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Large scale electronic structure calculations using the Lanczos method

Lin-Wang Wang, Alex Zunger
National Renewable Energy Laboratory, Golden, CO 80401, USA

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Abstract

The orthogonality requirement in either iterative diagonalization or conjugate gradient approaches to the single particle Schrödinger equation $\hat{H}\psi = E\psi$ leads to an overall N^3 scaling of the effort with the number N of atoms. We show that the Lanczos method circumvents this problem even when applied to all occupied states. Our implementation shows that the method is stable, exact, scales as N^2 for N around a few hundreds.

and is thus optimally suited for such mid-size (100 – 1000 atoms) quantum systems. The analogy between the basic Lanczos equations and Anderson's localization in a disordered one-dimensional tight-binding chain

is pointed out and used to gain some insights into improved convergence and stability of the method. For a 900-atom Si cluster tested here using pseudopotentials and a plane wave basis, the Lanczos method is about

Fig. 5. The Number of converged eigenvalues as functions of the Lanczos iteration index i. Since this system has 120 occupied

from Fig. 4, most of the eigenstates have been converged far before N_t is reached, so for each E_i^c, it is worth doing a few (5 to 10) inverse it-

erations for different matrix dimensions M (<

converged eigenstates generated at each sweep decay as a geometrical series.

(2) The Lanczos procedure described here is

stable. It guarantees that each converged eigen-

360Mbyte.

To test whether this procedure is stable, we

have repeated the calculation of the largest system $Si_{617}H_{316}$ using different starting random wavefunctions $u_1(r)$ in the Lanczos iteration (Eq. (6)). The two sets of the eigenvalues

within 0.0001% of the Lanczos results. For systems larger than Si the computational

times denoted by "E" in Table 2 have been estimated from the known scaling of the orthogonalization part (N^3 scaling) and the $H\psi(r)$ part (N^2 scaling). It can be seen from Table 2

References

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