Modification of Lanczos method for high fidelity and scalability for electronic structure calculations

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The applicable area of quantum chemistry has been expanded to large and complex molecular systems due to the remarkable advance of parallel computing. In this study, we propose a new way to calculate a large number of eigenpairs with degeneracies and evaluate its performance on high performance computing environments. The newly proposed method is to run multiple Lanczos iterations with orthogonally selected initial vectors. An enough number of independent Lanczos iterations found eigenpairs without missing degenerated eigenvectors in real molecular systems. Also, it shows a high parallel efficiency up to 4096 cores with a two-level parallelization scheme and better performance than the locally optimal block preconditioned conjugated gradient method which is widely used in electronic structure calculations.