The scientific bet for 1 million USD for "Orbital moment in NiO"

11 Jan 2000

From: sfradwan@cyf-kr.edu.pl
To: prl@aps.org
Subject: report LF7313 Radwanski (bet to dr Bron)
Date sent: Tue, 11 Jan 2000 16:07:01 +0100

From R. J. Radwanski
To: DAE, Dr W. E. Bron
Editor of PRL

Concerns: LF7313: "Orbital moment in NiO"
by R. J. Radwanski, Z. Ropka nad R. Michalski

Dear W. E. Bron, DAE of Phys. Rev. Lett.,

In my email of 14.12.1999 I have proposed to you the scientific bet for 1 mln USD from your side and 300 USD from my side about the importance of crystal field and spin-orbit coupling in description of NiO.
By this I confirm this bet and take the Editor as the executor of this bet.
I hope that you take the full responsibility for your decision as I am.

Sincerely Yours,
Ryszard Radwanski and Z. Ropka

PHYSICAL REVIEW LETTERS

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JACK SANDWEISS
Editor and Chairman
Divisional Associate Editors

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25 January 2000

Dr. R.J. Radwanski
Center for Solid State Physics
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Re: Orbital moment in NiO

By: R.J. Radwanski LF7313

Dear Dr. Radwanski:

I am writing in connection with your manuscript "Orbital Moment in NiO" LF7313, 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 manuscript.

However, as a matter of practice I review all such appeals in my capacity as Editor and Chairman of the Divisional Associate Editors. 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.

In this way, your e-mail of December 14, 1999 has come to my attention and I have studied the manuscript and the associated correspondence. After reading your responses I did decide that additional expert consultation was needed and I have now obtained a further careful analysis of the manuscript. The attached material is from the new referee. Unfortunately, I am now convinced that the manuscript is not appropriate for Physical Review Letters.

Since your appeal was not based on a procedural matter, I am not forwarding it to Dr. Blume. You may, of course, appeal to Dr. Blume if you wish. However, 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

Attached to negative decision of Chairman
of DAE Dr Sandweiss of 25.01.2000

Report of Referee D
on LF7313 "The orbital moment in NiO"

The model used by the authors is quite simple.
Overall, the description in the paper of what is actually done is poor. Starting from their assumption of a d^8 configuration, they only consider the lowest lying multiplet, ^{3}F. (In their second response to Yeung [Referee B], the authors argue that they don't need to do a full calculation - "it is not my business" - so I assume they didn't include the states from the higher multiplets. If they have, they don't give enough information about the calculations; at a minimum, the Slater F^2 and F^4 integrals would be needed.) I didn't have tables of the experimental Ni multiplets handy, but the ^{3}P state is probably on the order of 1 eV higher (based on multiplets of similar materials). With their claim (resub 10/20) that the crystal field splitting is 2.16 eV, this approximation is suspect.

Given these approximations, the authors then add in a term into the Hamiltonian, Eq. (1), that includes crystal field and spin-orbit effects. The first term in Eq. (1) has a normalization that yields an effect 1000 times (!) as large as B_4; I'll assume that the authors did this correctly, although the numbers don't seem quite correct to me. This term will break the degeneracy of the ^{3}F states into state compatible with the cubic symmetry. In solids, because of inversion and/or time-reversal symmetry, orbital moments are quenched. To get an orbital moment, the symmetry between m_l and $-m_l$ must be broken; the spin-orbit term does that. This fact is well-known and in text books, even if not generally appreciated. The authors get a spin moment of 1.99 (would expect 2 for ^{3}F state without spin-orbit). The value of the orbital moment will depend on the splitting of the different sublevels due to the parameters chosen in Eq. 1. I don't know if the parameters used, especially B_4, are reasonable, and the manuscript doesn't present compelling arguments either. (The spin-orbit term supposedly comes from some book, so perhaps that is reasonable.) However, I don't

doubt that a certain set of parameters will give the results listed. If one is doing a model calculation, it would be easy and useful to show how the results depend on the input parameters; the authors should have done this.

Up to this point, there is no contact made with the antiferromagnetic ordering of NiO; everything is single atom. Eq. 2, is a very simple way to couple the spins on different sites, basically using a semi-classical dipole-dipole interaction, with all the spins antiferromagnetically aligned. (The inter-site term should be $m_i.m_j$, where i and j are different sites. For translationally invariant AFM systems, the nearest neighbor m_j = - m_i, thus yielding Eq. 2.) This approximation ignores all the details of the electronic interactions that give rise to the coupling. (This is the basis for Yeung's comments about super-exchange, etc.) The authors point out that the orbital moment is increased by a factor of two compared to the single atom case. While the authors don't explain WHY, the answer is simply that H_{d-d} adds another L.S term:

$$m \cdot m = (L + g\ S) \cdot (L + gs) = L^2 + g^2\ S^2 + 2g\ L \cdot S$$

with a coefficient basically the same size as λ_{s-o}, i.e., -46 meV compared to -41 meV. (I *think* I did the conversion correctly; the fact that the orbital moment is twice as large suggests that this is correct.)

