Cornell University Library

We gratefully acknowledge support from the Simons Foundation and member institutions

arXiv.org > physics > arXiv:1107.3537

Search or Article-id

(Help | Advanced search)

All papers | Go!

**Physics > Chemical Physics**

# Quantum Monte Carlo facing the Hartree-Fock symmetry dilemma: The case of hydrogen rings

Peter Reinhardt (LCT), Julien Toulouse (LCT), Roland Assaraf (LCT), C. J. Umrigar (LASSP), Philip E. Hoggan (LASMEA)

*(Submitted on 18 Jul 2011)*

When using Hartree-Fock (HF) trial wave functions in quantum Monte Carlo calculations, one faces, in case of HF instabilities, the HF symmetry dilemma in choosing between the symmetry-adapted solution of higher HF energy and symmetry-broken solutions of lower HF energies. In this work, we have examined the HF symmetry dilemma in hydrogen rings which present singlet instabilities for sufficiently large rings. We have found that the symmetry-adapted HF wave function gives a lower energy both in variational Monte Carlo and in fixed-node diffusion Monte Carlo. This indicates that the symmetry-adapted wave function has more accurate nodes than the symmetry-broken wave functions, and thus suggests that spatial symmetry is an important criterion for selecting good trial wave functions.

| | |
|---|---|
| Comments: | 6 pages, 3 figures, 2 tables, to appear in "Advances in Quantum Monte Carlo", ACS |
| Subjects: | **Chemical Physics (physics.chem-ph)**; Computational Physics (physics.comp-ph) |
| Cite as: | **arXiv:1107.3537** [physics.chem-ph] |
| | (or **arXiv:1107.3537v1** [physics.chem-ph] for this version) |

**Submission history**

From: Julien Toulouse [view email]

**[v1]** Mon, 18 Jul 2011 19:39:34 GMT (46kb)

*Which authors of this paper are endorsers?*

Link back to: arXiv, form interface, contact.