Non-relativistic expansion of Dirac equation with spherical vector and scalar potentials†

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Since the 1970s, the density function theory (DFT) in both the non-relativistic and relativistic frameworks has succeeded in microscopically describing the ground-state and excited-state properties of thousands of nuclei in a 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)]

In 2012, Guo[3)] first applied the similarity renormalization method (SRG)[4,5)] to perform the non-relativistic expansion of the Dirac equation. By using SRG, the Dirac Hamiltonian can be transformed into a diagonal form after infinite steps of unitary transformations, *i.e.*, the eigenequations for the upper and lower components of the Dirac spinors can be decoupled. Furthermore, the Hamiltonian $\mathcal{H}$ thus obtained was expanded in powers of $1/M$ (with M being the bare mass of the nucleon).

The results up to the $1/M^3$ order were calculated.[3)] However, the differences between the corresponding results and the exact ones were still approximately 1 MeV. Therefore, it is necessary to include higher-order corrections. In this work, the results up to the $1/M^4$ order are calculated, and the differences between the calculated and exact values are less than 0.2 MeV for all states.

From a simple observation, some geometric progressions are determined in the results of the conventional SRG method. This observation is reminiscent of the idea of resummation. In the reconstituted SRG method, replacing M with the Dirac mass $M^* = M+S$ (with S being the scalar potential) not only yields the non-relativistic expansion up to a certain order, but also sums up the terms that belong to their families up to infinite order. Consequently, the convergence of the reconstituted SRG is much faster than that of the conventional SRG. The spectrum of the Hamiltonian $\tilde{\mathcal{H}}$ thus obtained is shown in Fig. 1.

The Foldy-Wouthuysen (FW) transformation[6–9)] is another non-relativistic expansion method that has been widely used. Both the FW transformation and SRG method provide a systematic way to perform the non-relativistic expansion of the Dirac equation up to an arbitrary order. Thus, we also apply the FW transformation to a general case of the covariant DFT. In this work, the results with the FW transformation have also been obtained up to the $1/M^4$ order and compared with the corresponding results obtained using conventional SRG method. It seems that the FW transformation and the conventional SRG method produce the same results up to the second order, but they show differences from the third order. By introducing a block-diagonal transformation Ξ, we determined that the results obtained using the conventional SRG method are equal to those obtained using the FW transformation with an additional unitary transformation Ξ. Consequently, the spectrum of the single-particle energy obtained using the FW transformation is identical to that obtained using the SRG method.

With the applications of the SRG method and FW transformation, the bridge connecting the DFT in the relativistic and non-relativistic frameworks is now conceivable.

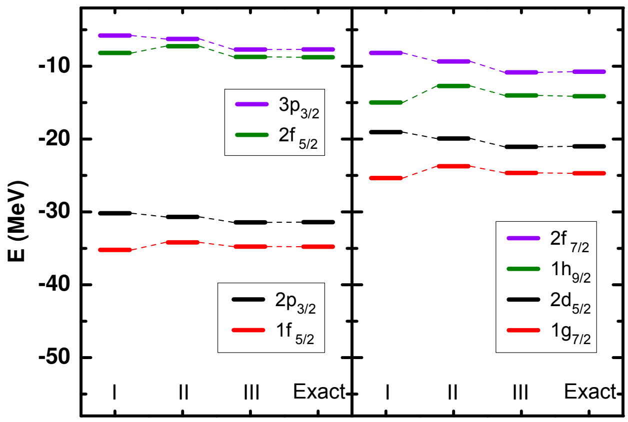

Fig. 1. Energy spectrum of $\tilde{\mathcal{H}}$ for the four pseudospin partners calculated using the reconstituted SRG method. The first, second, and third columns show the single-particle energies up to the first, second, and third orders, respectively. The last column, labeled "Exact," shows the eigenenergies of the Dirac equation.

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