

CORRIGENDUM

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To cite this article: Ion Mitxelena *et al* 2018 *J. Phys.: Condens. Matter* **30** 089501

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Corrigendum

Corrigendum: On the performance of natural orbital functional approximations in the Hubbard model (2017 *J. Phys.: Condens. Matter* **29** 425602)

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Received 21 December 2017

Accepted for publication 9 January 2018

Published 31 January 2018

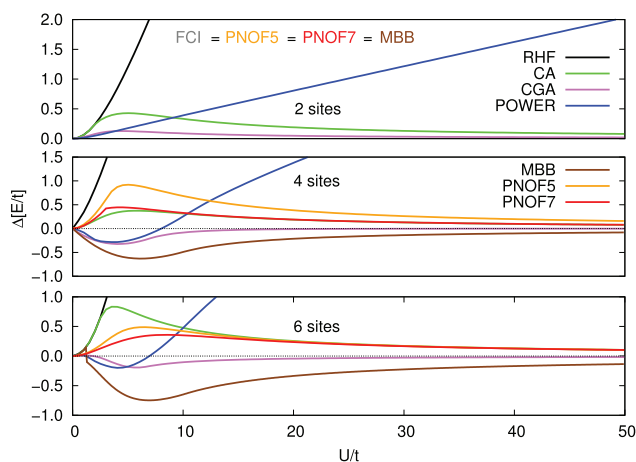


Figure 4. Differences in E/t values with respect to exact FCI obtained for the 1D homogeneous Hubbard model by using many NOFAs.

There was an error in the results corresponding to PNOF7 for the homogeneous four site square and six site hexagon Hubbard models reported in the article. Accordingly, the left

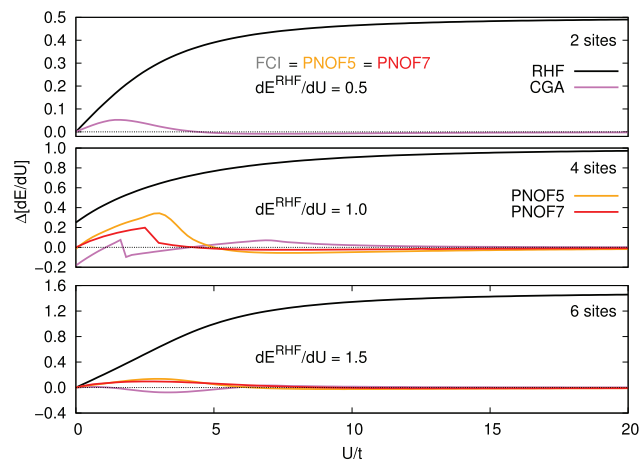


Figure 5. Differences in dE/dU values with respect to exact FCI obtained for many NOFAs.

side of figures 4–6 have been corrected in this corrigendum. Note that PNOF7 energies always remain above FCI (figure 4).

For the four site square, the PNOF7 double occupancy (figure 5) does not go parallel to the exact dE/dU , whereas

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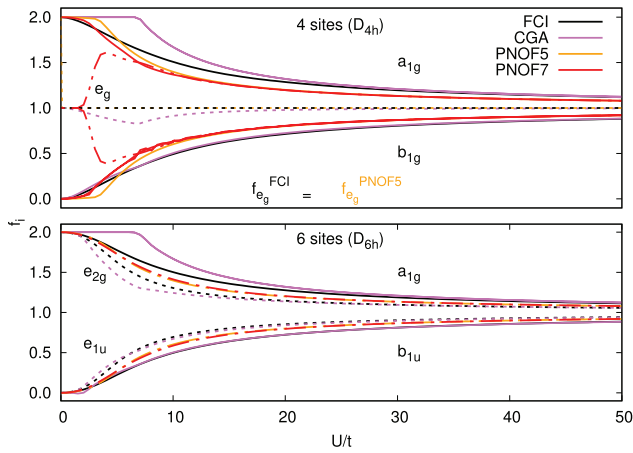


Figure 6. Natural orbital occupancies (spins summed) obtained for FCI, CGA, PNOF5, and PNOF7, in the four site square and six site hexagon Hubbard systems. Solid lines are used for non-degenerate occupancies, whereas dotted and dash-dotted lines correspond to degenerate occupancies.

the PNOF7 natural orbital occupancies (figure 6) are not always adapted to the symmetry of D_{4h} point group. PNOF7 yields two configurations of orbitals depending on the correlation regime. In the region $U/t \leq 2.7$, natural orbitals remain adapted to the symmetry, however, for $U/t > 2.7$ PNOF7 leads to localization in the natural orbital representation. Orbitals adapted to the symmetry can be retrieved by a unitary transformation that leads to the canonical representation

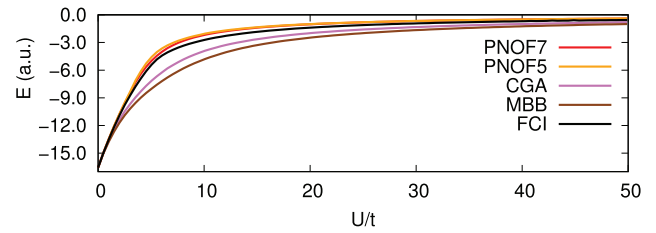


Figure 10. Exact and approximate energies for the ten site Hubbard model including an Aubry–André on-site potential, for many U/t values.

as we have shown for six site hexagon Hubbard model in the article.

For the six site hexagon, no significant changes appear for PNOF7 double occupancy (figure 5) and natural orbital occupancies (figure 6).

Finally, for the ten site Hubbard model including an Aubry–André on-site potential, the MBB and CGA energies have been corrected. In contrast to figure 10 of the article, MBB and CGA are able to reproduce the asymptotic behavior as U/t gets larger, although, energies are always below the FCI ones (figure 10). We thank Mr Robert Schade for his kind comments regarding the MBB energies.

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