UNSW SYDNEY

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The referee report for the PhD thesis by Sergey D. Prosnyak "Theoretical study of the properties of nuclei using atomic-molecular systems".

The thesis consists of Introduction, four Chapters, and Conclusion. Introduction and Chapter 1 present a general introduction in the field and general description of methods used in the work. Conclusion section summarises results of the thesis.

The original research results of the candidate are presented in Chapters 2, 3, 4. The focus of the research is in application of sophisticated numerical methods to calculations of several physical properties.
Chapter 2 addresses the influence of the finite nuclear size on the hyperfine structure.
Chapter 3 is aimed at isotopic shifts in atomic spectra.
Chapter 4 considers time and parity symmetries violating energy shifts in molecules induced by the interaction mediated by a hypothetical axion-like particle.

This is a heavily computational work. I have no doubts in the computational results. I think that the candidate deserves awarding the PhD degree. However, I have comments on physical results and on significance and interpretation of the results. Lack of physical interpretation in some cases disappoints me. My comments are the following.

1) Page 29. What is b_N in Eq.(2.2), how b_N depends on κ? This dependence is qualitatively important. Eq.(2.2) implies that $\delta \propto R_c$ at $Z\alpha \ll 1$ for both $s_{1/2}$ and $p_{1/2}$ states. However, it is clear that $p_{1/2}$-correction must be much smaller than the $s_{1/2}$-correction. It would be also appropriate to compare the ϵ and the δ corrections analytically.

2) Pages 30-31 present magnetic moments and hyperfine constant corrections for even-odd nuclei in single particle approximation, the Schmidt line approximation plus the single particle spin-orbit contribution. Usually for magnetic moments the spin-orbit contribution is smaller than 10% of the " Schmidt" contribution. On the other hand the many-body core polarisation contribution that is not accounted in the presented analysis can be as large as 40-50%. I presume that the same is true for the hyperfine constant corrections. If so, what is the point to account for the spin-orbit correction missing the many-body one?

3) Page 32. The author claims that Eqs.(2.14),(2.15) are valid for the 1s-state of a hydrogen-like ion. I think that they are equally valid for any s-state of an ion or a neutral atom. This is because the electron potential energy at $r \sim R_c$ is enormous compared to the electron binding energy.

4) Page 34. The author neglects the QED Karplus-Klein correction to the Hyperfine constant. Why is it neglected? This correction is about 1% for s-states at Z=81. By the way, for a multi-

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electron ion or neutral atom there is also a comparable correction to the hyperfine cosnstant from polarisation of inner electronic shells (PRB **63**, 042504 (2001)).

5) Page 34. Eqs (2.23),(2.24) do not make sense to me, at least I do not understand them. In the sentence after these Eqs. I conclude that the magnetisation distribution is not a property of a particular nucleus. Why the author does not present simple analytical expressions for δ and ϵ?

6) This comment is relevant to the entire Chapter 2, but specifically I am asking this in relation to Section (2.1.4). It would be appropriate to discuss where the most precise tabulated values of magnetic moments come from. I hardly believe that magnetic moments of ^{203}Tl and ^{205}Tl presented in Table 2.2 with nine digits can come from atomic or molecular measurements. Most likely this is from NMR in solids/liquids with "paired" electrons (band insulators). At least Eq.(2.39) is equally applicable to band insulators. I do not quite like the notation μ^{uncorr} since the diamagnetic shielding σ is not related to electron correlations in usual semantics. However, this is just a notation. I'll return to this point in comments **9,10**. By the way, Table 2.2 presents nuclei charge radii with five significant digits! Where do they come from?

7) Page 41. As far as I understand Eq.(2.41) corresponds to the cylindrical gauge for the vector potential. Why the author uses the cylindrical gauge, not Landau gauge or any other gauge?

