Possible Design and Development of Ultra-high Strength Permanent Magnet Based on Fundamental Conceptual Change in Magnetism

Yoshiyuki Kawazoe
(New Industry Creation Hatchery Center, Tohoku University, Sendai, Japan)

After the discovery of neodymium magnet $Ne_2Fe_{14}B$ in 1984 by Dr. Masato Sagawa, no permanent magnets better than that have been commercialized over 35 years. As a matter of course, a number of developments have been done to improve its properties. In the long history of magnet development, basically experimental findings have led the improvements. Theory basically contributes to explain the phenomena realized by experimental studies. We have proved the fundamental and serious misunderstanding in the origin of magnetism, which has been explained in the standard textbooks that exchange interactions between electrons reduce the system energy for the magnetic ground state. This misunderstanding originated in the old and famous paper by Slater in 1929 just after the invention of quantum mechanics (Ref. 1) which explains well the Hund's first rule (Among the degenerated low-lying states, the highest spin state is the ground state.), and is still introduced in the standard textbooks in magnetism. However, when Slater developed his theory, he did (could) not include the effect from the nucleus, and simply electron-electron interactions were considered.

Slater's explanation of magnetism has been claimed by Davidson (Ref. 2) and other researchers. They basically solved the magnetic ground state in high accuracy including all the interactions between nucleus and electrons, and proved that the effect from nucleus-electron interaction contributes most to reduce the system energy to realize the magnetic ground state, where electron-electron exchange energy even increases the energy. However, these studies are only considered to be for specific cases, and not accepted as a general aspect of magnetism. We have solved the magnetic ground state in atoms and molecules in high accuracy and proved that the Davidson's theoretical explanation holds in general for the magnetism in atoms and molecules (Ref. 3). We have proved based on checking the virial theorem satisfaction. By this way, most of the standard theories in magnetism such as Slater's perturbation theory for Hund's rule, Heitler-London model for hydrogen ground state, Hubbard model for magnetic and superconducting states, etc. are fundamentally incorrect, since they violate the virial theorem (for the equilibrium state V/T=-2 should hold, and this is a necessary condition for all Coulombic systems.).

Recent progress in computer power has made it possible to apply the density functional theory (DFT) to compute numerically the magnetic ground state. Although DFT is called *ab initio* simulation, within the theory it is not possible to determine the electron exchange-correlation functional and the researchers introduce parameters, such as LDA+U, hybrid functional, etc. which try to fit to the experimental observations (therefore, not *ab initio* but phenomenology). These phenomenological methods can be checked by virial theorem satisfaction; violation means incorrect. We therefore know now exactly what we should do to be able to predict new permanent magnet; what we should do is to solve the quantum mechanical equation without any parameters. Although this is costly, it is important to have good guidelines for theoretical prediction of new magnet without experimental help, which is time consuming and costly.

We have successfully performed several theoretical predictions of new magnets; (1) Atom cluster based high magnetic moment magnets, (2) Two dimensional magnets with only light weight elements, (3) Carbon based magnets, etc. These new magnets have been predicted with confidence, because we have solved the Schroedinger equation for magnetic ground state with no parameters for fitting to experiments.

References

1) J. C. Slater, "The Theory of Complex Spectra", Phys. Rev. 34, pp. 1293-1322 (1929).
2) E. R. Davidson, "Single-Configuration Calculations on Excited States of Helium", J. Chem. Phys. 41, pp.656-658 (1964).
3) T. Oyamada, K. Hongo, Y. Kawazoe and H. Yasuhara, "Unified Interpretation of Hund's First and Second Rules for 2p and 3p Atoms", J. Chem. Phys., 133[16], pp.164113-(1-19), (2010).