The authors' model is quite simple and the results will depend on the parameters chosen. Important quantum effects are completely ignored. The utility of such a model is not in getting accurate numbers, but rather in giving new insight into the physics of the system; in my opinion, the authors have failed to do so. The authors argue that including spin-orbit is necessary and that this is an important point of the paper. I would claim that the effect of spin-orbit in generating orbital moments (and determining magneto-crystalline anisotropy, for example) is well-known. Moreover, if the authors set λ_{s-o} to zero in their model, but kept eq. 2, they should also get an orbital moment. Again, in my opinion, I don't think there is anything of significance in the paper beyond what is already known, even if this exact calculation has not been published previously. Having a simple model just because it is simple is not sufficient; there must be new insight gained.

My feeling is that even if the manuscript were rewritten, this is not a paper that would have any impact in the field; it would just be ignored.

RJR Answer to Chairman of PRL-DAE dr J. Sandweiss and Answer to the referee report D

1 Febr 2000

From: sfradwan@cyf-kr.edu.pl
To: prl@aps.org
Subject: appeal LF7313 Radwanski (Sandweiss)
Copy to: blume@aps.org
Date sent: Tue, 1 Feb 2000 18:29:06 +0100

From R. J. Radwanski
To: Chairman of DAE of Editor of PRL
Jack Sandweiss

Concerns: LF7313: "Orbital moment in NiO"
by R. J. Radwanski, Z. Ropka nad R. Michalski

Dear Chairman of DAE of Phys. Rev. Lett., J. Sandweiss

In the answer to your letter of 25.01.2000, just obtained by post, with the negative decision about a/m paper I challenge your referee (D). Although I appreciate very high referees of PRL I maintain that it is the next referee that is wrong, not me. It proves that our paper is really important.
At beggining I have three remarks:
1. I hope that the main goal of PRL is to serve the scientific community in order to search the scientific truth,
2. I hope that PRL assures the honest scientific treatment, if so, how I have the possibility to inform the scientific community about the problem - can I publish payed 1 page announcement, otherwise nobody takes the real responsibility for these erroneous referee reports,
3. Why so sophisticated scientific discussion is going in letters not in open? I consider it as the violation of fundamental scientific rules.

Next, please be informed that I have made the scientific bet with DAE W. E. Bron for 1 million USD and according to me this bet is established already (11.01.2000). It is the real responsibility -however I would like to announce it for the stronger obligation for both sides.

Coming to the referee report D.
I appreciate it.
I fully understand all arisen arguments.
And I do not agree with his thinking.

I fully agree that "the utility of such a model is not a getting accurate numbers, but rather in giving new insight into physics of the system" and I draw completely opposite conclusion. Exactly, my model provides new insight. I could say that it is so new that 4 experts of PRL cannot see it. The new insight is seen in a number of papers waiting for publication in PRL (the referee is not aware of them) that offers "new insight" for a great number of important presently problems of 3d magnetism.
I do not agree that "important quantum effects are completely ignored." Nonsense. Just the essence of my theory is that in a solid 3d ions preserve much of their atomic-like properties what reflects in the existence of the discrete energy spectrum. Please note that in the band-theory of solid the spectrum energy is continuous. Thus my theory is "quantum" in contrary to presently-in-fashion solid state theories.
The report is dishonest as the referee D does not inform where I can find the proper description of NiO, otherwise it is the discussion about nothing. Next, I do not claim that I invent crystal field and spin-orbit coupling. This what I generally claim is that the well-known spin-orbit coupling, calculated years ago by Blume and Watson (1963), have to be taken into account in description of 3d-ion compounds, NiO in this case. In combination with it is the existence of the atomic-like discrete energy spectrum in the electronic structure of 3d-ion containing compounds. My paper and the general claim should be considered in the present discussion in renowned journals including PRL. The s-o coupling is not taken into account at presently-published papers even in PRL (PRL 83 (1999) 4828, PRL 83 (1999) 4136, and many others). It is not always explicitely written but in PRB 53 (1996) 7158, p.7164 left column 16b, and J. Phys. Cond. Mat. 11 (1999) 6553, p. 6553 line 6b it is honesty written (what I really appreciate).

At the end, doubts of referee D about a factor 1000 in B_4 and the crystal field shows that Ref. D is very, very out of the subject; "everybody" knows that the CF splitting equals for the term F to 1080 B_4 (ref. 5, ch. 7), it is really "elementary" knowledge. It means that the "elementary knowledge" is not so elementary.

All these things proves that the subject is not so easy, the referees have "problems", the knowledge about the crystal field is not so established, and ... it is the highest time for normal open discussion.

Finally, **in order to make our discussion responsible for both side I propose the scientific bet with the inputs twice larger compared to the Bron one i.e. 600 USD from my side and 2 millions from your side provided that you maintain your negative decission that unables the normal open scientific discussion.**
I think that it is honest bet - we have to take the real responsibility for our decisions. You do not loose so much - please take the subsequent declaration of the referee D. It is in contrary to me - I am paying from my private money.

