0.1 Report on Workshop

Quantum Monte Carlo in the Apuan Alps V

International Workshop
Saturday 25th July - Saturday 1st August 2009
The Apuan Alps Centre for Physics @ TTI, Vallico Sotto, Tuscany
`www.vallico.net/tti/tti.html`

Sponsors: Psi-k, CCP9
Organizer: Mike Towler

Conference web page: `www.vallico.net/tti/qmcitaa_09/conference.html`

The fifth Cambridge international workshop devoted to the quantum Monte Carlo (QMC) method took place in late July 2009. The event was organized and run by Mike Towler of Cambridge University, and was held in the pleasant setting of his 15th century monastery in the beautiful mountain village of Vallico Sotto in Tuscany. Workshops at this venue are generally intended to gather together limited numbers of expert physicists to discuss subjects of topical interest where there is an ongoing requirement for new insights. This workshop - like the previous four - appeared to be succeed very well in its stated purpose, and all participants enjoyed a varied programme of interesting lectures and discussions.

The quantum Monte Carlo method is an important and complementary alternative to density functional theory when performing computational electronic structure calculations in which high accuracy is required. The method has many attractive features for probing the electronic structure of real atoms, molecules and solids. In particular, it is a genuine many-body theory with a natural and explicit description of electron correlation which gives consistent, highly-accurate results while at the same time exhibiting favourable (cubic or better) scaling of computational cost with system size. It is the *only* known highly-accurate method which remains tractable for systems with more than a few tens of electrons; indeed, solid-state applications of more than 2000 electrons were reported during the workshop.

Here is a (by no means exhaustive) list of interesting themes presented and discussed at this year's event:

- Insights into QMC and other numerical simulations from trajectory-based interpretations of quantum mechanics (specifically, de Broglie-Bohm pilot-wave theory)
- Various new forms of many-particle wave function, including a new completely general form of Jastrow correlation factor which allows the inclusion of arbitrary higher-order terms.

- QMC calculation of weak interactions.
- The exploitation of new petascale parallel hardware to do quantum Monte Carlo calculations.
- Forces and the optimization of geometries in QMC.
- A completely new algorithm for doing QMC in a 'Slater determinant space'.
- A very wide-range of applications of QMC to atoms, molecules, surfaces, solids and various model systems.

As is usual with events at this venue, formal lectures were restricted to the mornings, and participants were encouraged to spend the remainder of each day thinking about and discussing the topics at hand. For those so inclined, a wide variety of activities were organized for each afternoon, often involving mountain walks and cave exploration.

1 Programme

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Sunday 26th July
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8.30am  : Mike Towler (5 minutes)
        - "Welcome to Tuscany"
8.35am  : Mike Towler (50 minutes)
        - "Pilot waves, Feynman path integrals, and quantum Monte Carlo"
9.30am  : Dario Alfe (50 minutes)
        - "Water graphene binding energy curve from diffusion Monte Carlo"
10.30am : Pablo Lopez Rios (50 minutes)
        - "The Jastrow factor"
11:30am : Richard Needs (50 minutes)
        - "Applications of ab initio random structure searching"

Monday 27th July
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8.30am  : Michele Casula (50 minutes)
        - "Hexatic and mesoscopic phases in the 2D quantum Coulomb system"
9.30am : Ken Esler (50 minutes)
        - "Recent developments in QMC for periodic systems"
10:30am : Alston Misquitta (50 minutes)
        - "The dispersion energy: an introduction and some surprises"
11.30 am: Martin Krupicka (25 minutes)
        - "Comparison of QMC and ab initio methods for eight constitutional
            isomers of C4H6"
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Tuesday 28th July

8.30am : Lucas Wagner (50 minutes)
- "Using QMC to optimize geometries"
9.30am : Matthew Foulkes (50 minutes)
- "Point defects and diffusion in alumina"
10.30am : Roberto Dovesi (50 minutes)
- "State of the art in the ab initio treatment of crystalline solids with a local basis set. The case of the CRYSTAL code, and its CRYSCOR son"
11.30am : Mariapia Marchi (25 minutes)
- "Resonating Valence Bond wave function with molecular orbitals: application to diatomic molecules"

Wednesday 29th July

8.30am : Shiwei Zhang (50 minutes)
- "Is the homogeneous electron gas homogeneous?"
9.30am : Neil Drummond (50 minutes)
- "Quasiparticle effective mass of the 2D homogeneous electron gas"
10.30am : Ching-Ming Wei (50 minutes)
- "QMC studies of (i) transition metal clusters, and (ii) surface adsorption".
11.30am : Robert Lee (25 minutes)
- "QMC and the 1d electron liquid"

Thursday 30th July

8.30am : Michel Caffarel (50 minutes)
- "A new type of trial wave function for electronic structure calculations with QMC"
9.30am : Norbert Nemec (50 minutes)
- "Diffusion Monte Carlo: exponentially inefficient for large systems"
10.30am : George Booth (50 minutes)
- "Quantum Monte Carlo in a discrete space"
11.30am : Martin Korth (50 minutes)
- "'Mindless' QMC benchmarking"

Fri 31st July

8.30am : John Trail (50 minutes)
- "Optimum and efficient sampling for variational quantum Monte Carlo"
9.30am : Ryo Maezono (25 minutes)
- "DMC study of an atom immersed in a jellium sphere"

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10am : Andrew Morris (50 minutes)
        - "BEC-BCS crossover in ultracold atomic gasses within Quantum Monte Carlo"
11am :  Priyanka Seth (25 minutes)
        - "QMC studies of the first row atoms"
11.30am : Gareth Griffiths (25 minutes)
        - "Post-cotunnite phase of TeO2 from random structure searching"

Poster presentation
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Raffaella Dimichelis
"Ab initio quantum mechanical simulation of systems with helical symmetry:
  carbon and chrysotile nanotubes"
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All presentations should be downloadable from the conference web site.

2 List of participants

There were 28 scientific participants in the meeting from 7 countries, accompanied by 12 family members. Their names and affiliations were as follows:

Dario Alfè (UCL, London, U.K.)
George Booth (Cambridge University, U.K.)
Michel Caffarel (Université Pierre et Marie Curie, Paris, France)
Michele Casula (Ecole Polytechnique, Paris, France)
Raffaella Demichelis (University of Torino, Italy)
Roberto Dovesi (University of Torino, Italy)
Neil Drummond (Cambridge University, U.K.)
Ken Esler (University of Illinois, U.S.A.)
Matthew Foulkes (Imperial College, London, U.K.)
Gareth Griffiths (Cambridge University, U.K.)
Bohshiang Jong (Cambridge University, U.K.)
Martin Korth (University of Münster, Germany)
Martin Krupicka (Slovak Academy of Sciences, Bratislava, Slovakia)
Valentina Lacivita (University of Torino, Italy)
Robert Lee (Cambridge University, U.K.)
Pablo Lopez Rios (Cambridge University, U.K.)
Ryo Maezono (JAIST, Japan)
Mariapia Marchi (SISSA, Trieste, Italy)
Alston Misquitta (Cambridge University, U.K.)
Andrew Morris (Cambridge University, U.K.)
Richard Needs (Cambridge University, U.K.)
Norbert Nemec (Cambridge University, U.K.)
Priyanka Seth (Cambridge University, U.K.)
John Trail (JAIST, Japan)

Mike Towler (Cambridge University, U.K.)
Lucas Wagner (University of California, Berkeley, U.S.A.)
Ching-Ming Wei (Academia Sinica, Taiwan)
Shiwei Zhang (William and Mary College, U.S.A.)