K112962 OTKA FINAL REPORT

Beyond Hermiticity: open quantum systems

2014.09.01 – 2018.08.31, extended to 2019.08.31

Preliminaries and scope

Open quantum systems differ from isolated ones in that they are in interaction with their environment, as the result of which they require more sophisticated mathematical approaches. The description of isolated quantum systems can be performed within the traditional Hermitian constructions of quantum mechanics. In addition to normalizable (bound-state) solutions and real energy eigenvalues, the description of open quantum systems requires also non-normalizable (scattering), as well as complex-energy (resonance) solutions of the wave equations. For this, the extension of the usual Hermitian mathematical constructions is necessary. Due to the previous experience of the research team, the actual problems aimed at the present project were taken from nuclear physics and quantum mechanics.

In nuclear physics bound, scattering and resonance states all appear naturally. The description of bound states is essential in understanding the structure of nuclei, while scattering and resonance states appear in nuclear reaction phenomena, i.e. in the interaction of nuclei with other particles. The complete understanding of nuclear physical systems and processes requires both nuclear structure and reaction studies.

In quantum mechanics in general, non-Hermitian extensions of the traditional Hermitian theoretical models have been known for a long time. In the past 20 years, the investigation of such theories has got more emphasis due to the introduction of PT-symmetric quantum mechanics. Here special complex potentials are considered, which, however, show many features similar to real potentials. From the mathematical point of view, PT-symmetry was found to be a special case of pseudo-Hermiticity, a specific generalization of Hermiticity. This theory spread to several branches of physics, and it became especially successful in optics, where it stimulated the study of optically active systems.

Results

Here we arrange the results in a sequence dictated by the internal logic of the subject, which may differ from the chronological order of the published articles.

Nuclear theory – phenomenological potential models

The interaction of a nucleus with another particle can be described phenomenologically in terms of potential models. This approach allows the incorporation of bound, scattering and resonance states in a natural way, and can be extended to complex potentials too. In order to describe interacting system as an open quantum system, these states have to be discussed in a unified mathematical framework. On the other hand, the actual shape of the potential has strong effect on the wave functions and thus on any physical quantity derived from them. It is therefore important to investigate the consequences of refining the potential shape, e.g. in the cut-off region, i.e. where it goes to zero. These studies can be performed using both analytical and numerical methods.

The Berggren completeness or Bergren basis is composed of bound states, scattering states along a complex contour and decaying resonances between the contour and the real k-axis. The basis states are eigenstates of a phenomenological nuclear potential. These eigenstates are calculated by using numerical integration of the radial equation and some cases can be tested by comparison to analytical solutions, if they are available. Analitical solutions exist only for special potentials, and we perfomed test calculations in these cases. The Cox-potential is one of these cases, and a comparison of the energies calculated exactly with the result of the diagonalization in Berggren basis was performed in [NTP.1]. It was shown that even shadow poles of the S-matrix could be calculated with acceptable accuracy.

In most of our calculations numerical solutions were performed by our computer code JOZSO published in [NTP.2.], and its results are more accurate than those of other codes.

In [NTP.3] we compared our JOZSO calculations with previously known analytical results for zero angular momantum. Deviations in the pole distribution were explained by the cut-off of the Woods-Saxon (WS), and the generalized WS potentials (GWS).

In [NTP.4.] we changed the forms of the WS and GWS nuclear potentials by attaching polynomial tails to them. The cutting off of the exponential tails of the WS and GWS potentials changed the distribution of the poles of the S-matrix considerably. When we modified the tails of the potentials by attaching Hermite polynomial tails to them, the tails reached the zero value smoothly at finite ranges of the potential. Reflections of the resonant wave functions could take place at different distances. Similar effect was observed for the pole distribution when we dumped the tail of the WS potentials [NTP.5].

A new and previously unknown result was the demonstration of the repulsion of close-lying resonances in the cut-off WS potential [NTP.6].

In [NTP7] the square well potential was smoothed with a finite range smoothing function, in order to get a new, simple, strictly finite range (SSQW) form as a new phenomenological nuclear potential. The SSQW potential becomes exactly zero smoothly at a finite distance. If the smoothing range is four times the diffuseness of the Woods-Saxon shape, the bound and the narrow resonant energies in a CWS potential are reproduced reasonably well.

Based on the results of the one-dimensional Scarf II potential, the radial version of this potential was studied [NTP.8]. For this, the origin was defined at an arbitrary value on the real x axis, and the s-wave solutions were constructed from the two independent solutions of the one-dimensional Schrödinger equation, after prescribing the appropriate boundary conditions. The resulting potential possesses both a well and a barrier, and can be applied to describe certain nuclear physical systems. The $S_0(k)$ S-matrix was constructed analytically, and its poles were determined to locate the bound, anti-bound and resonance solutions. The relation between the bound-state solutions of the one-dimensional and radial potentials was studied. It was shown that these two problems are related to each other in a way similar to the case of the one-dimensional Rosen-Morse II and the generalized Woods-Saxon potential.

