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Investigating electron structure with the GW method

We are living in an era that millions of books can be stored in a disk of a coin's size, trains can float above the rail and reach a speed of 500 km/h. These fascinating inventions, having changed our living style, are brought by the development of material science. Materials are composed of atoms, and the atoms can be seen as electrons moving around the nuclei. Thus the properties of materials are decided by the way how the nuclei are arranged and how electrons interact with each other. To push the frontier of material research forward, we want to understand the interactions in a microscopic level.

Quantum mechanics is a powerful tool in the modern physics, especially when the investigated system is microscopic. Based on the wave-particle duality and the quantization of some observables (energy, momentum, etc.), the quantum theory managed to explain the experiment results of black-body radiation and photoelectric effect, which was a puzzling reef for the ship of classical theory. Applications of the theory leads to a variety of revolutionary and promising ideas, including lasers, quantum computing, etc.

One simple example of a microscopic quantum system is the single electron system: a single electron, perhaps our most familiar subatomic particle, trapped in some potential. The single electron system, having the clearest electron structure, can be well described by the Schrödinger equation. This simple model can be used to explain some phenomena, like the spectrum of hydrogen atom.

Is that good enough? To be an optimistic physicist, we can say that more complicated multi-electron cases can be dealt with the same procedure, by constructing a set of Schrödinger equations, as we usually do in classical mechanics and fixing the Hamiltonian correspondingly. However, this is too idealistic. The electrons are correlated with each other by Coulomb interactions, which means the complexity of the Hamiltonian. To make matters worse, the number of equations is fairly enormous. For instance, a bulk of semiconductor may contain 10^{30} electrons. It may be easy to monitor someone restrained in his house, while to watch over everyone in Stockholm is quite another story, not to say when there are 10^{30} objects looking exactly the same.

That is, we need smarter methods to solve the many-body problem. In this project, we will try to simplify a powerful approximation, the GW method. The GW method can be used to deal with large and complicated system, however, the computation is time and resource consuming. We aim to use the uniform electron gas system to get some direct and detailed information about the method, so that we can get higher efficiency when applying it to real and novel materials.

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References

[1] Ferdi Aryasetiawan and Olle Gunnarsson. The *GW* method. *Reports on Progress in Physics*, 61(3):237, 1998.