





Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry

21 January - 2 February 2008

Miramare, Trieste, Italy

Quantum Monte Carlo (QMC) methods are among the most successful approaches for computing the properties of interacting quantum many-body systems. For a variety of problems in physics and chemistry, QMC techniques have been employed to provide answers in cases where standard methods such as density-functional theory or Hartree-Fock methods are shown to be inadequate, and post-Hartree-Fock methods are too computationally expensive.

This Advanced School follows the "School on Continuum Quantum Monte Carlo" held at the ICTP in January 2004. After introducing the basics of the methods and giving a broad overview of the field, the School will focus on new developments in methodology and applications.

Lectures will be held during the morning sessions, while afternoon sessions will be devoted to hands-on tutorials.

TOPICS:

- Introduction: Random walks, Variational Monte Carlo, Projection Monte Carlo, Path Integral Monte Carlo;
- Improved wave functions and wave function optimization techniques, computation of forces and observables;
- Lattice Regularized Diffusion Monte Carlo, Auxiliary-Field Monte Carlo for any single-particle basis set, Auxiliary-Field Monte Carlo for spin/isospin-dependent problems, Coupled Electron-Ion Monte Carlo, Worm Algorithm and Diagrammatic Monte Carlo.

LECTURERS:

D.M. Ceperley (UIUC)
C. Filippi (Leiden)
W.M.C. Foulkes (Imperial, London)
S. Moroni (DEMOCRITOS, SISSA)
N. Prokofiev (UMass, Kurchatov)

K.E. Schmidt (Arizona State)
S. Sorella (DEMOCRITOS, SISSA)
C.J. Umrigar (Cornell)
S. Zhang (William and Mary)

<u>CALL FOR CONTRIBUTED POSTERS</u>: During the activity there will be a Poster Session. Abstracts should be submitted **no later than 30 November 2007** to the Activity Secretariat, at the address indicated below. Please send file attachments in PDF format.

AS A PART OF THE ACTIVITY, A TWO-DAY MINIWORKSHOP will be held from 1 to 2 February 2008. The programme will be posted at the School web site.

PARTICIPATION:

Application to the activity is open to a limited number of selected advanced undergraduates, graduate students, post-doctoral researchers, faculty and research scientists from all countries that are members of the UN, UNESCO or IAEA. A good working knowledge of elementary quantum mechanics is required, some experience with numerical methods is useful. Computer laboratory sessions will make use of the UNIX operating system. As the School will be conducted in English, participants must have an adequate working knowledge of that language. The main purpose of the Centre is to help researchers from developing countries through a programme of training activities within the framework of international cooperation. However, scientists from developed countries are most welcome to attend.

As a rule, travel and subsistence expenses of the participants are borne by their home institutions. Some ICTP funds are available for a limited number of applicants who are nationals of, and working in, developing countries. Such financial support is available only to those attending the entire School. As scarcity of funds allows travel to be granted only in a few exceptional cases, every effort should be made by candidates to secure support for their fare from their home country. There is no registration fee to attend this activity.

The closing date for the receipt of requests for participation is <u>5 October 2007</u>

Interested participants should fill in and submit the Online Application Form that can be found at: http://agenda.ictp.it/smr.php?1929. Kindly send any file attachments in PDF format.

Secretariat: SMR.1929 - Advanced School on Quantum Monte Carlo Methods in Physics and Chemistry c/o Ms. N. Ivanissevich the Abdus Salam International Centre for Theoretical Physics Strada Costiera 11, I-34014 Trieste, Italy

ICTP Home Page: http://www.ictp.trieste.it/



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ORGANIZERS:

Claudia Filippi (Leiden, The Netherlands)

Saverio Moroni (DEMOCRITOS, SISSA, Trieste, Italy)

Sandro Sorella (DEMOCRITOS, SISSA, Trieste, Italy)

Cyrus J. Umrigar (Cornell University, Ithaca, NY, USA)

Shiwei Zhang (College of William and Mary, Williamsburg, VA, USA)

DEADLINE for applications:

5 October 2007

SCHOOL WEB PAGE:

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