Deep Learning Solves the Schrödinger Equation, a Fundamental Problem in Quantum Mechanics.

The Schrödinger equation (SE) is a keystone of quantum physics, and it governs all phenomena of the microscopic world. Solving this equation helps predict the behavior of quantum systems such as molecules which means that the chemical and physical properties can be obtained with plausible accuracy. This has significant implications in advancing our technology and industrial capability to a comparable level with the sci-fi version of the future. However, solving the SE appears extremely difficult and is resource-intensive and time-consuming work. Additionally, an exact solution is not mathematically accessible with the current numerical and analytical methods due to the complexity of the problem. But, thanks to the emergence of deep learning, it is possible now to obtain a solution with an unprecedented combination of accuracy and computational efficiency.

Deep learning has transformed many technologies and scientific areas, and now it can assist with solving the SE. If this task succeeds, needless to say, that is an extraordinary breakthrough.

To solve the SE, researchers need a high-dimensional mathematical entity, dubbed wave function, that describes the behavior of electrons in a molecule. When dealing with many electrons, the relationship between these electrons must be incorporated in the wave function, which renders it very complicated. Most techniques used by researchers to represent the wave function are impractical to make calculations on a system of many atoms. Therefore, the focus is diverted into determining the system's energy instead of the wave function, but that limits how much we can predict from the system. Here, deep learning can enter the arena and be utilized in finding a good representation of the wave function.

Artificial neural networks (ANN) can be a new way to represent the wave function of many electrons. To do that, we need the exemplary network architecture and to build the fundamental physics property of the electrons in this network. In particular, the exchange principle; states that if two electrons exchange their places, the wave function should change sign. We turn into the Quantum Monte Carlo method (QMC) to effectively use such a network, which provides an accurate solution with an acceptable computational cost. The idea is to integrate ANN as a wave function representative in the QMC method. This procedure has the potential of exceeding all state-of-the-art QMC methods in terms of accuracy and computational complexity.

The deployment of deep learning to tackle the problem of SE is still fundamental research in its foundation, and there are many challenges yet to overcome in this subject. But it is an innovative approach to a long-standing problem in molecular and material science. To date, this new approach shows tremendous progress, which holds big promises and excites the scientific community about the possibilities it opens up.