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Ground-state QMC with QMCPACK (180' lab)

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

Topics

- VMC simulations of benzene
<http://cms.mcc.uiuc.edu/qmcpack/qmc07/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/qmc07/ch04.html>
 - time step
 - local approximation : non local DMC

Final scheme: non local DMC

Three steps in the evolution of the walkers: the non local move is the new one introduced in the non local DMC scheme

$G_{DMC}(x \rightarrow y, \tau)$ **diffusion + drift (with rejection)**

$$w_{DMC}(x) = \exp \left\{ -\tau \left[K + V_{loc}(x) + \sum_y V^+(y, x) - \Lambda \right] \right\}$$

$p(x \rightarrow y) = T^{FN}(y, x) / w_T(x)$ **non local move (heat bath)**

$$w_T(x) = \exp \left[-\tau \sum_y V^-(y, x) \right]$$

$w(x) = e^{-\tau(E_L(x) - \Lambda)}$ **weight with local energy**
(it includes the contribution from both diffusion and non local move)



2007 Summer School on Computational Materials Science
07-16-2007 New pairing wfs and methods for non local pseudopotentials (Casula)

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- 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