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Report on the Habilitation Thesis submitted by Dr. František Knapp

Prelude: In recent years nuclear theory has gained new momentum, both from the conceptual and the practical-numerical side. Important steps forward were the introduction of advanced many-body theoretical and numerical methods and a new understanding of nuclear interactions by effective field theory (EFT).

The new era of nuclear physics demands excellence in fundamental nuclear many-body theory and high skills in development and application of appropriate numerical method, combined with high-performance computing. An indispensable ingredient is the access to powerful computing hardware which is required for solving in a finite time huge systems of coupled equations approaching easily dimensions of a billion or more. The coordinated handling of these resources is essential for successful research in modern nuclear theory. František Knapp belongs without any question to the rare species capable of managing this task.

Scientific Achievements: A close look to Dr. Knapp's published work reveals two achievements of general importance for a successful career: First, over the years his research has reached and maintained a high level of quality; establishing him as an internationally recognized expert in nuclear structure theory, as convincingly documented by publications in scientific journals of the highest international reputation and sharp peer reviewing rules. Second, he has been able to establish and maintain collaborations with international research groups of high profile.

Most of his papers are the result of teamwork - as is good practice in the field and necessary for tackling the very involved research issues. That implies co-authoring in alphabetical and/or rotating order. A look over the international nuclear theory community shows that this scheme is typical and necessary for successful research work in this field. In practice two schemes are found: Either research is done in a large local group, or in collaborative research units formed spontaneously for investigations of special topics. The collaborative scheme, informal and flexible, with distributed contributors from a variety of locations and institutions, is especially well suited, Around the world, it is successfully practiced by small research groups becoming competitive by joining forces. Obviously, that has been the approach of Dr Knapp.

The published work documents very well the achievements and continuous progress of František Knapp's research activities. As emphasized in the thesis, the research is centered around two main topics: the theory of nuclear collective motion and advanced shell model calculations. A common feature of the research in these two fields is the use of modern concepts and advanced numerical algorithms.

Nuclear collective motion is manifested in two corner stones of historical importance, namely low-energy vibrational modes and giant resonances at higher energies. Between these two defining traditional kinds of collective modes, in recent years the widely – and still controversially – discussed pygmy modes were unexpectedly discovered. Since then, their description has attracted large attention. In Dr. Knapp's work, these distinct phenomena are described in a unified manner with the extended multi-phonon model (EMPM), formulated in collaboration with partners in Italy. In various collaborative papers, Dr. Knapp has contributed to the theoretical formulation and applications of these highly desired extensions of nuclear structure theory. The works collected under section A of the thesis are important contributions for tearing down some of the persisting theoretical and numerical barriers in nuclear theory. For many years, the modelling of collective modes was restricted to lowest-order particle-hole i.e., two-quasiparticle descriptions, corresponding to a harmonic approximation. In the EMPM that limitation is overcome by the inclusion of multiple phonon states. The interactions between configurations of different phonon content introduce anharmonicities by which dissipative effects are incorporated into the modelling of nuclear spectra. That extension is essential for describing the observed fragmentation pattern and the related fine structure in nuclear spectra. In the EMPM the underlying dynamical polarization effects are treated on a sound theoretical basis by using a microscopic approach.

The advantage of approaches like EMPM is the applicability to low and high energy modes, in principle limited only by the available computing power. Moreover, the EMPM scheme contains elements of an effective field theory because it allows in principle a systematic treatment in terms of many-body diagrams from single phonon to many phonon dynamics. In practice, however, that goal is not yet fully achieved but works like those of F. Knapp are important preparatory steps. The equation-of-motion approach is one of the methods of choice, as explained in the thesis. In the thesis, the obstacles encountered in multi-phonon models are discussed very clearly, giving the reader an understanding of the quite involved theoretical and numerical work.

The microscopic approach utilized by Dr. Knapp derives the internal structure of phonons in a self-consistent manner in terms of multi-quasiparticle states. The quasiparticle basis by itself is determined self-consistently by Hartree-Fock-Bogolyubov theory. Hence, the multi-phonon picture is in fact congruent to a many particle-many hole shell model approach. As the latter, it accounts fully for the Fermion nature of nucleons by introducing the proper norm. These aspects of the model are elucidated repeatedly in the thesis and the publications.

