Predictive computing for condensed matter

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Introduction

We are pursuing methods to solve the many-body quantum problem accurately and efficiently.

Our collaboration includes a suite of high-accuracy electronic structure approximations.

These methods all use different techniques to tame the high dimensionality of the many-body quantum problem.

Computational problem

Coupled many-dimensional partial differential equation

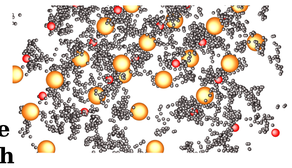
$$\hat{H}\Psi_i(\mathbf{R}) = E_i\Psi_i(\mathbf{R})$$

$$\mathbf{R} = \{\mathbf{r_1}, \mathbf{r_2}, \ldots\}$$

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 - \sum_{i\alpha}\frac{Z_\alpha}{r_{i\alpha}} + \sum_{ij}\frac{1}{r_{ij}} + \sum_{\alpha\beta}\frac{Z_\alpha Z_\beta}{r_{\alpha\beta}}$$

Methods

Continuum quantum Monte Carlo

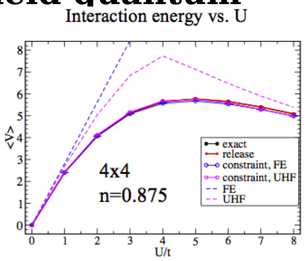


Random walk in high dimensional space
Walkers are the positions of all electrons, or paths of all electrons

Abbamonte, Ceperley, and Wagner are investigating the performance of these methods when applied to challenging materials like the high temperature superconductors.

An application is highlighted in the accompanying poster.

Full configuration interaction and auxilliary field quantum Monte Carlo (FCI-QMC and AFQMC)



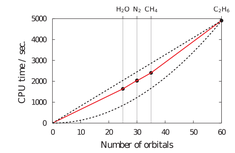
Random walk in the space of determinants

Zhang is an inventor of the AFQMC method as applied to realistic materials and is working to extend its applicability to larger systems. There are three major activities: (1) obtaining effective Hamiltonians using truncated orbitals, (2) calculation of excited states, and (3) approaching the exact solution (pictured)

Chan and Clark are pursuing methods of extracting more information regarding the response properties of quantum simulations from FCI-QMC.

References:
Booth and Chan. J. Chem. Phys. 137 191102 (2012)

Monte Carlo Moller-Plesset perturbation theory (MP2)



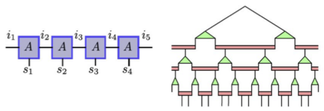
Start from a separable solution of the Schroedinger equation, apply perturbation theory to include particle interactions

Efficient quantum chemistry technique, but still suffers from poor scaling: O(N^5)

Hirata has developed a Monte Carlo implementation of MP2 that is very efficient and scalable to large computationsl resources.

References:
Hirata and He, J. Chem. Phys (in press 2013)
Willow, Kim, and Hirata. J. Chem. Phys. 138 164111 (2013)
Willow, Kim, and Hirata. J. Chem. Phys. 137 204122 (2012)

Density matrix based approaches



Instead of sampling a large space, enforce structure on the wave function for efficient computations.

For one dimensional problems, often obtains near exact solutions, but for higher dimensionality is more challenging to implement.

Ryu is studying the theory of tensor networks and classification of the graphs. Chan is developing software and techniques that implement various density matrix decompositions of the many-body wave function.

References:
M. Nozaki, S. Ryu, and T. Takayanagi, JHEP 10, 193 (2012)
Software for density matrix-based chemistry and model solutions: http://www.princeton.edu/chemistry/chan/software/

Computational bottlenecks

4-point matrix elements:

Many of the methods require one to know the matrix elements of the Hamiltonian in a one-particle basis. This is given by integrals of the form

$$M_{pqrs} = \int \phi_p^*(\mathbf{r_1})\phi_q^*(\mathbf{r_2})\frac{1}{r_{12}}\phi_r(\mathbf{r_1})\phi_s(\mathbf{r_2})d\mathbf{r_1}d\mathbf{r_2}$$

Evaluation and storage of the many matrix elements requires a large amount of computer time and data management.

Determinant row updates

The limiting factor of the continuum QMC calculations is the update of a determinant and its derivatives on changing a single column or row. Typically the Sherman-Morrison algorithm is used, in conjuction with a method invented by Clark.

Better determinant updates would lead to much more efficient high accuracy calculations.

Summary

An important component of our collaboration is the implementation and progression of multiple comparable high accuracy methods.

The methods all obtain valuable information about many-body quantum systems using high performance computing.

Faster implementations will have large impact in physics and chemistry

Keep updated on our progress athttp://predictive-scidac.org

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