factor is very useful, as will be shown later.

9.7.4 Determination of C_{IG} factor from the IG energy balance of H₂ ortho-I molecule.

We are familiar with the Newtonian gravitational field, electrical field and magnetic field. The IG fields and potentials are quite more strong than any other fields and potentials we are familiar with. Then let formulate the energy balance between the hadron structures by the IG potentials, according to the considerations discussed in §9.7.2. For the whole system including the CL space we may expect, that the following balance exists:

IG(CP) energy = IG(TP) energy

Applying this balance for the H2 ortho-I system, we get:

$$E_{IG}(CP) = E_X + 2(E_q) + 2(E_K)$$
 (9.14)
where:

 $E_{IG}(CP)$ - is the IG(CP) energy

 E_q - is the IG energy spent for creating the positive unit charge of the proton

 E_{K} - is the kinetic energy of the electron.

 E_X - energy potential that we must identify

The energy E_X may appear some of the energies shown in Fig. 9.15. Our task is to identify it.

Consideration (a): The Eq. (9.14) characterizes the system without considering the quantum quasishrink effect.

For the electrical charge energy we will use the following expression:

$$E_q = hv_c = m_e c^2 \tag{9.15}$$

The kinetic energy of the electron with first harmonic velocity is

$$E_k = 0.5m_e \alpha^2 c^2 = h v_c \alpha^2$$
 (9.16)

Substituting Equations (9.13, (9.15) and (9.16) in Eq. (9.14) and solving for C_{IG} we get:

$$C_{IG} = (2hv_c + hv_c\alpha^2 + E_X)(L_q(1) + 0.6455L_p)^2 \qquad (9.17)$$

 E_X could be some of the energies of H_2 molecule. Expressed in eV it could not exceed 16 eV. For such range the value of the C_{IG} factor (reference to energy balance in eV) in fact changes insignificantly - only at 5th significant digit.

If $E_X = 0$, then $C_{IG} = 5.265108 \times 10^{-33}$

If $E_B = 9.7189 \text{ eV}$ $C_{IG} = 5.265127 \times 10^{-33}$ It is quite possible E_X energy to be equal to $E_{\rm B}$ that is the difference between the dissociating limit and the metastable state. It has been determined in §9.6.3 and given by Eq. (9.13). It is more convenient, however, in further analysis to consider this potential to the right side terms in the more universal Eq. (9.17). Then the value for CIG factor when used in energy balance in eV is:

 $C_{IG} = 5.26508 \times 10^{-33}$

9.7.5 Definition of emitted photon energy as an excess energy in the total energy balance involving IG energy of the system

A. Photon emission (absorption)

In the derivation of the factor C_{IG} the quantum quasi-change effect has not been taken into account, but C_{IG} is not sensitive to potential in a range of few electronvolts. For determination of the photon energy, however, this effect has to be considered.

Using again Eq. (914) with substituted terms $(E_{IG}(CP) \text{ from Eq. } (9.13) \text{ and other terms}) \text{ and } di$ viding on the unite charge q in order to obtain the balance in electronvolts we get:

$$\frac{C_{IG}}{q(L_q(1) + 06455L_p)^2} = \frac{2E_q}{q} + \frac{2E_K}{q} + E_X$$
(9.18)

The quantum quasishrink effect will affect the orbital length $L_{a}(1)$. So we have to find the proper function affecting this parameter. In fact there are two ambiguous trends of the system:

Trend (1) The electron tries to fall to lower quantum orbit, whose trace length is distinguished by one Compton wavelength λ_{SPM} .

Trend (2) The system tries to keep the present status by small decrease of the internuclear distance

We will analyse firstly the effect of Trend (1) by some approximate method. From Eq. (9.17) we have seen that the IG field energy is much larger than other energies, so a small change of internuclear distance means a large energy change in the range of system energy E_{SYS}.

