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Referee report for the PhD Thesis of Mohammad Hassan Naddaf 30 May 2023

The PhD Thesis of Mohammad Hassan Naddaf titled **"Simulation of the dynamics and geometry of the broad line region in active galactic nuclei"** prepared under the supervision of Prof. Bożena Czerny develops a 2.5D version of the Failed Radiatively Accelerated Dusty Outflow (FRADO) model, introduced in a 1D version by Czerny & Hryniewicz (2011), and works out several observable predictions to make comparisons with observations.

The thesis is presented in 6 chapters. Chapter 1 is a broad introduction to current knowledge of Active Galactic Nuclei (AGN), providing background and motivation for the research. Chapter 2 derives key formulae needed for the 2.5D FRADO model. Chapters 3, 4, and 5 are published multi-author papers on which the candidate is the first author. Chapter 6 is a brief summary and outline of prospects for future work.

Chapter 1 begins with some historical material on the discovery of AGN, followed by a sketch outlining current understanding of AGN structure as supermassive black holes being fed from an accretion disc, the x-ray corona around the black hole, photo-ionised broad and narrow emission-line regions, enclosed by a dusty torus, and sometimes emitting jets. The unified model of AGN is then noted, with different AGN types interpreted as different viewing angles on the axisymmetric accretion flow, and AGN are placed in a cosmological context tjat motivates ongoing efforts to use AGN as standard candles to address the Hubble tension. A detailed discussion follows on the Broad Line Region (BLR) which produces the broad and variable emission lines in AGN spectra, including several proposed models, evidence for dust in the BLR, and dust-based BLR models. The chapter concludes with a brief overview of the thesis.

The writing in Chapter 1 is generally good, with only a few grammatical errors per page that could be corrected by more careful proofreading. Throughout this chapter the material presented is well linked to relevant literature. It provides ample evidence that the candidate has a broad and deep understanding of the background and current issues in the field, motivating the research undertaken and presented in the thesis.

Chapter 2 formulates the mathematical framework for the 2.5D FRADO model. The equations derived detail primarily how radiation pressure acts on dusty gas parcels above the accretion disc. Each gas parcel is assumed to conserve mass, momentum and energy while being accelerated by Newtonian gravity of the black hole and by incident radiation from the underlying flat steady-state blackbody accretion disc. Balancing heating and cooling, the dust temperature rises until dust is sublimated at $T = 1500$ K, after which the trajectory is a ballistic orbit. A useful 'polar patch' approximation is introduced to emulate the shielding effect that allows dust to survive long enough for the upward radiative acceleration to launch the trajectory above the plane before the dust evaporates with increasing exposure to irradiation from the hotter central regions of the accretion flow.

I found Chapter 2 difficult to read, due to grammatical errors and imprecision in defining some of the symbols used in the equations. It seems to paraphrase the Appendix of the Chapter 3 publication, which is much clearer. For example, Eqns (2.1) thru (2.7) employ many symbols that could be defined by reference to Fig 2.1, but this reference is not encountered until 1 or 2 pages later. The discussion of Fig. 2.2 makes the point that the radiative force on a tilted surface element can act in a direction different from that of the incident radiation. Eqns (2.9) and (2.10) then express the radiation pressure normal to the surface element, with factors of $\cos\alpha$ for full absorption and $2\cos^2(\alpha)$ for full reflection, where α is the tilt angle. The $\cos\alpha$ factors then vanish in Eqns (2.11) and (2.12). What is missing here is an explicit definition of the changed meaning of $d\Omega$ in Eqns (2.11) and (2.12) in terms of the effective cross sections $\sigma^{\rm rad}$ and $\sigma^{\rm sca}$, which in turn need to be defined in terms of integrals over the surface elements of the dust grain. There seems to be an implicit approximation that the dust particles are spheres so that integrating over their surface cancels the sideways accelerations. Alternatively, summing over N randomly oriented dust particles in a gas parcel reduces the sideways acceleration by $1/\sqrt{N}$. The confusion induced by the imprecision in Chapter 2 somewhat degrades my confidence that the candidate fully understands and can communicate clearly the relevant small-scale physics. I recommend that the clarity of Chapter 2 be significantly improved.

Chapters 3, 4, and 5 are published papers presenting the candidate's major contribution to the field. In my view these are well presented and provide an important advance of the field by developing a 2.5D version of the 1D FRADO model introduced in Czerny & Hryniewicz (2011).