Nuclear theory – microscopic few-body models

Microscopic models allow high-precision calculation of physical quantities using well-founded interactions of the constituent particles. It is also possible to incorporate in them three- or more-body interactions. However, due to their mathematical complexity, they can be usually applied only to systems with limited particle number. Nevertheless, they can account for various delicate phenomena *occurring for loosely bound states of nuclei. Furthermore, these techniques can also be applied to atomic systems, which are dominated by the Coulomb force.*

It is known that in Coulombic systems the wave functions must be described by the so-called Kato's cusp conditions in coordinate regions, where charged particles get close to each other. The importance of the fulfilment of the Kato cusp condition has been demonstrated for double photoionization. For the description of this phenomenon in two-electron atoms we used Hylleraas and Kinoshita type wave functions. We prescribed the correct cusp conditions for this wave function and derived the cusp equations for the expansion coefficients appearing in the Kinoshita expansion. We determined new basis functions, based on the standard Hylleraas and Kinoshita types, which exactly satisfies the Kato's cusp conditions [NTM.1, NTM.2].

The surface integral formalism of quantum scattering theory is valid not only for two-body scattering but it can be extended to scattering of three charged particles. Another adavantage of this formalism is that it handles the short- and long-range interactions on an equal footing. The Coulomb-distorted plane wave plays a basic role in this framwork. We studied the partial wave expansion of this function and published a computer code to calculate it numerically [NTM.3].

We joined the Nuclear Astrophysical group of Atomki in describing certain aspects of the $^{17}O(p,\gamma)^{18}F$ reaction. This reaction plays an important role in hydrogen burning processes in several different stages of stellar evolution. The rate of this reaction must therefore be known with high accuracy at the relevant temperatures in order to provide the necessary input for astrophysical models. The purpose of the joint work was to provide consistent and precise cross section values in a wide energy range for the said reaction, with special attention to the low-energy side, where measurements are more difficult to carry out. Our theoretical contribution was an R-matrix analysis of the experimental data, which eventually strengthened the reliability of the extrapolated zero energy astrophysical S factor. The results also provided a constraint for the theoretical cross sections [NTM.4].

We studied resonance states in radiative capture reactions using quasi-separable potentials. This procedure allows an easier treatment of non-local effects that can be extended to three-body problems. Using this technique, the neutron and proton radiative capture cross sections on the ^{12}C nucleus were calculated. The results obtained show good agreement with the available experimental data. The experimental phase shifts are also well reproduced, and can be extended to multi-channel problems in a straightforward way [NTM5].

Experimental data indicate that ^{31}Ne is one of the heaviest halo nucleus discovered so far. The possible ground state of ^{31}Ne is either 3/2- coming from the p-wave halo or 1/2+ coming from the s-wave halo. Using the Glauber model for knockout reactions, we have studied the one-neutron removal reaction from the deformed projectile ^{31}Ne incident on carbon targets. The calculated longitudinal momentum distributions and cross sections have been analyzed and compared with experiments. Our results indicate that ^{31}Ne has the spin-parity 3/2-. The inclusive longitudinal momentum distribution is not very sensitive to deformation [NTM.6].

Nuclear theory – algebraic models

The nucleus is an interacting many-body system, and its microscopic description can be prohibitively difficult for large particle number. However, the relevant degrees of freedom can be reduced, e.g. when the nucleus is pictured as a system of two, or a few clusters, which are, themselves, nuclei in their own right. The most typical cluster configurations contain a core nucleus and one or more alpha-particles, *which are tightly bound structures of two protons and two neutrons. The description of the cluster states of the unified nucleus can further be simplified using symmetry principles and algebraic techniques. In these studies, both the structural aspects and the reaction mechanisms have to be considered, which can both rely on algebraic methods. Obviously, the applicability of these methods is not restricted to cluster models only.*

We have carried out symmetry-related studies concerning both nuclear structure and reactions, as well as their relations.

From the structure side we have studied the quantum phases of a shell model which incorporates Hamiltionian with isoscalar and isovector pairing. Such a model has a three-dimensional phase diagram, that can be illustrated by a tetrahedron. Previously only two-dimensional phase diagrams have been studied. Both sd-shell (^{20}Ne, ^{20}O) [NTA.1], and pf-shell nuclei (^{44}Ti) [NTA.2] have been investigated.