Let analyse the effect starting from the dissociation limit where Lq(1) could be considered unchanged and moving in direction of shorter r_n . At this point the orbit length is $L_q(1)$ and its trace length contains approximately 137 numbers of Compton wavelengths. Changing the number of the Compton wavelength by one, the next stable quantum orbit may contain 136 numbers, following by 135 and so on. It is convenient to denote the change of these numbers by integer parameter Δ . Let denote the quasishrink length by a prime index ('). Then for the quasishrink trace length we have:

$$L_{Tq}' = L_{Tq} \left(1 - \frac{\Delta}{137}\right) \approx L_{Tq} (1 - \alpha \Delta)$$

If assuming that the shape of the quantum orbit in a quasishrink space is preserved, then a similar expression should be valid for the size of the quantum orbit, but the term $\alpha\Delta$ should be multiplied by the factor π . This comes from the following considerations: The trace length of the Lq(1) is λ_c/α . We may make from the same length a circles with a diameter $d = \lambda_c/(\pi\alpha)$. If λ_c changes due to the quantum quasi-change effect we have $\Delta d = \Delta \lambda_c/(\pi\alpha)$. We see that α is multiplied by a factor a factor π . Now if considering that the distance is defined by a Hippoped curve with a same trace length the condition is the same - α is multiplied by a factor π . Consequently, we arrived to the expression.

$$L'_{q}(1) = [L_{q}(1)](1 - \pi \alpha \Delta)$$
(9.19)

The obtained expression is only approximate, because we have still take into account the ability of the IG field to control the Compton wavelength in strongly oriented E-field.

The effect of Trend (2)

Eq. (9.19) has only one dimensional spatial dependence whose variable parameter is Δ . But the proximity E-filed controlled by the IG field is a three dimensional. The possible parameters from Eq. (9.19) that could be affected are only α and Δ . Obviously some additional dependence of Δ parameter should exist. We may try to find this dependence by empirical way. Following the logical considerations about quasi-change space we may define the first unknown parameter as a power degree on α , and the second one as a power degree on Δ .

Then the expected function $L'_q(1)$ will take a form:

$$L'_{q}(1) = [L_{q}(1)](1 - \pi \alpha^{x} \Delta^{y})$$
(9.20)

The quantum number Δ (integer) was referenced to the dissociation limit of the vibrational ladder. In order to use quantum numbers referenced to this point we substitute $\Delta = v_m - v$ where: v - is the vibrational number (also integer) and v_m - is its maximum value, previously obtained

and v_m - is its maximum value, previously obtained (Eq. (9.10). If replacing L (1) from Eq. (9.18) by U (1)

If replacing $L_q(1)$ from Eq. (9.18) by $L_q(1)$ given by Eq. (9.20) and expressing the internuclear

change as a function of the vibrational number υ we get:

$$\Delta E = \frac{C_{IG}}{q[[[L_q(1)](1 - \pi \alpha^{x}(\upsilon_m - \upsilon)^{y})] + kL_p]^2} - \frac{2E_q}{q} - \frac{2E_K}{q} - E_X$$
(9.21)

where: k = 0.6455 a coefficient defining the locus position of the proton (Hippoped curve)

The obtained balance difference in comparison to the first and second terms is quite small, so the system reacts in order to restore the accurate balance. This reaction is in a form of emission (absorption) of a photon.

When the energy difference of (9.21) is positive, a photon with the same energy will be emitted. In such way the IG energy balance in the system is restored. So we may consider ΔE as a photon energy. Then plotting Eq. (9.21) in function of v, we try to obtain a best fit to the (0-v) and (1-v) optical transitions sets, by selecting the unknown parameters *x* and *y*.

Fig. 9.23 shows a step-like plot of ΔE in function of v with x = 4, and y = 2, together with the vectors E_0 and E_1 . The argument v is shifted at half step in order the middle of the step to be between the two sets of observation data given by vectors E_0 and E_1 . The vertical scale is drawn reversed in order to reference to energies to the necessary zero level that appears in the top of the drawing (similar as the vibrational curve shown in Fig. 9.15.



Fig. [9.24]. Calculated, ΔE , and estimated vibrational levels by the optical transitions E_0 and E_1 for H_2 ortho-I

The shown vibrational levels are in fact contributed from the momentary balance disturbance from both sides of the equilibrium point of vibration. The energy difference ΔE works symmetrically for positive and negative quantum displacement, so they appear with same vibrational levels as shown in Fig 9.24. Examining the dependence of the obtained plot from the parameter E_X we find that only its vertical position is influenced (it is a same if E_X is included as part of C_{IG}). The best vertical fit is obtained at $E_X = 6.26$ (eV). In Fig. 9.23 this level is shown by a dashed line. The difference between the theoretical plot and the levels obtained by the optical data is shown in Fig. 9.25.



