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Resonating Valence Bond wavefunctions for electronic simulations[1]

SANDRO SORELLA, Democritos National SImulation Centre and SISSA

We discuss several progress for the simulation of strongly correlated electrons, based on an efficient implementation of the Resonating Valence Bond (RVB) theory with Quantum Monte Carlo (QMC). Due to very important advances[1] in the energy optimization of strongly correlated variational wave functions, it is now possible to optimize several variational parameters with remarkable efficiency even within a stochastic approach such as QMC. In this way it is possible to describe very accurately the electronic correlation by a first principle many-body wave function, that can be extended to fairly large electronic systems. Indeed a remarkable improvement of the Hartree-Fock theory is provided by the so called RVB wave function introduced by P.W. Anderson in the context of High-Tc superconductivity[2]. For instance, by means of this paradigm, it has been possible to perform a realistic and accurate simulation of the benzene dimer, where we have found that the RVB correlation of the benzene ring plays a crucial role in the dimer bonding[3,4]. Finally we consider the still controversial low-temperature and high-pressure phase diagram of Hydrogen by using the same RVB wavefunction. We use a novel second order Langevin dynamics by introducing a consistent friction tensor, allowing to remain in thermal equilibrium even with very noisy forces, namely determined by QMC with very short runs. This allows us to simulate finite temperature systems ($\simeq$ 100 H) with very high efficiency, while the variational parameters are consistently optimized during the ionic dynamics.

[1] See C. J. Umrigar, J. Toulouse, C. Filippi, S. Sorella and R. G. Hennig, cond-mat/0611094 and references therein.

[2] P. W. Anderson Science 235, 1196 (1987).

[3] M. Casula, C. Attaccalite and S. Sorella J. Chem. Phys. **121** 7110 (2004).

[4] S. Sorella, M. Casula and D. Rocca in preparation.

[5] C. Attaccalite and S. Sorella in preparation.

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