

Extended constrained-search theory and its applications

Masahiko Higuchi¹ and Katsuhiko Higuchi²

¹*Department of Physics, Faculty of Science, Shinshu University, Matsumoto 390-8621, Japan*

²*Graduate School of Advanced Sciences of Matter, Hiroshima University, Higashi-Hiroshima 739-8527, Japan*

higuchi@shinshu-u.ac.jp (corresponding author)

The pair density (PD) functional theory has recently attracted particular interest because it provides the obvious way to improve on the density functional theory (DFT) [1-9]. Ziesche first proposed the PD functional theory about a decade ago [1,2], and then many workers followed his work and have developed a variety of approaches [3-9].

Very recently, we have proposed an approximate scheme for calculating the PD on the basis of the extended constrained-search theory [10–14]. By introducing a noninteracting reference system [10,11], the resultant PD corresponds to the best solution within the set of PDs that are constructed from a single Slater determinant (SSD). This PD functional theory has two kinds of merit. The first is that the reproduced PD is necessarily N -representable. This is a strong merit because the necessary and sufficient conditions for the N -representable PD are not yet known exactly. The second merit is the tractable form of the kinetic energy functional. The kinetic energy functional cannot exactly be written by using the PD alone. Some approximation is required. In this theory, we have successfully given an approximate form of the kinetic energy functional with the aid of the coordinate scaling of electrons [10].

On the other hand, a significant problem remains in that approach [10]; namely, there exists the possibility that the solution might be far from the correct value of the ground-state PD. This is because the search region of the PDs may be smaller than the set of N -representable PDs. In order to improve the PD functional theory, we have to extend the search region of the PDs to the set of N -representable PDs as closely as possible.

In this paper, we present a density functional scheme for calculating the PD by means of the correlated wave function.[15] The Jastrow wave function is adopted as the correlated wave function. By using the lowest-order approximation to the Jastrow wave function PDs, the search region for the ground-state PD is substantially extended as compared with our previous theory [10, 11]. The variational principle results in the simultaneous equations that are practicable to calculate the ground-state PD [15].

References

- [1] P. Ziesche, *Phys. Lett. A* **195**, 213 (1994).
- [2] P. Ziesche, *Int. J. Quantum Chem.* **60**, 1361 (1996).
- [3] A. Gonis, T. C. Schulthess, J. van Ek, and P. E. A. Turchi, *Phys. Rev. Lett.* **77**, 2981 (1996).
- [4] A. Gonis, T. C. Schulthess, P. E. A. Turchi, and J. van Ek, *Phys. Rev. B* **56**, 9335 (1997).
- [5] A. Nagy, *Phys. Rev. A* **66**, 022505 (2002).
- [6] A. Nagy and C. Amovilli, *J. Chem. Phys.* **121**, 6640 (2004).
- [7] P. W. Ayers, *J. Math. Phys.* **46**, 062107 (2005).
- [8] P. W. Ayers and M. Levy, *J. Chem. Sci.* **117**, 507 (2005).
- [9] P. W. Ayers, S. Golden, and M. Levy, *J. Chem. Phys.* **124**, 054101 (2006).
- [10] M. Higuchi and K. Higuchi, *Physica B* **387**, 117 (2007).
- [11] M. Higuchi and K. Higuchi, *J. Magn. Magn. Mater.* **310**, 990 (2007).
- [12] M. Higuchi and K. Higuchi, *Phys. Rev. B* **69**, 035113 (2004).
- [13] K. Higuchi and M. Higuchi, *Phys. Rev. B* **69**, 165118 (2004).
- [14] K. Higuchi and M. Higuchi, *Phys. Rev. B* **71**, 035116 (2005).
- [15] M. Higuchi and K. Higuchi, *Phys. Rev. A* **75**, 042510 (2007).