UCRL- 87544
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UCRL--C7544 MASTER

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The Jahn-Teller Effect: Its Hiistory and Applicability

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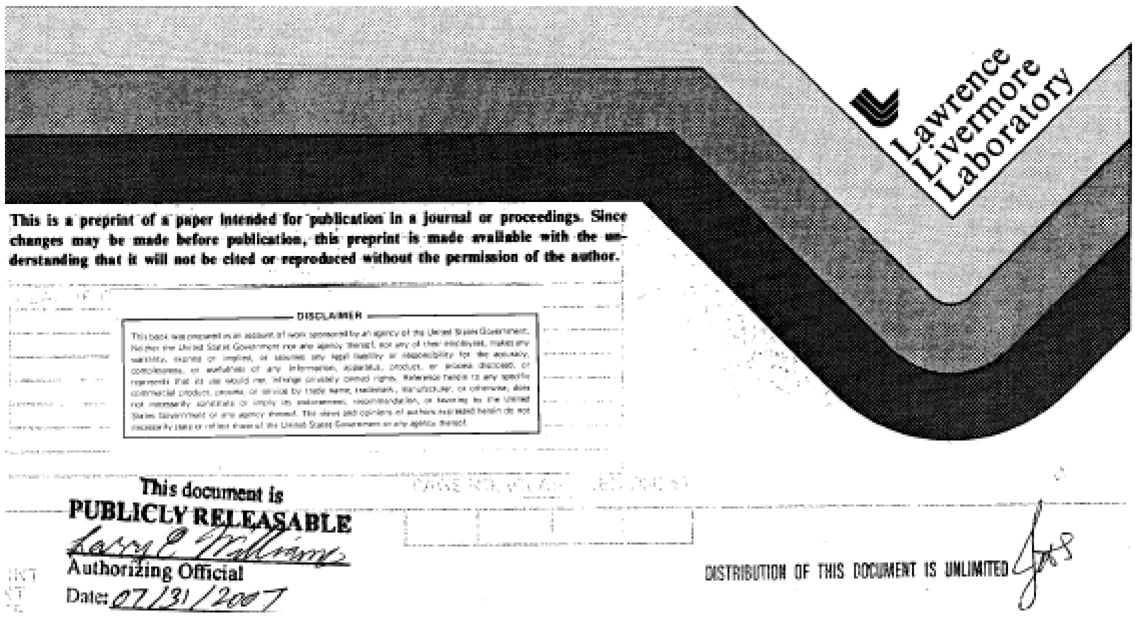
This paper was presented at 10-th International Conference

on Group-Theoretical Methods in Physics

The University of Kent at Canterbury, Great Britain ,August 31, 1981



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THE JAHN-TELLER EFFECT: ITS HISTORY AND APPLICABILITY

Abstract

The interactions between Teller, Renner, Jahn and Landau which led to the formulation of the Jahn-Teller effect are discussed. The applicability of Jahn-Teller type of theory to superconductivity and the explanation proposed by the use of Goldstone particles are assessed.

I'm afraid I am about to expose you to a multiple disappointment. My talk is going to have relatively little to do with the announced topic. It differs from many previous topics in that I hope it will be understood by everyone except possibly the speaker. I would like to say a few words about the origin and history of my all-too-brief cooperation with Professor Jahn. As far as I know (for I don't know what was in Jahn's mind), our collaboration had its origin in a rather straightforward paper that one of my students, Rudolph Renner, wrote in Gottingen shortly before Hitler took over. After that, I had to leave Germany and went to Copenhagen for a year. I am still very grateful that I was able to come to this country (Great Britain) following that time. During the war, Renner became involved in weather prediction, and he never returned to physics -one of the casualties of the war.

The topic of Renner's paper was the CO_2 molecule--three atoms on a straight line. This molecule can bend, and any given bent conformation can be described in terms of independent bends in .two mutually perpendicular planes. This then is a doubly-degenerate vibration of' the simplest kind. That is how simple group theory was in those days.

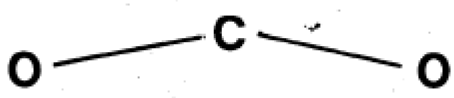

Fig. 1. The C02 molecule in a bent configuration-the

simplest example of a degenerate state.

However, there was a little difficulty. Electronic excitation of the CO_2 molecule into a degenerate state will, of course, split the degeneracy by the vibration. The splitting turns out to be quadratic in energy: the equilibrium configuration may remain in a straight line. If the carbon now rotates against the two oxygen atoms because of the degeneracy, the electrons must rotate with it. The Born-Oppenheimer separation between electronic and nuclear motion becomes disturbed, and the breakdown of the simple harmonic oscillator picture produces a much more complicated spectrum.

A few months after Renner finished his work, I was in Copenhagen and met a young Russian physicist who unfortunately is no longer with us, Nobel laureate Lev Landau. Although the Jahn-Teller theorem did not exist at that time, he told me about it. He said that a symmetric polyatomic molecule in a degenerate electronic state would lose its symmetry. I disputed this idea by virtue of Renner's successful Ph.D. thesis. After a little discussion, Landau, who was somewhat stubborn, gave in.

A further few months later, I came to London and looked for further exceptions to Landau's hypothesis. I met Jahn and discussed the problem with him. Jahn had the ability to get very busy indeed, and in a very short time, he showed that the Jahn-Teller theorem is valid for all molecules except those in which the atoms lie in a straight line. In the case of twofold degeneracy based on spin (or as Eugene Wigner likes to say, based on time inversion), there is no effect, while four- and sixfold degeneracies can be split down to the twofold but no lower.

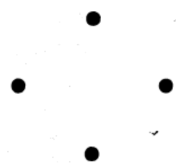

Fig. 2. Square configuration of a tetratomic molecule.