Chapter 3 clearly outlines the assumptions and approximations used in building the 2.5D FRADO model. It describes a 3D FRADO model that is not yet fully implemented. A major simplification, yielding a practical advantage in computational simplicity and speed relative to hydrodynamical models of accretion flows, is the neglect of pressure gradients, so that streamlines are test particle trajectories that do not interact. An important further innovation is the approximate treatment of the shielding effect, in two versions that are tested and compared. Snapshots of individual cloud locations help to justify the neglect of inter-cloud interactions. Interesting details are presented of the trajectories launched from different radii, for a typical 10^8 solar mass black hole and for 3 accretion rates 0, 1 and 2 dex below the Eddington limit. At the Eddington accretion rate trajectories launched near the inner edge of the BLR achieve escape velocity, while those at lower accretion rates or larger launch radii rise to a crest and fall back onto the disc. This important transition will likely help to explain qualitative differences in the emission lines for AGN above and below the Eddington limit. Many relevant issues are discussed covering the capabilities and limitations of the 2.5D FRADO model, and prospects for testing based on BLR emission profiles and time delays from reverberation mapping studies.

Chapter 4 is a short paper discussing the innovative method used to approximate the shielding effect. To some extent it covers the same material as in Chapter 3, but adds a comparison of the BLR size and shape for two different treatments of the shielding effect. The model BLR sizes, computed for Eddington ratios 0.01, 0.1, and 1.0, are tested in comparison with observed BLR sizes derived from reverberation mapping studies. The observed BLR radii scale with luminosity as $R \propto L^{1/2}$, with a bias toward smaller BLR radii for AGN above the Eddington limit. Adopting same power-law slope to extrapolate the model BLR sizes, for a $10^8\,M_\odot$ black hole and fixed 39° disc inclination, the model nicely covers the the observed range, and the model also exhibits a bias to smaller sizes at higher Eddington ratios. This successful quantitative comparison is very encouraging.

Chapter 5 develops in a simplistic way BLR velocity profiles for the 2.5D FRADO model. The model grid now considers 4 black hole masses ($\log(M/M_\odot) = 6$, 7, and 8), 2 dust/gas ratios (1 and 5 times solar), and three inclination angles (15°, 30°, and 45°). Photoionisation and radiative transfer inside the cloud, and consequent anisotropic radiation from the cloud, are neglected. Instead the line emission is assumed to be isotropic and to scale with height z above the disc plane, and the mass of lofted material is assumed to scale with radius as $R^{-5/2}$. Despite these extreme approximations, the resulting line profile predictions are interesting. Symmetric double-peaked line profiles are found for sub-Eddington models, and asymmetric single-peaked profiles with the peak shifted to the blue for models in which cloud trajectories reach the escape velocity. The asymmetric single-peaked profiles are shown to agree remarkably well with MgII and Hβ line profiles in a composite quasar spectrum constructed in the literature by averaging observed spectra of quasars at many different redshifts. This agreement is encouraging, although it is not really a strong test due to the arbitrary assumptions noted above, and the decision to compare with the composite quasar spectrum rather than the more detailed information from reverberation mapping studies of individual objects. The double-peaked model line profiles at low accretion rates do not match typical observed profiles, for example. I would be interested to see the corresponding model predictions for velocity-delay distributions, which should be straightforward to produce, and are available in the literature for comparison. But this is a good target for future research.

The summary and forward look in Chapter 6 briefly recapitulates the background that motives the work, and outlines the main advances achieved by the candidate's development of the 2.5D FRADO model, as presented in the 3 published papers. A further paper interpreting Broad Absorption Line AGN is noted, as are plans for future developments.

Summary

I regard the thesis to be one of the stronger ones that I have encountered in recent years. The successful development of the 2.5D FRADO model is an important advance in the field and opens the door for future developments. Apart from minor typographical corrections, my main recommendation is to improve the poor quality of presentation in Chapter 2 to bring it closer to the standard set in the rest of the thesis.

Conclusion

In summary, I consider the doctoral thesis of Mohammad Hassan Naddaf to be a valuable contribution to current research on modeling the broad emission-line regions of active galactic nuclei, and to meet the criteria prescribed by law for a doctoral dissertation. Therefore, I request that this dissertation be admitted to a public debate.

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