EXPECTATION VALUES DYNAMICS OF QUANTUM SYSTEM WITH SINGULARITIES VIA PROBABILISTIC EVOLUTION APPROACH, PSEUDO EXPECTATION VALUES, WEIGHTS, PERTURBATION EXPANSION AND PADE APPROXIMATION

SUMMARY

Since every physical system, living or non-living, is made up of quantum systems, understanding the dynamics of quantum systems is important in diverse fields of science and quantum dynamics has become an active field of research in recent decades. Yet, existing tools are not enough to exactly solve the dynamical equations for most quantum systems. In this thesis study, strong mathematical tools that have been developed in our research group's studies supervised by Professor Metin Demiralp are used to overcome this non-solvability, combined with other tools and new ideas to propose efficient mathematical algorithms to deal with the difficulties arising from the singularities in Hamiltonian systems. To this end, Hydrogen-like and screened Coulomb potential systems has been the other main focus of the study.

Probabilistic Evolution Theory (PREVTH) is one of the mentioned tools and has been devoloped mainly to solve inital value problems of first order autonomus explicit ODE sets, but also has been used successfully in recent studies to construct expectation value dynamics for certain quantum systems. The main idea of using PREVTH for quantum dynamics applications is to investigate the dynamics of the systems without explicitly solving Schrödinger equation, as it is not exactly solvable for most quantum systems. PREVTH enables us to use linear algebra tools and then can be manipulated by using Kronecker algebra.

Thesis is organised as follows. Second section focuses on constructing the mathematical model for quantum systems under consideration in a way to ease the investigations.

In the third section, PREVTH is revisited to construct expectation value dynamics. An ODE set over expectation values of quantum mechanical operators which then can be solved by using PREVTH, is constructed using Poisson Bracket algebra. This means Poisson brackets of momentum and position operators with system Hamiltonian are evaluated. This set of system's fundamental operators is not multinomially closed under the Poisson Bracket operation. To this end, new operators might be defined using existing operators and introduced to system's operator basis set to obtain a closed set under Poisson bracket operation. To achieve a concise format, a vector $\widehat{\mathbf{s}}$ including the basis set operators as elements is defined and called "system vector ". The Poisson bracket of system vector with Hamiltonian is expressed as an infinite Kronecker power series in system vector and then approximated by taking the first n term into consideration, resulting in nth degree multinomial right hand side. Here another tool which we have called "space extension "is used to achieve conicality. A recursive formula is obtained between the expactation values of extended space elements by applying Fluctuationlessness Theorem. An implementation has been done for Hydrogen-like systems.

The fourth section focuses on singularities through Fluctuation Approximation based investigations. Assuming that the evolution of expectation value of an quantum operator can be expressed as a Maclaurin series, it is shown that this series is actually the equivalent of fluctuation expansion if the system Hamiltonian is autonamous. Implementation for Hydrogen-like systems shows that fluctuations may not be evaluated for every operator due to the singularities in system Hamiltonian. To overcome this, one way would be chosing an appropriate wave function, but this will reduce the set of inital wave functions. Another way might be constructing a different structure for the operator to suppress the singularity which seems more appropriate for this study. The image of initial wave function under Hamilton operator may also not stay in the same space with the inital wave function due to the Hamiltonian singularities. And more generally, staying in the space under $\widehat{H}^j$ does not guarantee to stay in the space under $\widehat{H}^{j+1}$ where j is a positive integer. The space which is closed under all positive integer powers of Hamilton operator will be spanned by the eigenfunctions of Hamilton operator. Since constructing this space is not an easy way to go, working in the space spanned by the image functions seems a better option. To this end, singularity suppressing structure has been searched first, to be introduced as a weight operator into the integrals that are needed to be evaluated. This leads to a new definition for the expectation values which we call “pseuodo expectation values ”and can be considered as weighted expectation values. Although they are not the actual expectation values, they still can give information about the system. Implementing these findings to hydrogen-like systems converted the process of evaluating the integrals into derivation and linear algebra operations.

The fifth section is focused on derivation of perturbation series expansions for the energy and the relevant wave function of a screened Coulomb potential system.The perturbed problem is defined by manipulating system’s Schrodinger equation, and instead of introducing an artificial perturbation parameter to the equation, screening parameter is taken as the perturbation parameter. Expanding all operators and functions appearing in the equation into Maclaurin series with respect to screening parameter, relevant recursions are obtained in an uncomplicated way. Perturbation components and convergence issues are investigated.The state identity number seems to have impact on convergence, as well as asymptotic behaviors of Maclaurin coefficients of the screening function. These perturbation based investigations are also used to evaluate expactation values and fluctuations of position and momentum operators. It has shown that phase spaces based on momentum and position are not good options to investigate system dynamics. Taking initial wave function from Hamilton eigenspace, spaces based on Hamilton and position operators are shown to be more convenient. Also it has seen that Maclaurin series in screening parameter for expectation values are divergent for all screening parameter values. However investigations on asymptotic behaviour shows that this divergence can be converted into convergence. To this end, Borel sum type applications have been considered. Trials and searches carried out for this purpose has shown that the diagonal sequences in Padé table seem to be more fruitful. Satisfactory results have been obtained using the main diagonal sequences for energy perturbation series. Also it has been found that the Padé approximant sequence with denominator polynomial’s degree greater than numerator polynomial’s degree by 2 as giving the best approximation for the expectation values. Numerical implementations have been proposed and graphics for energy perturbation approximants have been obtained by MuPAD scripts. The main contribution of this section is showing that accurate information can be produced from diergent series.

The sixth section finalizes the thesis remarking important findings in itemized format. There have been also some other trials that have failed or not haven't been finalized for quantum systems, yet brought important findings in mathematical sense. The most fruitful ivestigations from those trials also given in additions section. The first one proposes a method for PREVTH applications where second degree right hand side can not be achieved. The second one proposes a detailed Mathematical Fluctuation Theory based investigation to evaluate time dependent expectation values.