Minimax Isometry Method

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A compressive sensing approach for the Matsubara summation of many-body perturbation theory is presented. By constructing low-dimensional, almost isometric subspaces of the Hilbert space we obtain optimum imaginary time and frequency grids that allow for extreme data compression of fermionic and bosonic functions in a wide temperature regime. The method is applied to a low-scaling algorithm[1] of the random phase[2] and GW approximation[3, 4] of the grand potential for insulating and metallic compounds.

References

- M. Kaltak, J. Klimeš, G. Kresse, J. Chem. Theory Comput. 10, 6, 2498 (2014).
- [2] M. Kaltak, J. Klimeš, G. Kresse, Phys. Rev. B 90, 054115 (2014).
- [3] P. Liu, M. Kaltak, J. Klimeš, G. Kresse, Phys. Rev. B **94**, 165109 (2016).
- [4] M. Grumet, P. Liu, M. Kaltak, J. Klimeš, G. Kresse, Phys. Rev. B 98, 155143 (2018).