

Minimization Principle for Linear Response Eigenvalue Problem with Applications

Ren-Cang Li *

April 5, 2012

Abstract

The linear response eigenvalue problem arising from the calculation of excitation states of many-particle systems, a hot topic among computational material scientists today for materials design to advance energy science. It is a large scale nonsymmetric eigenvalue problem (up to tens of millions in dimension) but has many of the symmetric eigenvalue problem's characteristics as this talk will show. We'll present a new minimization principle for the sum of the first few smallest positive eigenvalues, Rayleigh quotient-like projection matrices, and Cauchy-like interlacing inequalities. We will explain how this new minimization principle relates to some of the remarkable results of Kovač-Striko and Veselić (1995). Subsequently, we'll develop the best approximations of these smallest positive eigenvalues by a structure-preserving subspace projection. Based on these newly established theoretical results, we'll present conjugate gradient-like algorithms for simultaneously computing the first few smallest positive eigenvalues and associated eigenvectors. Finally, numerical examples will be presented to illustrate essential convergence behaviors of the proposed conjugate gradient-like methods with and without preconditioning.

*Department of Mathematics, University of Texas at Arlington, P.O. Box 19408, Arlington, TX 76019
(rcli@uta.edu.)