Non-relativistic expansion of Dirac equation by the reconstituted Foldy-Wouthuysen transformation†

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In the past few decades, the density functional theory (DFT) has been successfully applied in both the non-relativistic and relativistic frameworks to describe the ground-state and excited-state properties of thousands of nuclei in a microscopic and self-consistent manner. However, the connection between these two frameworks remains unclear. The non-relativistic expansion of the Dirac equation is considered to be a potential bridge connecting these two frameworks.[1,2)]

Recently, the reconstituted similarity renormalization group (SRG) method was proposed.[3)] Compared to conventional methods, the reconstituted SRG method not only showed a much faster convergence, but also yielded single-particle densities $\rho_v(\boldsymbol{r}) = \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})$ that are closer to the exact values. Moreover, for the single-particle scalar densities $\rho_s(\boldsymbol{r}) = \psi^\dagger(\boldsymbol{r})\gamma_0\psi(\boldsymbol{r})$, the γ_0 matrix should be transformed in the same manner as the Dirac Hamiltonian. However, the original Dirac Hamiltonian is operated with infinite steps of unitary transformations in both the conventional and reconstituted SRG methods. Therefore, the calculations of single-particle scalar densities are not trivial in SRG methods.

Meanwhile, with the consideration of the strong scalar potential, we further applied another well-known technique, the Foldy-Wouthuysen (FW) transformation, to the general cases in the covariant DFT and performed the corresponding expansion up to the $1/M^4$ order.[4)] With the present FW transformation, all the unitary transformations involved hold explicit forms. On this basis and with inspiration from the reconstituted SRG method, we developed the reconstituted FW transformation. By replacing the bare mass M with the Dirac mass M^* and defining the corresponding new operators, the contributions related to the higher powers of the quotient of the scalar potential and the bare mass are absorbed into the lower orders.

As a step forward, the so-called picture-change error,[5,6)] *i.e.*, the difference between the densities calculated in the Schrödinger picture and those obtained in the Dirac picture, has also been investigated through calculations starting from basic field operators. After considering such picture-change errors, *i.e.*, the relativistic corrections, both the single-particle vector and scalar densities become much closer to the exact results. In addition, the difference between ρ_v and ρ_s originates from the $1/M^{*2}$ order, as does the relativistic correction $\Delta\rho$. Therefore, the relativistic corrections also play a crucial role in the difference between the vector and scalar densities.

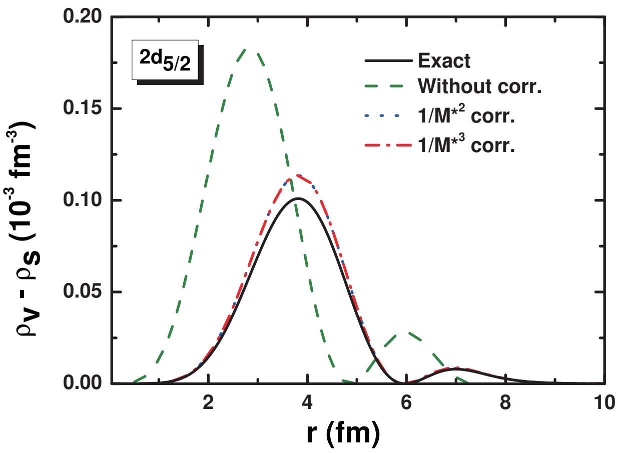

Fig. 1. Difference between the single-particle density and the single-particle scalar density for the neutron $2d_{5/2}$ state of nucleus ^{208}Pb.

By taking the $2d_{5/2}$ state of ^{208}Pb as an example, the difference between the single-particle density and the single-particle scalar density is shown with the black solid line in Fig. 1. The result without any relativistic correction is shown with the olive dashed line, while the results calculated with the consideration of relativistic corrections up to the $1/M^{*2}$ and $1/M^{*3}$ orders are shown with the blue dotted and red dash-dotted lines, respectively. It can be seen from Fig. 1 that the differences between the results without the relativistic corrections and the exact values are systematic. There are differences in the positions of peaks and nodes as well as the amplitudes. In contrast, the results with the relativistic corrections remarkably reproduce the behavior of the exact values, particularly in terms of the positions of peaks and nodes.

Based on the above discussions, the reconstituted FW transformation is a promising method to connect the relativistic and non-relativistic DFTs for future studies.

References
1) P. G. Reinhard, Rep. Prog. Phys. **52**, 439 (1989).
2) M. Bender, P. H. Heenen, P. G. Reinhard, Rev. Mod. Phys. **75**, 121 (2003).
3) Y. X. Guo, H. Z. Liang, Phys. Rev. C **99**, 054324 (2019).
4) Y. X. Guo, H. Z. Liang, Chin. Phys. C **43**, 114105 (2019).
5) M. Douglas, N. M. Kroll, Ann. Phys. (N. Y.) **82**, 89 (1974).
6) B. A. Hess, Phys. Rev. A **33**, 3742 (1986).

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