Recent Progress in Many-Body Theories (RPMBT22)



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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.

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