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An application of the shift-invert Lanczos method to the non-equilibrium Green's function method

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Describing transport properties of a many-body fermionic system is one of the most important topics in many fields of physics and chemistry.
To simulate the electronic properties of nanodevices, the non-equilibrium Green function method (NEGF) has been widely employed.
However, this method suffers from substantial numerical costs for a calculation of the Green function.
To overcome this problem, we propose a novel approach to significantly reduce the numerical cost of the NEGF by utilizing the shift-invert Lanczos method, where eigenstates of a Hamiltonian in the middle of the spectrum are selectively calculated.
We apply this procedure to model Hamiltonians for induced-fission reactions and demonstrate its effectiveness.
For instance, for a Hamiltonian with 66103 dimensions, we find that this method reduces the computation time by about a factor of 30 compared to a direct evaluation.

Primary author(s) : UZAWA, Kotaro (Kyoto University)

Co-author(s) : Prof. HAGINO, Kouichi (Kyoto University)

Presenter(s) : UZAWA, Kotaro (Kyoto University)

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