On the reaction side we have proposed an extension of the statistical pre-equilibrium (exciton) model of nuclear reactions [NTA.3]. This generalization includes cluster emission and heavy ion collisions. The motivation for this work came from the study of the exotic shapes of nuclei, like superdeformed, hyperdeformed, etc. states. The problem of their population is in the intersection of the structure and reaction studies, inasmuch both aspects are essential in planning these kind of experiments. These shape isomers are much more likely to be detected in heavy-ion reactions than in those induced by light projectiles (nucleons, deuterons, alpha-particles).

Our most important results in relation with nuclear symmetries are related to a new symmetry, called multi-configurational dynamical symmetry (MUSY). It connects different structure configurations, and gives a bridge also to reaction channels. This symmetry was invented previously by us in relation with cluster configurations, therefore, it was also called multi-channel symmetry, referring to the reaction channels that define the cluster configurations.

Within the present project we have elaborated new aspects of the MUSY. In particular, we have shown that MUSY is the common intersection of the quartet and cluster models [NTA.4, NTA.5]. The quartet model is a simplification of the shell model. Furthermore, in the algebraic description of these configurations the SU(3) gives uniquely the quadrupole deformation of state. Thus we can say that the MUSY is the intersection of the three fundamental structure models: the shell, collective and cluster models for a multi major shell problem [NTA.4, NTA.5.]. Furthermore, via the cluster configurations the MUSY has a direct connection to reaction channels.

MUSY is able to give unified description of the detailed spectra of different configurations in different energy windows. As a consequence it has considerable predictive power. In [NTA.5] we have shown how the high-lying ^{12}C+^{16}O cluster spectrum can be predicted from the quartet-model description of the low-lying well-established bands of the ^{28}Si nucleus. The prediction turns out to be in good agreement with the resonance spectrum of the ^{12}C+^{16}O reactions. A similarly remarkable agreement was observed between the experimental spectrum of the high-lying 0^+ states, and the predicted states of the ^{4}He+^{24}Mg clusterisation in [NTA.6].

MUSY can incorporate not only binary cluster configurations and reaction channels, but other ones, too. In [NTA.7] the three-alpha-cluster states of the ^{12}C were studied. Concerning this widely discussed problem we have shown that different symmetries may result in very similar spectra, therefore, the investigation of all the measurable physical quantities is needed for the selection of the various proposed symmetries.

There are further complex symmetries based on the cluster structure of nuclei. One is the cluster supersymmetry scheme introduced earlier for the description of neighbouring light nuclei in the A=18 to 20 mass region. The states of these nuclei are assigned to the *same* supermultiplet, which introduces strong constraints concerning and the energy spectra and transitions. The supersymmetry scheme contains three Neon isotopes (with A=18, 19 and 20), and the cluster states of ^{22}Ne were also studied previously. In order to fill the gap at A=21, the alpha-cluster states of ^{21}Ne were studied in the algebraic framework [NTA.8].

Quantum mechanics – Extensions of solvable Hermitian potential problems

PT-symmetric potentials form a special class of complex potentials: their real and imaginary components are even and odd functions of the coordinate, respectively. Constructing the PT-symmetric extension of solvable real (Hermitian) potential problems is an important contribution to the understanding of PT-symmetric, and in general, pseudo-Hermitian quantum systems. However, there are real potentials too, for which a non-self-adjoint extension of the formalism is necessary: this is the case for some singular potentials. Finally, studying potentials beyond the range of solvable cases considered up to now (Natanzon-class) is an important task. The results may serve as the starting point towards the non-Hermitian extension of these potentials.

The class of Natanzon (and Natanzon confluent) potentials is a rather general family of potentials for which the Schrödinger equation can be solved in terms of hypergeometric (and confluent hypergeometric) functions. We presented a systematic construction of the PT-symmetric version of these potentials and discussed how known potentials can be obtained as members of these potential classes [QM.1].

We discussed a phenomenon found in some exactly solvable PT-symmetic potentials and demonstrated that it occurs for any PT-symmetric Natanzon-class potentials for which the breakdown of PT symmetry can occur. The accidental crossing of energy levels occurs when the potential possesses two series of bound-state levels discriminated by the q=+/- quasi-parity quantum number, and a potential parameter is tuned to specific values. Then energy levels with different n and q become degenerate, and the corresponding wave functions become linearly dependent [QM.2].

Following the invitation of C. M. Bender, a chapter on exactly solvable PT-symmetric potentials was completed for a monograph that gives a comprehensible account of PT-symmetric quantum mechanics. The chapter contains 40 pages, about 100 references, and summarizes the status of the field in a self-contained form. It discusses the techniques of generating exactly solvable potentials as well as their classification. The adaptation of these methods to PT-symmetric complex potentials is presented and illustrated with numerous examples [QM.3].

