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Optimization of harmonic oscillator basis for static and dynamic calculations

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Abstract.

Density functional theory (DFT) is the only microscopic framework nowadays which allows the description of all nuclei across the nuclear chart [1]. In most of the calculations, it employs the basis set expansion approach in which the wave functions are expanded into the basis of harmonic-oscillator (HO) wave functions [2]. Paradoxically, the parameters of such bases were never globally optimized: both in non-relativistic and covariant DFTs they were defined by the fit to a few nuclei more than thirty years ago. The present investigation focuses on the improvement of the accuracy of the description of static and dynamic physical observables in moderately sized fermionic basis within the framework of covariant DFT. The optimization of the basis allows to reproduce exact (i.e. infinite basis) solutions in the basis truncated at full N_F fermionic shells with high precision. The 30 keV accuracy in the reproduction of binding energies calculated in the infinite basis is achievable at $N_F = 20$ for meson exchange functionals [3], but mass-dependent basis reaching $N_F = 34$ in superheavy nuclei is required for point coupling functionals for the same accuracy [4]. The impact of basis extension to $N_F = 50$ has also been investigated for the monopole, dipole, quadrupole, and octupole resonances calculated in the relativistic random phase approximation (RRPA) and its extension by the particle-vibration coupling dubbed as relativistic time-blocking approximation (RTBA) for a selected set of spherical nuclei [5]. A considerable sensitivity of the strength distributions to the HO basis size is found, especially for low-spin resonances in the light neutron-rich nuclei.

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References

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