Smoothed Particle Method for the Real-Space Electronic Structure Calculation

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In large-scale calculation such as hydrodynamics analysis, Smoothed Particle Hydrodynamics (SPH) is used as a typical mesh free particle method, and is very convenient and applicable for dealing with complex shapes, large deformations, and free surfaces. Currently, SPH is used in various fields for solving non-hydrodynamic partial differential equations such as the wave equation, Maxwell's equations, and Poisson's equation. However, it lacks sufficient accuracy. To realize a similar level of accuracy, many more particles are necessary than mesh points in the finite difference method (FD). Thus, it has not been evaluated sufficiently in quantum mechanical problems, because they require fairly high accuracy. As a higher-accuracy method in an improved method of SPH, Modified Smoothed Particle Hydrodynamics (MSPH) has recently been developed. Although various improved versions of SPH have been proposed, it is reported that MSPH has higher accuracy than other versions.

We have applied MSPH to quantum mechanical problems. The Schrödinger equation of a harmonic oscillator and the hydrogen atom are solved. Since we can analytically obtain exact solutions for these problems, it is quite efficient to evaluate MSPH in the quantum mechanical problems. The calculated results for MSPH are in good agreement with the analytical solutions. As a result, we have successfully shown that MSPH is efficient, and can therefore be applied to quantum mechanical problems with adequate accuracy. The results of using this method are also compared with those of the traditional FD and the standard SPH. The accuracy, however, depends on the arrangement of the particles. To obtain high accuracy, many particles should be distributed in the area where the wave function changes significantly.

In this paper, we demonstrate the importance of non-uniform particle distribution. Since the electron density of molecules is localized for example, fewer particles are necessary in the low electron density region and many particles are distributed in the high electron density region. We have introduced the smooth particle arrangement based on the electron charge density, and show the efficiency of MSPH in the electronic structure calculations.