We described the finite PT-symmetric extension of the square well potential. This project was inspired by results concerning the PT-symmetric Rosen-Morse II potential $V(x)=v/\cosh^2(x)+ iw \tanh(x)$, which has similar structure, and which was found to exhibit unusual features among PT-symmetric potentials. We determined the general solutions and constructed the T transmission and R reflection amplitudes. We searched for the poles of T to identify the bound-state solutions. It turned out that only solutions with real energy eigenvalues can be found, in agreement with the results concerning the PT-symmetric Rosen--Morse II potential. We attributed this finding to the asymptotically non-vanishing imaginary potential components [QM.4]. As a further link between the two potentials, we constructed their common limit: the potential containing a real Dirac-delta function with an imaginary step function. We poved that the solutions of this potential are obtained in the same form by taking the appropriate limit of both potentials [QM.5].

Eigenvalue problems of differential operators play a central role in quantum physics. The mathematical study of singular potentials and the self-adjoint extension of the corresponding operators inspired a mathematically oriented study concerning hypergroups [QM.6, QM.7]

We studied a class of potentials beyond the Natanzon class, by considering solutions of the Schrödinger equation in terms of the bi-confluent Heun equation. We applied the general methods to the sextic oscillator as a specific example by expanding its solutions in terms of Hermite functions. We showed that for the reduced version of this potential, i.e. without quartic term, the solutions can be written in a polynomial form, and reproduced solutions obtained earlier within the framework of quasi-exactly solvable potentials [QM.8]. Later we considered the general problem and non-polynomial solutions. However, with special choice of the parameters polynomial solutions can be obtained, and we showed that these match with the QES solutions of sextic oscillator [QM.9]. We also considered the QES solutions of the sextic oscillator to describe shape phase transitions of nuclei within the Bohr Hamiltonian. With this we extended our previous results, by which the energy spectrum and the electric quadrupole transition rates could be calculated exactly for solutions containing polynomials up to second order. Now we also included polynomials up to third order after showing that exact results can be obtained by calculating analytically the three real roots of a cubic algebraic equation [QM.10].

As another extension of solvable potentials beyond the Natanzon class, we considered the rationally extended harmonic oscillator potential, the solutions of which are obtained in terms of X_1-type exceptional Laguerre polynomials. We considered a rather general form of supersymmetric quantum mechanical transformations to generate potentials from the harmonic oscillator potential. In our pedagogical work we showed that the extended harmonic oscillator potentialcan can be construct within this formalism. The same formalism was used to demonstrate that these latter potentials satisfy the requirement of shape invariance [QM.11].

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Changes with respect to the original plans

Personnel:

There was a change in one of the junior participants: József Kovács replaced László Vajtay (see the explanation on the web-based report). This change had no effect on the total quantity of the work force (FTE) planned originally.

Budget:

Significantly less money was spent on ***Travel and conferences*** than planned. The reason was mainly that our participation at conferences turned out to be cheaper than expected for two reasons: 1. We often attended conferences as invited speakers, so the registration fee and accommodation costs could be spared. 2. The number of conferences organized outside Europe turned out to be lower than expected.

Also less funds were spent on ***Miscellaneous costs*** than expected. The reason for this is two-fold: 1. Originally the domestic costs of conference visits (travel within Hungary to the airport) were planned at this item, while due to regulations introduced later these costs were eventually counted at conference visits. 2. We expected a larger number of foreign visitors.

The costs for ***Investments*** turned out to be higher than planned. The main reason is that originally softwares were planned at ***Consumables***, but later, with the change of regulations they were counted at ***Investments***. It has to be added that the Budget plan was developed according to the regulations that were in effect at the time of submitting the proposal and later the Contract with OTKA.

Cost for ***Consumables*** also turned out to be higher than planned. The reason is that we used the allowed range accountable at this item to spend the extra funds left over at other items.

We initiated in April 2019 the relocation of the extra funds from ***Travel and conferences*** to ***Personnel costs***, ***Indirect personnel costs*** (salary + social security fee) and ***Investments***.

Research:

There were minor deviations from the Work plan, which may be justified by the partially changing focus of the research trends during the five years of the project. The most significant change was that we were unable to establish a link between the formalism of complex scaling and PT symmetry, or, in general, pseudo-Hermiticity. The reason may be that in PT symmetry typically one-dimensional systems are discussed, while in the complex scaling problems defined in 3 spatial dimensions are considered. Perhaps a different realization of pseudo-Hermiticity would be needed to reach our aim. It has to be noted though, that we are unaware of any advance in the literature in this field. There are also some results that are related to topics not planned five years ago, but the investigation of which became timely during the project [NTP.7, QM.3, QM.8, QM.9].