

RELATION BETWEEN PFAFFIAN AND NEERGAARD-WUST FORMULA TO EVALUATE HARTREE-FOCK-BOGOLIUBOV NORM OVERLAP KERNELS

Makito Oi¹, Yang Sun² and Takahiro Miusaki¹

¹Institute of Natural Sciences, Senshu University, Tokyo 101-8425, Japan

²Department of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai 200240, China

Evaluation of norm overlap in the Hartree-Fock-Bogoliubov (HFB) theory has been a long-standing theoretical problem as well as a challenge from a numerical point of view. In 1960s', a formula was proposed by Onishi and Yoshida to provide an analytical form to evaluate the HFB norm overlap. However, its application to numerical investigations faced a difficulty coming from the so-called "sign problem". The sign problem is originated from the presence of the multi-valued complex function (square-root operation) of the Onishi formula. Although Hara, Hayashi and Ring managed to circumvent the sign problem in particular cases by introducing fine-mesh discretization approach, their approach was found not to be always feasible, in particular, for cranked HFB states to deal with high-spin nuclear states.

Recently, a new formula was proposed by Robledo, which is expressed in terms of the Pfaffian. This new formula is free from the sign problem due to an elimination of the square root operation in the Onishi formula in an algebraic way. This success is basically owing to the relation between the Pfaffian and the determinant.

In 1980s', soon after the work by Hara, Hayashi and Ring, Neergaard and Wust proposed an alternative method to evaluate the HFB norm overlap. For unclear reasons, their work was ignored by the majority of the community.

We found recently that Neergaard and Wust (NW) method is equivalently effective as the Pfaffian formula by Robledo, even in the numerical applications. We even noticed that there are cases that NW method works faster than the Pfaffian formula in its numerical implementations. We would like to present how NW method is related to the Pfaffian from a theoretical point of view.