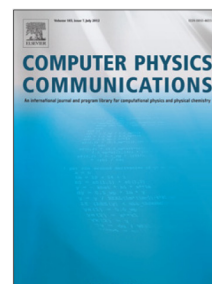


Accepted Manuscript

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PII: S0010-4655(17)30237-0
DOI: <http://dx.doi.org/10.1016/j.cpc.2017.07.017>
Reference: COMPHY 6277

To appear in: *Computer Physics Communications*

Received date: 3 December 2016
Revised date: 16 May 2017
Accepted date: 19 July 2017

Please cite this article as: E. Vecharynski, J. Brabec, M. Shao, N. Govind, C. Yang, Efficient block preconditioned eigensolvers for linear response time-dependent density functional theory, *Computer Physics Communications* (2017), <http://dx.doi.org/10.1016/j.cpc.2017.07.017>

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Efficient Block Preconditioned Eigensolvers for Linear Response Time-Dependent Density Functional Theory

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Abstract

We present two efficient iterative algorithms for solving the linear response eigenvalue problem arising from the time dependent density functional theory. Although the matrix to be diagonalized is nonsymmetric, it has a special structure that can be exploited to save both memory and floating point operations. In particular, the nonsymmetric eigenvalue problem can be transformed into an eigenvalue problem that involves the product of two matrices M and K . We show that, because MK is self-adjoint with respect to the inner product induced by the matrix K , this product eigenvalue problem can be solved efficiently by a modified Davidson algorithm and a modified locally optimal block preconditioned conjugate gradient (LOBPCG) algorithm that make use of the K -inner product. The solution of the product eigenvalue problem yields one component of the eigenvector associated with the original eigenvalue problem. We show that the other component of the eigenvector can be easily recovered in an inexpensive postprocessing procedure. As a result, the algorithms we present here become more efficient than existing methods that try to approximate both components of the eigenvectors simultaneously. In particular, our numerical experiments demonstrate that the new algorithms presented here consistently outperform the existing state-of-the-art Davidson type solvers by a factor of two in both solution time and storage.

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