

Quantum-mechanical aspects of the L. Pauling's resonance theory.

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Abstract: The L. Pauling's resonance theory analyzed using principle of quantum superposition, that is the principle of superposition "wave function", which is the main positive principle of quantum mechanics. The principle of quantum superposition is essentially a basic property of the wave function. By example of benzene molecule is shown that the principle of quantum superposition, and hence the quantum mechanics in general is in insurmountable conflict with the resonance theory.

Keywords: L. Pauling's resonance theory, benzene, the principle of quantum superposition, quantum mechanics, the superposition of "wave functions", the wave function.

INTRODUCTION.

The basis of mathematical apparatus of quantum mechanics constitutes assertion that the state of a quantum system can be described by a certain function of the coordinates $\psi(q)$ called a wave function (the square of the modulus of this function determines the probability distribution of coordinate values) [1]. In the L. Pauling's resonance theory [2, 3], the wave function ψ is used to describe the distribution of electrons in molecules and especially illustrative is example of benzene molecule. Therefore, the resonance theory (on the example of the benzene molecule) can be analyzed from the point of quantum mechanics using the principle of quantum superposition.

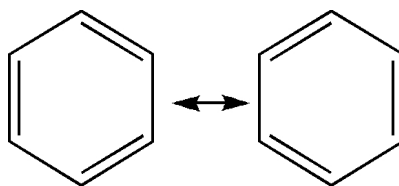
RESULTS AND DISCUSSION.

For example, consider two quantum states (actually existing) are described by wave functions ψ_1 and ψ_2 . From the principle of superposition [1, p. 21] it should be clearly, that their linear combination ($\psi_3 = C_1\psi_1 + C_2\psi_2$) will be the third quantum state (as actually existing), which will be described by a wave function ψ_3 . What does it mean? The fact that the measurement of a

certain physical value d in the state $|\psi_1\rangle$ will result d_1 , and for measure a value for of d in the state $|\psi_2\rangle$ will result d_2 . When the third quantum state $|\psi_3\rangle$ is realized, then when measuring a physical quantity, the quantum system will take the values d_1 and d_2 with probabilities, respectively, $|C_1|^2$ and $|C_2|^2$. That is, in a quantum state $|\psi_3\rangle$ when we will have many dimensions sometimes d_1 value and sometimes d_2 (with certain known frequency). But this is in resonance theory can not be.

We describe for simplicity resonance of two Kekule structures (resonance structures) excluding structures Dewar. Then, the resonance theory it is assumed that $|\psi_1\rangle$ is a quantum state 1, which is describes a resonance structure 1 and $|\psi_2\rangle$ is a quantum state 2, which is describes a resonance structure 2.

Wave functions ψ_1 and ψ_2 for the resonance structures 1 and 2 (Kekule structures):



The linear combination of the ($\psi_3 = C_1\psi_1 + C_2\psi_2$) is normally the third quantum state $|\psi_3\rangle$, which is described by a wave function ψ_3 and will describes the actual benzene molecule (resonance hybrid). The coefficients C_1 and C_2 will specify the contributions of resonance structures (Kekule structures, for our case $C_1/C_2 = 1$, $|C_1|^2 = |C_2|^2 = 0.5$) in a real molecule of benzene (resonance hybrid), which can not be described by separate resonance structures. And now it is important to note that the real molecule of benzene it really real and unique, and can not have a discrete description, ie the measurements we will never "see" the one Kekule molecule (resonance structure 1), then another (resonance structure 2), and this is directly contrary to the principle of quantum superposition. Moreover, adopted in theory of resonance Kekule structure, ie resonance structures are ideal structures that do not exist in reality, because they have all the bonds are equal, and this is despite the alternation of single and double C-C bonds, which in reality are different length. Therefore, the principle of quantum superposition (for resonance theory) is not executed,

even for quantum states $|\psi_1\rangle$ and $|\psi_2\rangle$, because as resonance structures is not reality, and any physical quantity (real) we can not measure.

If, however, as the resonance structures we take the real "curved" Kekule structures with ties that have different lengths, then the resonance theory does not make sense, since the transition from one structure to the other will vary internuclear distance. But then the principle of quantum superposition is applicable to all three quantum states (for $|\psi_1\rangle$ and $|\psi_2\rangle$ it is obvious, and for $|\psi_3\rangle$ will be the one "twisted" Kekule structure, then the other, at 50 : 50). In fact, no change bond lengths have therefore chemistry is not applicable.

Especially notice, that resonance structures (Kekule structures with the same C-C bonds) is not electronic tautomers. Real benzene molecule is unique and no tautomerism exist. Incorrect represent benzene molecule as transitions between electronic tautomers (electrons in benzene does not migrate from one bond to another). There is a single benzene molecule, which has a constant electron distribution in time and which can not be represented by a discrete description. Therefore, it is accepted in resonance theory that every resonance structure contributes to the a real molecule (resonance hybrid) (usually chemists determined the contribution by the "eye"). And the third quantum state $|\psi_3\rangle$ describes the real benzene molecule, which represents something between a resonance structures (remember the contribution of each resonance structure to the real structure (resonance hybrid)).

CONCLUSION.

By example of benzene molecule is shown that the principle of quantum superposition, and hence the quantum mechanics in general is in insurmountable conflict with the resonance theory. And so the assumption is that real benzene molecule (resonance hybrid) that is a cross between a resonance structures is genius chemical assumption, though not strictly from the standpoint of quantum mechanics, but that made it possible to qualitatively and quantitatively describe the benzene molecule, which could not represent a single formula. This example clearly shows that in

fundamental matters of chemistry did not reducible to physics, here there is a "chemical" highlight. And yet, the same L. Pauling's resonance theory literally changed the chemistry, had a profound influence on the minds of chemists (I'm not talking about the pedagogical impact of resonance theory), and for a long time is not a textbook on organic chemistry where there are no resonance theory. Nevertheless it should be noted that when complication of the molecule (pyridine, naphthalene, anthracene, and so on) quantitative calculations becomes difficult (for the correct calculation of naphthalene is necessary to consider of about 40 resonance structures) and therefore started to use the MO method.

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