Numerically, multi-phonon calculations are a demanding task. The computational efforts are comparable to other many-body schemes, as to be expected. An advantage of multi-phonon approaches, however, is that the computations can be optimized by use of an angular momentum coupled basis and by various pre-diagonalization steps. In the listed publications, papers are found which are especially devoted to the optimized diagonalization techniques. In general, the EMPM approach accomplishes those steps by a sequence of preparatory calculations, starting with an HFB single particle basis, the definition of single phonon states in Quasiparticle Tamm-Dancoff Approximation (QTDA) or, accounting for ground state correlations, by using the Quasiparticle Random Phase Approximation (QRPA). Both kinds of phonons are used to construct the higher order multi-phonon state vectors.

Closely related to multi-phonon theory is the question of ground state correlations. Thes are virtual excitations leading to admixtures of second and higher order particle-hole components into the mean-field ground state as obtained in Hartree-Fock theory. Dr. Knapp has addressed this important aspect of nuclear many-body theory in a non-perturbative approach based on the EMPM.

František Knapp has contributed also to solve the problem of spurious states, appearing in nuclear structure calculations because of broken symmetries. The most prominent case is the breaking of translational invariance by the nuclear mean-field, which produces a strongly collective isoscalar excitation in nuclear dipole spectra but, of course, is not an intrinsic excitation of the system but a translation mode of no special interest for spectroscopic work. The problem is that the spuriousity is to some degree part of any dipole state. In the EMPM methods have been developed to remove these admixtures, thus projecting the spectra on the true intrinsic excitations. An interesting application addressed in one of the papers is the EMPM description of a light nucleus like ^{4}He, typically thought to be out of reach for such approaches.

A distinct aspect of the EMPM studies, making the approach distinguishable from other multi-phonon models, is the use of modern nucleon in-medium interactions combined with the so-called V_{lowk} regularization scheme. This allows to implement directly well established and tested nucleon-nucleon interactions into the many-body calculations. Moreover, such methods pave the way to implement interactions of chiral effective field theory (EFT), providing systematic improvements of the calculations by inclusion of closed classes of diagrams of increased complexity.

Section B of the thesis is devoted to many-body shell model theory and numerical applications therewith. Importance sampling algorithms, serving to prepare and optimize the iterative diagonalization of large matrices of dimension up to $N=10^9$, were studied and implemented numerically. These methods are mandatory for so-called No Core Shell Model (NCSM) calculations avoiding the formerly necessary separation of the nuclear configuration space into an inert core part and an active valence sector. A major and important difference to multi-phonon descriptions is that the many-body shell model does not rely on the use of a spherical basis. Hence, such many-body approaches provide the appropriate tools for investigations of non-spherical nuclei of arbitrary deformation.

The NCSM approach, at present constrained to light nuclei, is considered of a high future potential for ab initio calculations with QCD-inspired chiral interactions for practically all nuclei, thus avoiding most of the additional intermediate steps and approximations as necessary by today. Quantum computing might be essential for such large-scale studies of fundamental character.

Status as a Researcher: In his work, František Knapp has addressed demanding issues of nuclear many-body theory, methods for numerical simulations, and applications of detailed spectroscopic studies in light to heavy nuclei. The research activities are centered at the theory of collective nuclear motion and modern nuclear shell model methods. Both areas are in rapid evolution, to which Dr. Knapp has contributed several important results. The (published) work was done within larger collaboration which, however, is typical for nuclear structure research. Modern nuclear structure theory covers a broad spectrum of subtasks requiring specialization and concentration on a selection of research issues. Topics, content, and quality of the research are well documented by publications in peer-reviewed journals of highest reputation and scientific standards.

Although ranking schemes should be used with care and their relevance should not be overemphasized, tools like the h-index still give a useful orientation on the reception of a researcher and his work by the international community and the closer peer group. František Knapp is listed with an h-index of 15, an i10-index of 18, and a total of presently 537 citations of his research papers. These scores are a very good result for an early career researcher. Dr. Knapp has achieved already a reputation on the international level as a serious and successful scientist, once again confirming the high quality of his research and the promising potential as a mature scientist and skilled researcher.

Plagiarism: The plagiarism checks have led to insignificant results on an overall relevance level of less than 1%. In all indicated cases standard formulations were found which are widely used in research papers on nuclear structure theory.

Closing remark and recommendation: Definitely, František Knapp belongs to the high sector of the upper half of early career researchers in nuclear structure theory in his age group. The achieved status and reputation are promising for excellent future perspectives on fruitful, creative, and inspired and successful work. Habilitation and possibly promotion to an advanced academic status will surely help to accelerate his scientific career further and tighten his status as an independent researcher by his own right. Under scientific aspects and in view of his research records, Dr. Knapp fully qualifies for habilitation.

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