The forced oscillator method incorporating with the fast time-evolution algorithm

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In condensed matter physics, the eigenvalue analysis of large matrices is often the most fundamental part. As sizes of matrices become large, calculations by conventional methods become difficult since computing times as well as required memory space grows rapidly. So far, many algorithms suitable to treat very large matrices have been developed. Among these, the forced oscillator method (FOM) [1] has offered a quite different scheme for computing spectral densities, eigenvalues and their eigenvectors of large-scale matrices, in addition to computing linear response functions of both classical and quantum systems [2].

The most time-consuming part in the FOM is to solve lattice-dynamical equations of motion. With an ordinary time-integrating method, a long computing time is needed for obtaining reasonable accuracy. We demonstrate that the fast time-evolution method (FEM) [3] remarkably enhances the efficiency of the FOM. The FEM enables us to calculate or simulate the state of a dynamical system at arbitrary time t with extraordinarily high speed and accuracy, not requiring the intermediate time-developed state. The computing time of the FOM incorporating the FEM is greatly reduced by about an order of magnitude compared to the case using the conventional time-integrating method. In this report, we demonstrate with example the high performance of the FOM. The emphasis will be on the presentation how the FEM effectively accelerates the calculation of eigenvalues and eigenvectors.

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