Solving the Schrödinger equations of interstellar molecules

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Schrödinger equation is the most fundamental equation in quantum mechanics and it governs most of phenomena in molecular science including space chemistry of interstellar molecules. In spite of that importance, however, the exact solutions of this equation have not been able to be solved for over 80 years. Recently, Nakatsuji was successful to propose a new general theory, the free complement (FC) method, for solving this equation [1] and theory was also extended to solving the relativistic Dirac equation [2]. In the tests with a few electron systems, the extremely accurate results could be obtained [3] and the stringent tests of the exactness of the obtained wave functions indicate how accurately the FC wave function can provide close to the exact solutions [4]. With different from ordinary quantum chemistry, the FC method is based on the idea that the exact wave function should be obtained by a functional of the Hamiltonian. Therefore, the adequate wave functions are automatically generated by the system's Hamiltonian itself and this feature is significant for space chemistry that appears the various unusual situations and environments.

We have applied the present method to various atoms and molecules [5] and also interstellar species with the environments of space. In the latter case, the following situations are rather significant: the accurate excited states and theoretical spectra, non Born-Oppenheimer (non-BO) calculations which include the quantum effect of nuclear motion [6], solving the relativistic Dirac equation [2], and atoms and molecules in an extreme environment such as under the strong magnetic fields [7]. For example, the non-BO calculations can provide the vibronic and rotational states including all the quantum effects of electron and nuclear motion, whose theoretical results are directly comparable with the observations and/or experimental results. For the last topic, the Universe's strongest magnetic field was observed on Magnetar object surface in space and the quantum mechanical calculations in magnetic fields become realistically important.

Thus, the present method indicated a high potentiality to be helpful for doing space chemistry in Schrödinger accuracy. We now continue to develop the methods and computational algorithms to be more easily applicable to more general atoms and molecules.

References

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This answer understands the term â€œSchrA¶dingerâ€™s equationâ€ in its general sense, that is, the governing equation of quantum mechanics, of possibly many particles. In general we donâ€™t know how, and people try very hard to find new and clever ways of...Â This involves advanced experimental setups, manipulating a few atoms (or molecules, or photons), often at extremely low temperature (close to the absolute zero). This is â€œcheatingâ€ in some sense because as scientists we want to solve the SchrÃ¶dingerâ€™s equation independently and confront the theoretical predictions with experiments.Â Because the Schrodinger equation cannot always be solved analytically. The electronic SchrÃ¶dinger equation describes fundamental properties of molecules and materials, but can only be solved analytically for the hydrogen atom. The numerically exact full conguration-interaction method is exponentially expensive in the number of electrons. Quantum Monte Carlo is a possible way out: it scales well to large molecules, can be parallelized, and its accuracy has, as yet, only been limited by the exibility of the used wave function ansatz. Here we propose PauliNet, a deep-learning wave function ansatz that achieves nearly exact solutions of the electronic SchrÃ¶dinger equ... The SchrÃ¶dinger Equation is a crucial formalism at the center of quantum mechanics. It is used to work out how quantum systems are, and how they evolve. It is also very much a challenge to solve precisely for a system made of more than a few particles, with approximations use in most cases. Computational methods are used to solve the equation for many systems, and a new study published in Nature Chemistry has put forward a new method.Â Solving the equation can provide insights into the formation and behavior of molecules that several of the current methods canâ€™t provide. This has often been too laborious to be worth it, hence why this method could be a game-changer. PDF | A local SchrÃ¶dinger equation (LSE) method is proposed for solving the SchrÃ¶dinger equation (SE) of general atoms and molecules without doing | Find, read and cite all the research you need on ResearchGate.Â Solving the Schro. Â¨ dinger Equation of Atoms and Molecules without Analytical Integration Based. on the Free Iterative-Complement-Interaction W a ve Function. H. Nakatsuji By solving Newtonâ€™s equation we can determine the position of a particle as a function of time, whereas by solving SchroÂ¨dingerâ€™s equation, what we get is a wave function Î¨(x, t) which tells us (after we square the wave function) how the probability of nding the particle in some region in space varies as a function of time. It is possible to proceed from here look at ways and means of solving the full, time dependent SchroÂ¨dinger equation in all its glory, and look for the physical meaning of the solutions that are found.Â metal, or gas molecules contained in a bottle, this model serves to describe very accurately. the quantum character of such systems.