

APPEAL TO CHAIRMAN of DAE

Krakow, 18.02.1999

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The Chair of Div. Ass. Editors
via
DAE, Prof. Z. Fisk
via
Editor of Phys. Review Letters

LE6925: Relativistic effects in the electronic structure of $3d$ -ion

Dear Professor,

In the answer to a letter of the Editor of PRL of 12.01.1998 containing the negative decision of Divisional Ass. Editor (Dr Zachary Fisk) concerning my paper:

Relativistic effects in the electronic structure for the $3d$ paramagnetic ion (LE6925)

I put the appeal to the Editor-in-Chief of the APS with information to the Chairman of the APS.

I have large respect to Dr Z.Fisk. I would like to keep this respect to Dr Z.Fisk but the report of 12.01.1998 is unjust and unfair. I cannot believe that it was written by Dr Z.Fisk. I expect that it was signed by Professor only. Thus, I ask you to reconsider that decision.

I repeat conclusions of my paper: the relativistic effect of the spin-orbit coupling has enormous influence on the low-energy electronic structure of the $3d$ magnetic ions and consequently on electronic and magnetic properties of $3d$ -ion compounds at low- and the room-temperature region. This temperature region is of great importance for the solid state physics.

The argument of DAE that presented result by me "do not appear to be useful, in the sense that might explain phenomena in particular 3d systems that have not been understood" is completely unjustified.

Writing that "the effects predicted occur at small energies and no case has been made by the author that they influence importantly the physical properties of a know system" indicates on, saying delicately, a bad altitude. Already in the abstract is written "these states affect electronic and magnetic properties at low and room-temperature regions". Secondly, in my paper the applicability to Ni^{2+} compounds, to the spectroscopic g factor, is discussed. The derived magnetic moment of the Ni ion of 2.15-2.20 μ_B is in very good agreement with experimental data. I point out that it was calculated from the microscopic Hamiltonian in papers up to now it is a simply assumed value. Next example has been given for the Fe^{2+} ion impurity in MgO. The values for the separations like $E_g - T_{2g}$ are consistent with the optical experiments.

Coming to the objection of "small energies" I say that these small energies are just the energies studied in solid-state physics, i.e. energies below 25 meV corresponding to low and room temperatures. In this paper the consequences of my calculations have not been discussed due to the length problem. They are the subjects of earlier papers submitted to Phys. Rev. Lett. LA6485 and next papers BFK631, LL6379, LL6530. But, in fact, I have expected that the consequences of such energy levels are easily deduced by the physicist. It turns out that it is not the case. On other side when I wrote more elementary paper like "Influence of spin-orbit interactions on the cubic crystal-field states of the d^4 system (LA6567) [Acta Physica **9-10** (2007) 46] it was refused as being known or/and too simple. So, this DAE referee report should be taken as the proof that the knowledge about the CEF effects in 3d ions is very low. Dear Editor, please remember it for the discussion of my next papers.

Dear Professor Fisk. If you are really interested, where my results can be applicable I can say that in FeSi, for instance. You are co-author of a paper in Physica B **206-207** (1995) 810 about FeSi. You have found absorption lines at about 200, 300 and 770 cm^{-1} . Looking at my results given in Fig. 1 for the d^6 system I am pretty sure that they should be attributed to lines detected by you. For the purely cubic Fe surroundings excitations should be grouped about 300K and 750K (2λ and 5λ ; $\lambda = -150\text{K}$ in Table). ($1\text{cm}^{-1} = 1.44\text{K}$). These values are close to the observed by you values of 290K, 460K and 1130K. The off-cubic local symmetry in FeSi will extra spread these my 15 states. This is in agreement with more accurate studies of Damascelli *et al.* (Physica B **230-232** (1997) 787) who manage to reveal more lines. My CEF theory expects up 14 lines, thought some of them could be forbidden.

Although those authors and you have attributed these lines to phonon excitations I think that the theory, providing excitations in this energy region, cannot be ruled out without checking.

I am convinced that these results will be applicable to many, many $3d$ oxides. There are a number of my papers submitted to PRL and PRB about LaMnO_3 , LaCoO_3 , NENP, Haldane Ni compounds, the Jahn-Teller effect showing results of my theory to these particular compounds. And results are very beautiful.

In conclusion: I ask for publication of my paper that presents another point of view on very important problems of magnetism and electronic structure of $3d$ ions. It allows normal scientific and open discussion.

Sincerely Yours,
R. J. Radwanski

Technical remarks:

I have revised my original paper improving English and the reading fluency. The paper is prepared in the .tex file and is attached to this email. Please note, that Z. Ropka appears as the co-author (from Acknowledgements). The scientific content of the paper is the same in order not to be accused for an improvement during the referee process. The paper has been appended with "Note added during the referee process" in order to clarify the doubts of DAE. The figure 2 has been removed as it was shown for comparison reasons.

Table 1 and Fig. 1 are the same as original they are not prepared yet in .tex file. I hope I manage to do it in the nearest future. I expect your cooperation in Science.

R. J. Radwanski

REJECTION BY CHAIRMAN of DAE Jack Sandweiss

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15 July 1999

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Dear Dr. Radwanski:

I am writing in connection with your manuscript "Relativistic Effects..." LE6925, submitted to Physical Review Letters. As you know, appeals beyond the level of the Divisional Associate Editor are handled by the Editor-in-Chief, Dr. Martin Blume. However, Dr. Blume evaluates the appeal solely on the basis of the correctness and fairness of the procedures used in reviewing the paper. If I am convinced by the arguments presented I accept the manuscript for publication in Physical Review Letters. If not, I may forward the appeal to Dr. Blume.

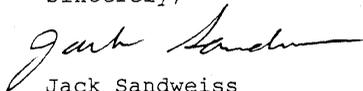
However, as a matter of practice, I review all such appeals in my capacity as Editor and Chairman of the Divisional Associate Editors. In this way, your letter of 18-February-99 has come to my attention and I have studied the manuscript and the associated correspondence. Unfortunately, I have decided that the manuscript is not appropriate for Physical Review Letters.

I do think that you have carried out an interesting calculation and that the relativistic effects of the electron motion, in the case you have studied, via the spin-orbit interaction, are important aspects of atomic physics. However, that such effects are present is not, at this time, surprising. Nor do the effects overturn in, any basic way, our understanding of systems you have studied. In my opinion, the best course of action would be for you to write a more complete description of your calculations and submit the enlarged paper to a more specialized journal.

In this way, your work would become known, and appreciated, by the physicists who are working in this and related areas. For example, one of the major motivations of the search, and study, of the transuranic uranic elements is the increasing influence of relativistic effects on the behavior, and chemistry of these elements as the charge of the atomic nucleus becomes greater. A more complete, comprehensive article describing your work would be much more likely to "reach" physicists in this field than would a brief letter, which would not have sufficient general interest to be appropriate for Physical Review Letters.

Since your appeal is not based on a procedural aspect, I am not forwarding it to Dr. Blume. You may of course, appeal to Dr. Blume but in my opinion, such an appeal is not likely to be successful.

Sincerely,



Jack Sandweiss
Editor and
Chairman of Divisional
Associate Editors
Physical Review Letters

JS:sc