UNSW SYDNEY

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The referee report for the PhD thesis by Dmitry V. Chubukov "Violation of fundamental symmetries in atoms and molecules: P, T -odd Faraday effect and P-odd optical activity."

The thesis addresses the following problems.
1) Calculation of parity violation in oxygen molecule.
2) Calculation of parity violation in parahydrogen molecule.
3) Calculation of parity violation in orthohydrogen molecule.
4) Optical activity of atomic vapours in a longitudinal electric field as a way to observe P and T violating interactions.
5) Optical activity of a molecular beam in a longitudinal electric field as a way to observe P and T violating interactions.

The central emphasis of the work is in application of the sophisticated numerical methods to calculations of parity and time violation effects in multi electrons atomic and molecular systems. Most importantly, results of these calculations may open new experimental ways for studies of fundamental interactions.

1) After a general introduction to the field the thesis begins from the analysis of parity violation in $b^1\Sigma_g^+ \to X^3\Sigma_g^-$ M1-transition in O_2 molecule. The M1-amplitude has been calculated previously in the literature, so the calculation is aimed at the E1-amplitude. The calculations are technically pretty involved and I trust that the results are correct. The obtained value of the parity non-conserving (PNC) E1-amplitude due to the nuclear weak charge,

$$E1 \sim 10^{-15} e a_B \ , \tag{1}$$

is consistent with a crude estimate. Another contribution comes from the PNC ee-interaction. This contribution is also calculated and it is 100 times smaller than that of the nuclear weak charge. The suppression by two orders of magnitude is expected, it is consistent with Eq.(8) in Ref.[21].

2) The next point is the molecule of parahydrogen where spins of protons are combined to zero. Here the M1-transition between two vibrational states of the electronic ground state is considered. The obtained E1 amplitude, Eq.(28),

$$E1 \sim 10^{-24} e a_B \tag{2}$$

is very small, 9 orders of magnitude smaller than that for oxygen (1). *It is necessary to explain where such dramatic difference comes from.* I understand that 2-3 orders of magnitude come from the standard Z^3 scaling, probably 4 orders come from the spin-orbit in hydrogen ($\alpha^2 \sim 10^{-4},\ \alpha = 1/137$). Is the rest of the suppression related to the adiabaticity parameter in hydrogen?

The contribution of the ee-weak interaction is also calculated. As expected, it is comparable to that of the weak charge, Eq.(8) in Ref.[21].

In this chapter the hypothetical experiment with optical activity of gaseous parahydrogen is discussed. When reading this section I've immediately got a question, what if one uses liquid parahydrogen? Of course in this case J cannot be large and hence some suppression from the electric quadrupole comes to the game. However, there are several gains from other factors. Of course in any case the effect is extremely small.

3) The molecule of orthohydrogen with spins of protons combined to S=1 is considered in Chapter 2. This case is interesting since the PNC effects are sensitive to the part of the electron-proton weak interaction that depends on the spin of proton. The same vibrational M1-transition is considered as that for parahydrogen. Of course in this case there are hyperfine components of the transition. The E1-amplitude obtained as a result of complex numerical

calculations is, Eq.(55),

$$E1 \sim 10^{-21} e a_B \tag{3}$$

So, it is 6 orders of magnitude larger than (1) and 3 orders of magnitude smaller than (2). *In my opinion a simple parametric explanation of these differences is absolutely necessary.* Numerical calculations can refine results up to factor 2-3. Orders of magnitude must be explained analytically. Is the difference between (2) and (3) due to the parameter of adiabaticity?

Right after Eq.(56) the author claims: "Note that, according to Ref. [99], the nuclear spin-independent PNC effects for the molecular system considered are negligible compared to the NSD-PNC one.". *I trust that this is a correct statement, but again in my opinion it is absolutely necessary to explain the statement parametrically.* Such a suppression must be evident without calculations. I suspect that if correct, the suppression of weak charge contribution is also related to the parameter of adiabaticity.

Similar to the case of parahydrogen, a hypothetical experiment with optical activity of gaseous orthohydrogen is discussed. Hence I have the same question, can one use liquid orthohydrogen?

4) Optical activity of atomic vapours in a longitudinal electric field is considered in the Chapter 3. There are two parts in this research.
(a) The first part is a calculation of atomic enhancement of the electron electric dipole moment. These are sophisticated numerical calculations which result in the enhancement factors for some states in several atoms. Overall the values of the enhancement factors agree with that known in the literature and also agree with simple estimates.
(b) The second part is a discussion of a hypothetical experiment on the optical activity of atomic vapours. The major idea is to enhance the optical length. There are three "handles" to realise the enhancement. (i) To work on far wings of the Doppler line shape to reduce absorption, similar to Fortson PNC experiment in Tl. (ii) Use cavity with mirrors. (iii) Use transitions with very long lifetime limited by the collisional broadening.

I have two comments related to the point **(b)**. The collisional line width in some cases is very small, about 100kHz. In this case effects of non-linear optics are expected to be very significant and this can influence the presented estimates. This problem is partially addressed in the end of Chapter 4. However, it will require further analysis in future.
The density in suggested experiments is low, $n \sim 10^{15} cm^{-3}$ and the electric field is rather high $E \sim 10^5$V/cm. In this situation it would be useful to comment on the possibility of electric discharge and leakage current.

5) Optical activity of a molecular beam in a longitudinal electric field is considered in Chapter 4. Specifically the PbF molecule is considered. Chapter 4 is a logical development of ideas considered in Chapter 3. With molecules there is an additional enhancement $\sim 10^3$ of electric dipole moment related to closeness of the rotational levels. All other gain factors considered in Chapter 3 remain in the game.

I am not sure that the natural line-widths used in the estimates are relevant to the problem. It seems that the relevant width is determined by the flight time of the molecular through the laser beam. If so this would reduce the presented estimates for angles of rotation.

In all the hypothetical experiments considered in the thesis systematic effects is a very serious issue. In this sense the molecular beam is probably the worst case. It would be useful to discuss possible systematic effects, at least briefly.

I've already commented on possible effects of non-linear optics for atoms. Similar effects must exist for the molecular beam experiment and they can influence the presented estimates. This issue is related to the shot noise of photons that is briefly discussed in the end of Chapter 4. This is a very interesting problem, somewhat similar to that considered in Ref.[69]. I hope that the problem will be addressed in future.

All in all, in his work D. V. Chubukov demonstrates a sufficient degree of technical capacity. The thesis is a contribution to the field of violations of fundamental symmetries at low energies. As always there are open questions, but this is normal and this will stimulate further development of the field. I recommend awarding Dmitry V. Chubukov the PhD degree.

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