Sincerely Yours,
Ryszard Radwanski
Z. Ropka

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Answer of Radwanski to ref. report D, 25.01.2000 obtained by post 1.02.2000, on the PRL paper: LF7313: "Orbital moment in NiO"
by R. J. Radwanski, Z. Ropka and R. Michalski

Dear Referee (D),
Thank you very much for your long report.
I appreciate it.
I fully understand all arisen arguments.
And I do not agree with your thinking.

Although I appreciate very high referees of PRL I maintain that you are wrong, not me. It proves that our paper is really important.

I fully agree that "the utility of such a model is not a getting accurate numbers, but rather in giving new insight into physics of the system" and I draw completely opposite conclusion. Exactly, my model provides new insight. I could say that it is so new that 4 experts of PRL cannot see it. The new insight is seen in a number of papers waiting for publication in PRL (the referee is not aware of them) that offers "new insight" for a great number of important presently problems of 3d magnetism.
I do not agree that "important quantum effects are completely ignored." Nonsense. Just the essence of my theory is that in a solid 3d ions preserve much of their atomic-like properties what reflects in

the existence of the discrete energy spectrum. Please note that in the band-theory of solid the spectrum energy is continuous. Thus my theory is "quantum" in contrary to presently-in-fashion solid state theories.
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At the end, doubts of referee D about a factor 1000 in B_4 and the crystal field shows that Ref. D is very, very out of the subject; "everybody" knows that the CF splitting equals for the term F to 1080 B_4 (ref. 5, ch. 7), it is really "elementary" knowledge. It means that the "elementary knowledge" is not so elementary.

All these things proves that the subject is not so easy, the referees have "problems", the knowledge about the crystal field is not so established, and ... it is the highest time for normal open discussion.

Finally, **in order to make our discussion responsible for both side I propose the scientific bet.** Please contact the Editor and say that you take the full responsibility for your report up to 1 millions USD.

I challenge you.
Your report unables the normal open scientific discussion.

Sincerely Yours,
Ryszard Radwanski
Z. Ropka

SIMPLE QUESTION TO THE EDITOR OF PHYS. REV. LETT.

From: sfradwan@cyf-kr.edu.pl
To: prl@aps.org
Subject: Report LF7313 Radwanski
Date sent: Tue, 1 Feb 2000 19:40:54 +0100

From R. J. Radwanski
To: Editor of PRL

Concerns: LF7313: "Orbital moment in NiO"
by R. J. Radwanski, Z. Ropka nad R. Michalski

Dear Editor,
I have sent to you email of 20.10.1999, see below, (reminder 9.11.1999, 23.11.1999, 14.12.1999) and up to today I did not get the answer for my simple question to your referees:

"What paper do you, i.e. the referee, consider as the most representative for theoretical understanding of NiO? So, provide the reference."

Please ask this simple question.

It indicates on unfair treatment of my papers in PRL. You cannot hide your responsibility basing on the unresponsible (anonymous) reports and using words: not suitable for publication. If your referees are not ready to answer so simple question it means that their report is good for nothing.

Still looking for the answers of your referees (A, B, C, D).

Sincerely Yours,
R. J. Radwanski

The American Physical Society

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MARTIN BLUME
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March 7, 2000

Professor R.J. Radwanski
Center for Solid State Physics
sw. Filip 5
31-150 Krakow
POLAND

Dear Professor Radwanski:

I have reviewed the files of four of your papers: LF7313, "Orbital moment in NiO"; LN6596, "Jahn-Teller-effect formation..."; LC7763, "Local off-cubic distortion...."; and LE6925, "Relativistic effects in the ...."; all of which were submitted to *Physical Review Letters*. The scientific review of your paper is the responsibility of the Editor of *Physical Review Letters*, and resulted in the decisions to reject your papers.

In reviewing manuscripts referred on appeal, the Editor-in-Chief must assure that the procedures of our journals have been followed responsibly and fairly in arriving at those decision. On considering all aspects of these files, I have concluded that our procedures have in fact been appropriately followed and that your papers received a fair review. Accordingly I must uphold the decision of the Editors.

I note that since May of 1997, you have been author or co-author of 20 manuscripts submitted to our journals for consideration. Six were submitted to *Physical Review B* (three Rapids, three Comments) and fourteen were submitted to *Physical Review Letters* (two were Comments). Evaluation of these manuscripts over the period has involved 34 different anonymous referees, six Editorial Board Members, and PRL Editorial Board Chair Dr. Sandweiss. None of the twenty manuscripts has been approved for publication. Because of the unusually large number of papers you have submitted in the last three years, the considerable effort required to evaluate each manuscript, and the repeated negative outcomes, I regret that we find it necessary to use the following procedures for consideration of your manuscripts, which shall apply to papers currently in process and to future submissions.

Henceforth, the senior editors of *Physical Review B* and *Physical Review Letters*, Dr. Adams and Dr. Wells, must be persuaded that a submission from you is appropriate for external evaluation before they will consult a referee. There will be no automatic appeal of a negative decision by them, whether or not it is supported by a referee report. They must be persuaded that an appeal is appropriate before it will take place. We regret the necessity of imposing this policy, but an inordinate measure of our resources going to a single author is unfair to everyone.

Sincerely,

Martin Blume

Martin Blume
Editor-in-Chief