Fig. 9.25. Difference between calculated and experimentally determined vibrational levels

The final expression for calculating the vibrational level of H_2 ortho-I molecule which configuration is shown in Fig. 9.12 is:

$$E_{v} = \frac{C_{IG}}{qr^{2}} - \frac{2E_{q}}{q} - \frac{2E_{K}}{q} + E_{X}$$
(9.23)

 $r = [[L_q(1)](1 - \pi \alpha^4 (\upsilon_m - \upsilon)^2)] + 0.6455L_p$ (9.23.a) where:

 E_{v} [eV] is the vibrational level of H₂ ortho-I molecule, Eq and E_K are given respectively by Eqs. (9.15) and (9.16); r - is the internuclear distance in function of vibrational number v

 $E_X = E_B = 6.26$ (eV).

The good match between the calculated results and experimental data allows to identify the energy levels of H_2 molecule in order to define the position of the vibrational ladder in respect to other experimentally determined energy levels - the binding and the dissociating energies (see Fig. 9.15).

The energy difference between level 0 and $v_m = 18$ obtained by Eq. (9.23) is 4.483 eV. This value is pretty close to the dissociation energy obtained experimentally $E_{DIS} = 4.478$ (eV). The energy difference between dissociation limit and the metastable state is $E_B = E_X = 6.26$ (eV). The binding

energy of H₂ is an accurately measured parameter: $E_{IP} = 15.426$ (eV) (E. McCormack et al., 1989). Then we obtain $E_A = 4.69$ (eV) that corresponds to the distance between the metastable state and the ionization limit.

It is found that the obtained parameter Eq. (9.23) provides exactly the same results if the offset value of 6.26 (eV) is ether a part of C_{IG} expression according to Eq. (9.17) or outside of it as in Eq. (9.23). Accepting the second option, allows C_{IG} factor to be defined independently of its involvement in any molecule and expressed accurately by known physical constants. Determined in such way it could be conveniently used in further analysis for more complex diatomic molecules.

$$C_{IG} = (2hv_c + hv_c\alpha^2)(L_q(1) + 0.6455L_p)^2 \qquad (9.17)$$

$$C_{IG} = 5.26508 \times 10^{-33} \left[\frac{\text{m}^5}{kgs^3} \right]$$
 (9.25)

According J. H. Black and A. Dalgarno, (1976) the excited H_2 by UV radiation (Lyman and Werner system) leads to "fluorecsence to the vibrational continuum of the ground electronic state, thus resulting in two separated atoms". The provided above analysis is in agreement with this concept.

The results obtained by the provided analysis lead to the following conclusions:

(a) The value of C_{IG} factor is pretty accurately expressed by known physical constants

(b) The equation (9.23) shows the IG field balance and its control function on the charge unity and internuclear distance.

(c) The H_2 ortho -I state could be regarded as a bonding structure between atoms in the molecules in case of valence proton without connected to it neutron. (In case of connected neutron - Deuteron Eq. (9.23) is slightly modified - see §9.8)

B. Energy scale ratio and signature about high precision accuracy in the total energy balance

The C_{IG} factor could be considered as a basic intrinsic matter parameter. It involves only an equivalent intrinsic gravitational constant, G_o , (for the mixture of two type intrinsic matter in CL space and in particles) and the intrinsic mass of the proton (or neutron, having in mind that the proton and neutron have exactly the same intrinsic matter, referred in BSM as intrinsic mass). The corresponding factor for Newtonian mass is

 $C_N = Gm_p^2 = 1.866772 \times 10^{-64}$

where: G -is the Newtonian gravitational constant and m_p - is the proton mass. Then the ratio between both factors is:

$$C_{IG}/C_N = 2.8204 \times 10^{31}$$
 (9.25.a)

The ratio (9.26) could be regarded as an energy ratio between the IG field and the Newtonian gravitational field. It indicates that IG energies are enormously large in comparison to the Newtonian gravitation energies. They in fact are responsible for the "infinities" in Faynman diagrams in particle collision experiments.

Having in mind the enormous ratio C_{IG}/C_N , one amazing feature of the H₂ system is apparent: the ability of the system to provide an extremely accurate balance of the total energy of the system.

C. Components involved in the total IG energy balance and the relations between them. Energy balance between IG(CP) and IG(TP) of the system

The extremely accurate balance of the total energy according to Eq. (9.23) leads to one question: *What is the driving mechanism, that is able to provide so accurate balance?* The possible answer is:

This could be the balance between the energy of IG(CP) and the energy of IG(TP) vectors of the whole system, including the CL space and the local gravitational field.

The system possesses self adjustable parameters as: the node distance for the local CL space and the E-field distribution inside the Bohr surface. The effect of Bohr surface integration also should be taken into account (involving synchronization between RL(T) of all FOHSs of the protons and the interaction of this commonly synchronized system with CL nodes).

