

Replay to referee 2

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Abstract

The following contains responses to the referee 2 comments copied from the SAIP2016 portal under ‘History – > View’. Referee comments, in blue, are followed by our answers in black.

Content: To be corrected; submitted on Fri 17 Nov 2017 at 12:11; Comments Referee 2

0.1 General comments

I am not very familiar with density functional theory, so I can only provide an outsider’s opinion. The paper applies a variation of a well-established technique to a standard lattice model of interacting electrons. The results don’t look particularly exciting, but are probably at a similar level to those appearing in the 2015 proceedings. I would therefore suggest that the paper be accepted, provided some editorial corrections are made. (So ‘To be corrected’.) I list these below.

0.2 Comments requiring answers

The capitalisation of ‘correlation’ and ‘exchange’ is not consistent:

fixed

KS as an abbreviation for Kohn-Sham is used before it is defined: There are some formatting issues directly after equation (1):

fixed

Is it correct that the bounds on the sums appearing in the Hamiltonian are determined by n_e , the number of electrons? Should this not be the number of lattice sites instead?

Thank you. We have corrected the error.

It is stated that the convexity conditions ‘leads to’ a simple two state ensemble. It is not clear to me what this means, or what the considerations really are here. This should at least be commented on.

It is an important point, but due to the limited length of the paper we did not give an explanation. The underlying concept and proof is relatively straight forward, but it requires some discussion and space in the paper to introduce the details. It is not a new concept and the interested reader can follow a discussion in the references given.

After equation (1): ”helps to determines” should be ”helps to determine”:

fixed

Four lines above equation (2): ‘product operator’ should probably be ‘operator product’:

fixed

The tilde on v^{KS} has become a subscript in some of the axis labels in the graphs:

Unfortunately subscripts do not exist in octave as in latex.

The sudden description of the finite chain as an ‘infinite square well’ in the captions of figures 1 and 2 could perhaps be commented on in the text.

We change ‘infinite well’ to ‘finite chain’ for consistency.

Three lines above figures 5 and 6 the 3.12% is missing a percentage sign.

fixed

In the second line of section 5 ‘We found that approximate’ should be ‘We found that the approximate’?

fixed

In the third last line of section 5 ‘a shape which is closely follows’ should be ‘a shape which closely follows’?

fixed

In the second last line of section 5 ‘include correlation’ should be ‘include correlations’

fixed

Check spelling, formatting and capitalisation in references 8, 11, 12 and 14.

reference checked

0.3 Criteria Evaluation

Does the article that you are being asked to review match your expertise? (On scale, + for yes or agree): Neutral

Are there any potential conflicts of interest if you review this article? (+3 for yes / -3 for no): Neutral

A1 Scientific merit: Is the work scientifically rigorous and accurate? Is it appropriate for the proceedings?: Neutral

A2 Clarity: Are the ideas in the paper communicated clearly and legibly? : Neutral

A3 Context: Is there sufficient discussion of the background for this work and suitable referencing?: Neutral

B1 Originality: Is the work relevant and novel?: Neutral

B2 Motivation: Does the problem considered have a sound motivation? All papers should clearly demonstrate the scientific interest of the results: Neutral

C1 Title: Is it adequate and appropriate for the content of the article?: Neutral

C2 Abstract: Does it contain the essential information of the article? Is it complete?: Neutral

C3 Diagrams, figures, tables and captions: Are they essential and clear?: Neutral

C4 Text and mathematics: Are they brief but still clear? If you recommend shortening, please suggest (below at comments) what should be omitted: Neutral

C5 Conclusion: Does the paper contain a carefully written conclusion, summarising what has been learned and why it is interesting and useful?: Neutral

C6 References: Are the references in the correct format? Are all references mentioned in the text and cited chronologically?: Neutral