8) I trust that the finite nuclear size correction $\approx 2\%$ for hydrogen-like s-wave ions presented in Table 2.3 are correct. To check the many-body calculations for 6p-states of atomic Tl I've performed my back-of-the-envelope calculation based on analysis of Tl hyperfine structure from Sov. Phys. Opt. Spectr. **44**, 3 (1978). According to this analysis the $6p_{1/2}$ hyperfine constant has $p_{1/2}$-weight 89% and $s_{1/2}$-weight +11% , hence the expected BW correction, $\approx (0.89*0.26+0.11)*0.02 = 0.007$, is consistent with +0.7% obtained in the thesis numerically. The $6p_{3/2}$ hyperfine constant has $p_{3/2}$-weight 622% and $s_{1/2}$-weight -522%, hence the expected BW correction, $\approx (6.22*0-5.22)*0.02 = -0.10$, is not quite, but still more or less consistent with -13% obtained in the thesis numerically. Actually I trust more the analytic calculation. This example illustrates that most if not all results of the thesis can be obtained analytically and it would be very instructive to compare results of the two methods.

9) The value of $\delta r_m^2 = ^{205} r_m^2 - ^{203} r_m^2 \approx 0.43 fm^2$ that follows from Fig. 2.2 on page 52 is the most intriguing result of the thesis. It dramatically contradicts to the widely accepted theory of saturation of nuclear forces. With saturation one expects $\delta r_m^2 = \frac{8}{15} 1.2^2 A^{-1/3} fm^2 = 0.13 fm^2$, here $A = 204$. Note that the pair ^{205}Tl, ^{203}Tl is a very clean case since the difference is just a pair of neutrons submerged to the BCS-condensate. Having this very intriguing result I would perform the analysis of magnetic moments of these nuclei presented in Table 2.2. I've already noted this in my comment 6). To do the analysis one has to perform an analytic calculation of the diamagnetic shielding factor σ in a band insulator with account of the finite nuclear size. This is pretty straightforward. Such an analysis would be much more reliable than the atomic hyperfine structure.

10) Page 57, I do not know the electronic structure of ReO_4^-, unfortunately the thesis does not present the spectra. However, almost for sure all electron angular momenta and spins are compensated to zero. Hence, this is like a band insulator and the calculation of the diamagnetic shielding can be performed analytically.

11) Page 60. Is δ in Eq. (3.1) what is later called F, $\delta = F$?

12) This is the question to the entire Chapter 3. The energy corrections NMS and SMS, Eqs.(3.2),(3.3),

how are they distributed over atomic shells, do they predominantly come from the inner shells or the valence electron contributes significantly? Probably for the total energy level shift inner shells dominate. However, for the transition frequency, say $6s^2S_{1/2} \to 6p^2P_{1/2}$ in Au, this is not obvious. It would be instructive to illuminate this point. Such understanding can greatly simplify the calculation.

13) Note that value of $\delta r_c^2 = 0.108 fm^2$ for ^{205}Tl, ^{203}Tl presented in Table 3.10 is practically consistent with that based on saturation of nuclear forces, see my comment 9).

14) Page 72 Chapter 4. What precisely is called the axionlike particle? If the particle interacts with electromagnetic field and gluons like axion then the constants g_N^s and g_e^p in Eq.(4.1) are not independent. Otherwise, this is just an arbitrary mediator with effective Hamiltonian (4.1).

15) Page 83 Table 4.1. I do not think that the lines of the Table with $m_a = 10^9, 10^{10}$eV have a physical meaning. These energy scales are above the QCD confinement scale $\sim$ 300MeV and hence the effective Hamiltonian Eq.(4.1) does not make sense.

To summarise. This work of Sergey D. Prosnyak demonstrates a sufficient degree of technical capacity. The thesis is a contribution to the field of computational atomic and molecular physics. As always there are questions and comments, but this is normal and hopefully this will stimulate further developments. I recommend awarding Sergey D. Prosnyak the PhD degree.

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