Now to offer an example of the Jahn-Teller theorem. Assume a non-existent tetratomic molecule such as is shown in **Figure 2**. In this case, electronic states can have a twofold electronic degeneracy. When this happens, they possess a quasi-angular momentum which can go to the left or to the right. Their wave functions proportional to exp(±inϕ). If there is no such degeneracy, the configuration of the square can be stable. Because it it symmetric, the potential energy will be symmetric about the minimum (see **Figure 3).** Assume a vibration of the type shown in **Figure 4**.

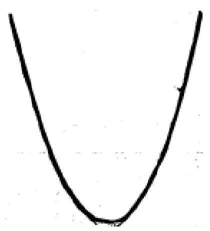

Fig. 3. Symmetric potential energy function. The vertical scale represents energy and horizontal displacement.

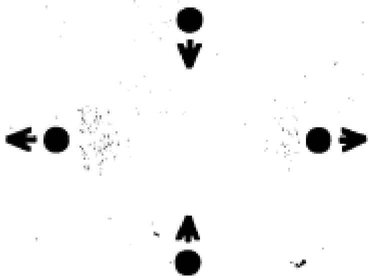

Fig. 4. Jahn-Teller active vibration of a square tetratomic molecule.

In this case, the pair of wave functions exp(±inϕ) will split into cosnϕ and sinnϕ which no longer have the same energy and instead have a potential of the form shown in **Figure 5**. same energy and instead have a potential of the f9rm shown in Figure 5. The two new equilibrium configurations are the rhombus (see Fig. 6) and the rhombus obtained by rotating this figure through 90^o.

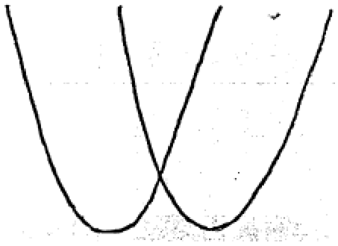

Fig. 5. Schematic form of the potential energy function for a double – degenerate electronic states suffering from Jahn-Teller splitting.

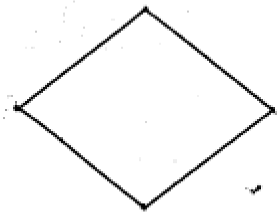

Fig. 6. Equilibrium configuration of a square tetratomic molecule which has undergone a Jahn-Teller distortion.

That is essentially all I have to say for my main talk. I have now arrived at the limits of my knowledge and can take no responsibility for what follows. If I had stayed in Britain, I would-have this with Jahn, but as it was, I didn't, and nothing came of it. Among chemists and spectroscopists, the theory has very wide application, e.g., to complicated molecules, such, as SF_6.

The interesting case for me is not the case of a degeneracy but that of a **near degeneracy**. In this case, there is not an exact coincidence of two or more energy levels, but there are infinitely many levels in a very narrow energy range. This occurs at the surface of the Fermi distribution in any metal. One should have (and I did have) the suspicion that such levels should be split. They do indeed split and produce crystals of lesser symmetry. Bismuth, for example is nearly symmetric but is disturbed by the Jahn-Teller effect. This is a somewhat trivial application.

A much more interesting application which has been discussed in the meantime is found in the very strange phenomenon of superconductivity. Although the application was completed by different methods, they were not necessary in order to demonstrate this application. In this case, the manner in which energy levels split is a little different from the one I just described. There are still infinitely many energy levels in a narrow range, but an energy gap can occur which can be related to the phenomenon of superconductivity.

For the Jahn-Teller effect to occur, displacements must give rise to interactions. I was looking in the right direction to explain superconductivity, but I did not recognize the kind of interaction which produces superconductivity. This type of interaction, which is somewhat peculiar, is connected with the energy states of the electrons. The repulsion between the electrons did not manage to produce an effect like superconductivity. The real trick was the fact that at somewhat greater distances, the electrons effectively attract each other. They distort the lattice, and this pair-wise attraction is more successful in distorting the lattice. Coupled with the phenomenon I have just described, we have the basis for superconductivity.

Now, to culminate this portion of my talk, I am going to talk about something which I'm not sure anybody including myself understands. In nature, particularly in group theory, we are interested in symmetries. It turns out that there are lots of symmetries, not all of which are perfect. There is no exception to this in the Jahn-Teller effect. In a degenerate state such as those which abound in rare-earth salts where the f-electrons are only slightly coupled to the lattice, a deviation in symmetry produces slightly separated minima.

In the theory of strong interactions, we have right and left symmetry. The weak interactions (which are only weak at “low" energies up to a GeV) may also be included for consideration of symmetry. However, these no longer have right-left symmetry at higher energy levels except when accompanied by an interchange of positive and negative charges. In the limited region which is accessible to us for study by β-decay, the violation of symmetry is weak. This is not true in general.

We may never be able to see the violation, of time-reversal symmetry on a microscopic scale. Why should nature want to be symmetric, and then, at the last moment, make up its mind not to be symmetric? One attempted explanation is to postulate Goldstone particles-particles of zero mass. According to Einstein, the creation of a particle is connected with an energy increase of mc^2. But think of particles with zero mass. The energy derived from putting such particles into a vacuum is nearly zero. Assume some interaction between Goldstone particles or between them and another particle. Then the original state of symmetry associated with the idea of a vacuum no longer be valid. There will be very many states of low energy. If there is an interaction, a state of symmetry could occur which is lower than that of the ideal vacuum. One can imagine a small deviation from symmetry. In the case of an up-and-down quark which in an ideal state may have equal energies, the difference of energies and thereby the deviation from symmetry could be quite marked.

Obviously I have talked about topics beyond the ideas on which Jahn and I collaborated. However, many of these are connected with the principles of the very simple examples with which Jahn and I amused ourselves.

References

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