Summer School 2007 - QMC : VMC using the QMCPACK code

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VMC using the QMCPACK code (120' lab)

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Link to Presentation slides (in PPT or PDF) format:

http://cms.mcc.uiuc.edu/qmcpack/qmcss07/

Quickstart

- On Tungsen cluster, change directory to scratch-global

```
cd scratch-global
tar xf ~/Li2.tar
tar xf ~/BulkCarbon.tar
```

- The tar file can be downloaded with wget

```
wget http://cms.mcc.uiuc.edu/qmcpack/qmcss07/input/li2.tar
wget http://cms.mcc.uiuc.edu/qmcpack/qmcss07/input/BulkCarbon.tar
tar xf li2.tar
tar xf BulkCarbon
```

Running jobs

Interactive jobs

bsub -Is -n1 -W 1:00 tcsh

Batch scripts are included for BulkCarbon.

Topics

- VMC simulations of Li2 (30)
  - QMC optimized Slater-type orbitals
  - Adding a Two-Body correlation function of Pade functor
  - Using a Two-Body correlation function of Wagner-Mitas functor
- Optimization of correlation functions (30)
- VMC simulations of Carbon (8-atom cubic diamond) (60)
  - RPA Jastrow
  - One/Two/Three-body Jastrow function

Comments

Li2/Carbon can be replaced by any other materials.