Summer School 2007 - QMC : Ground-state QMC with QMCPACK

This page last changed on Jul 18, 2007 by jnkim.

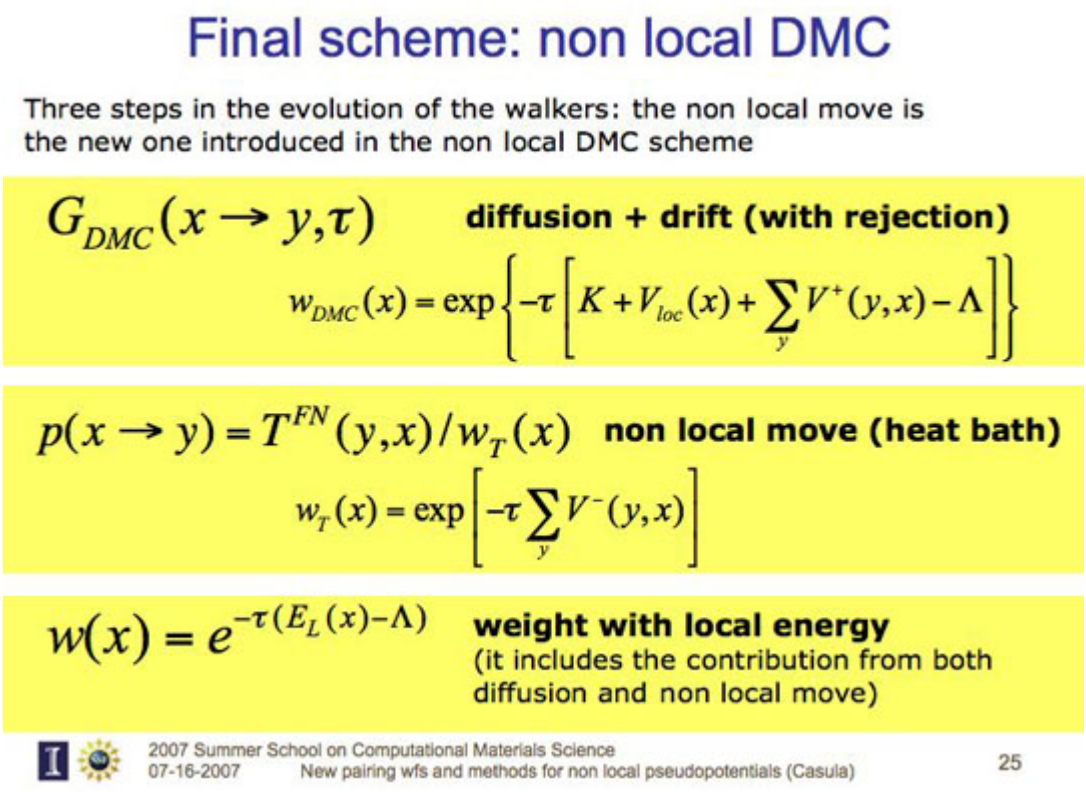
Ground-state QMC with QMCPACK (180' lab)

Jeongnim Kim

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

Topics

- VMC simulations of benzene
  http://cms.mcc.uiuc.edu/qmcpack/qmcss07/ch03.html
  - Pairing wavefunctions optimized by M. Casula: see the note prepared by Casula benzene.pdf
- DMC of bulk carbon
  http://cms.mcc.uiuc.edu/qmcpack/qmcss07/ch04.html
  - time step
  - local approximation : non local DMC



- DMC of Li2
  Li2.j2pade.dmc.xml
- Practical guides for using QMCPACK
  - http://cms.mcc.uiuc.edu/qmcpack/
  - http://cms.mcc.uiuc.edu/qmcpack/index.php/Working_with_external_packages

Comments