In such aspect, it could be considered that the mechanism providing the accurate energy balance of Eq. (9.23) is defined by the balance between the IG(CP) energy and IG(TP) energy of the whole system. In Chapter 2 §2.9.6.B it was accepted a priory, that the energy balance between both type of

intrinsic energies in CL space is expressed by the equation:

$$E_{IG}(TP) = 2\alpha E_{IG}(CP)$$

where: α - is the fine structure constant

This acceptance is successfully validated in §9.15.2 for derivation of total energy balance of simple diatomic molecules.

Analysing logically, let try to find to which of both IG energies anyone of the energy terms in Eq. (9.23) is related and also to shed a light on the IG energy involvement in the unit charge definition.

The term of Eq. (9.23) containing C_{IG} originates from E_{IG}, whose derivation was based on Eq. (9.13) with the presumption, that it is related with the IG(CP) field. According to Eq. (9.14) it supplies the energy for the proton electrical charge. Additionally, according to Eq. (9.23) it is able to regulate the proximity E-field of the proton (quantum quasishrink effect). In a same logic we can accept that it is involved in regulation of the E-field inside the Bohr surface of single not connected proton defining in such way the unite charge of the proton. In the latter balance, however, the IG(TP) field may also be involved. The unit charge according to BSM concept could not be defined without CL space environment with its CL node dynamics. Then we arrive to a conclusion that the following components may be involved in defining the unit charge:

IG(CP) field IG(TP) field CL space parameters

D. Range of vibrational motion of the protons in H_2 molecule

The range between min and max internuclear distance for analysed H2 molecule is obtainable directly by Eq. (9.23.a) if substituting v with v_m and with zero and take the difference. Having in mind that that the v = 0 is in the middle of the vibrational range, the obtained expression for the vibrational range is

$$\delta r = 2\pi \alpha^4 \upsilon_m^2 L_q(1) \tag{9.26}$$

For $v_m = 18$ the range of vibrations is only $\delta r = 7.866 \times 10^{-16}$ (m).

The obtained range is even smaller than the thickness of the proton core $t_p = 0.784 \times 10^{-12}$ m. However, the result is reasonable, when taking into

account, that the oscillating range is a few electronvolts, while the involved IG field energies are in megavolt range.

The analysis of diatomic molecules with discrete spectra presented in BSM_Appendix9_1 also shows quite small vibrational range in a length scale. This means, that the vibrational motion does not involve significant inertial interaction with CL space involving displacing and folding of CL nodes. Then for a practical considerations we may assume that the internuclear distance is unchanged. The rotational motion and its anticipated energy however exist. The negligible vibrational range in comparison to the internuclear distance allows to facilitate the theoretical analysis by the following considerations:

(a) The system does not spend vibrational energy for inertial interactions between the nuclei and the CL space, but only rotational. The transitions between different levels are pure quantum mechanical transitions related to the quantum quasi-change (space) effect.

(b) The system energy E_{SYS} could be accurately calculated, by operating with the parameters of the free (external) CL space including the length scale.

(c) The lack of detectable time delay in the Ramman process obtains a physical explanation.

The conclusion (b) has been already confirmed by calculation of E_{SYS} by Eq. (9.4) and compared with the value known as Average kinetic energy 15.98 (eV).

The conclusion (c) is confirmation of the discussion analysis about the Ramman scattering provided in §9.5.8.

The derived model of H_2 ortho-I could be regarded as one valence bonding system between two atoms. In many atoms, however, the valence connections involves Deuterons structures instead of protons. So it is necessary to obtain a similar equations between two Deuterons.

Summary

- The Intrinsic factor for IG(CP) forces between IG masses of two protons is derived
- The derived energy balance equation (9.23) provides a model of single valence electronic bonding system involving valence protons.

The bonding connection can be identified by analysis of the optical and PE spectrum.

- The process of photon emission or absorption is related with the momentum imbalance of the total energy of the system involving IG filed components.
- The size of the vibrational range estimated in external CL space is very small. This fact facilitates the task for estimation of the system energy, that for H_2 molecule matches the value of E_{VIP} potential (average kinetic energy). It also helps finding the spatial configuration of the molecule, by using the dimensions of the proton and the particular quantum orbit that have been defined in a normal CL space (ignoring the quantum quasi-change effect).

9.8 D₂ ortho-I molecule as a single valence bonding system in molecules.

Most of the atoms contain Deuterons in the external valence shell instead of protons. Some heavier atoms contain Tritii.

