Contribution ID: **173** Type: **Oral Presentation**

A comparison of purification schemes for treating the idempotency condition on the density matrix in electronic structure calculations

Thursday, 14 July 2011 13:45 (30 minutes)

<p>During the last 15 years there has been considerable interest in density matrix based methods for electronic structure calculations. The “difficult” problem of ensuring idempotency conservation of the density matrix through an appropriate purification scheme as well as the use of the “nearsightedness” and associated sparsity of the density matrix to achieve linear scaling with system size has been discussed by various authors.

In this study a density matrix based fictitious electron dynamics method for calculating electronic structure is used in a model nanoparticle calculation. This method uses an equation of motion that implicitly ensures the idempotency constraint on the density matrix. The effectiveness of this method compared to conventional purification schemes is discussed.

Important properties of the density matrix and its sub matrices, including its sparsity and conditions for effective linear independence of a column sub matrix of the density matrix are discussed and illustrated within the context of this model system. It is shown how the full density matrix can be reconstructed through a fast QR factorization of a column sub matrix using a Choleski factorization of its principal sub matrix.

Level (Hons, MSc,
   PhD, other)?

other

Consider for a student
   award (Yes / No)?

No

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

Primary author: Prof. HOFFMAN, Matthiam (UFS)

Presenter: Prof. HOFFMAN, Matthiam (UFS)

Session Classification: Theoretical

Track Classification: Track G - Theoretical and Computational Physics