It is quite logical to expect, that the D_2 will have similar oscillating behaviour, as H₂, but modified by the two neutrons. The neutrons are over the saddle point of each proton so the internuclear distance between the protons and deuterons is one and a same. Logically thinking the both deuterons will affect the degree of the quantum quasishrink space in the integrated Bohr surface. Consequently we may try to use the derived for H_2 molecule, Eq. (9.23), but searching for a proper correction factor for the term Δ^2 . This correction will affect the curvature. Another correction, affecting the vertical position of the vibrational levels should be related with E_B for D_2 . The C_{IG} factor obtained by H_2 model, however is intrinsic IG field parameter and should be used without change for D_2 case. So the second correction should be independent of C_{IG} factor.

The procedure is exactly the same as for H_2 and no need to be described in details. It is useful to show the PE spectra of D_2 and H_2 at one and a same observational conditions. Fig. 2.29 shows PE spectra of H_2 , HD and D_2 obtained at one and a same observational conditions (pressure and temperature) provided by J. E. Pollard et al. (1982). The optical spectrum provided by H. Bredohl and G. herberg (1973) denoted as Lyman band of Deuterium, matches the spectrum of D_2 ortho-I (according to BSM).



The 584 A photoelectron spectra of H_2 , HD and D_2 expanded from 200 Torr at 77K. (courtesy of J. E. Pollard et al. (1982)

By PE spectrum we obtain:

 $E_{VIP} = 21.23 - 5.05 = 16.18 \text{ eV}$. The identification of E_{VIP} only by the most populated bands of the optical spectrum for D₂ is not so obvious as in the case of H₂. But using the simultaneous signature of the vibrational levels in the PE and optical spectra, the identification of E_{VIP} level is still possible. If assuming that the Energy level E_B is close to the same energy level for H₂, then we have:

16.18-6.26 = 9.92 eV. Using the observed data presented by H. Bredohl and G. Herzberg, (1973), the obtained energy corresponds to the mean energy value of optical (0-4) and (1-4) transitions. The available observed spectral data are from (0-3) to

(0-10) for (0-v) set and from (1-3) to (1-12) for (1-v) set.

Following a procedure similar as for H₂, it is found that the optical transitions that match better the PE spectrum are again from (0-v) and (1-v) transitions. The largest vibrational level identified by PE spectrum matches well the identified optical transitions. In order to obtain a best fit between the optical transition sets and the calculated data, the Eq. (9.23) is used but with correction factors for the curvature (multiplying factor for the term $\alpha^4 \pi (\upsilon_m - \nu)^2$) and for the vertical positions value of E_X. The both correction factors are obtained by tuning of the calculated vibrational curve to the energy levels identified by the optical spectrum of D₂.

The obtained equation for the quantum vibrational levels for D_2 ortho-I state is:

$$E_V(v) = \frac{C_{IG}}{qr^2} + 6.235 - \frac{2E_q}{q} - \frac{2E_q}{q}$$
(9.27)

$$r = [[L_q(1)](1 - 0.5\pi\alpha^4(v_m - v)^2)] + 0.6455L_p \qquad (9.27.a)$$

where: C_{IG} - is given by Eq. 9.25;

 E_q - is a charge energy defined by Eq. (9.15) and E_k is the electron kinetic energy, given by Eq. (9.16).

The energy 6.235 eV is distinguished from the corresponding energy of 6.26 eV (for H_2) only by 0.025 (eV).

0.5 - is a correction factor for curvature.

The correction factor of 0.5 is reasonable if taking into account that every proton has a neutron in its saddle. This neutron may influence the strength and range of the quantum quasi-change effect (length scale) causing an extended vibrational curve with different curvature.

The deviation Δr from the equilibrium point for D₂, derived in a similar way as for H₂ (see Eq. 9.26) is given by the equation:

$$\delta r = \pi \alpha^4 v_m^2 L_q(1) \tag{9.28}$$

We see that the vibrational range for D_2 is twice smaller than for H2 molecule, due to the factor 0.5 that affects the curvature of the vibrational ladder. This is reasonable if taking into account that the internuclear distance will be little bit smaller and the effect of highly nonlinear IG forces is stronger.

The plot of calculated vibrational levels by Eq. (9.27) together with identified levels from op-

tical spectrum in UV range of D_2 are shown in Fig. 9.30.



Theoretically calculated by Eq. (9.27) vibrational levels (step line) and experimentally determined vibrational levels involved in (0-v) and (1-v) transitions (daimon points) for D₂ Lyman bands