Fwd: Your Submission COMPHY-D-23-00120

From:Hongcheng\x26nbsp;Ni<hcni@lps.ecnu.edu.cn>
Time:Monday, Jul 3, 2023 4:26 PM
To:Shanshan Song<51200920067@stu.ecnu.edu.cn>; 朱明宇<myzhu@stu.ecnu.edu.cn>

小宋，小朱：

审稿意见回来了，意见很正面，请按照要求修改。

附件中是提交版本（根据CPC要求修改过，和git上不同），请在提交版本基础上修改。

关于HF精度，我同意审稿人的说法。但是我们可以自己设定使用什么方法计算，比如，改用CASSCF计算，那么精度就又提高了。

请相应修改程序和文档、稿件，把使用不同方法的handler加进去。

-------- Forwarded Message --------
Subject: Your Submission COMPHY-D-23-00120
Date: 3 Jul 2023 04:11:11 -0400
From: Jimena Gorfinkiel <em@editorialmanager.com>
Reply-To: Jimena Gorfinkiel <j.gorfinkiel@open.ac.uk>
To: Hongcheng Ni <hcni@lps.ecnu.edu.cn>

Ms. Ref. No.: COMPHY-D-23-00120
Title: PyStructureFactor: A Python code for the molecular structure factor in tunneling ionization rates
Authors: Shanshan Song; Mingyu Zhu; Hongcheng Ni; Jian Wu
Computer Physics Communications

Dear Dr. Ni,

I have now received reviewers' reports on your submission. They have indicated that the manuscript would benefit from revision.

The reports are constructive and are enclosed below for your information. If you feel that you can suitably address the reviewers' comments, I invite you to revise and resubmit your revised version within the next 3 months. Please address carefully the issues raised in the comments and highlight in colour the changes made to the manuscript.

If you are submitting a revised manuscript, please also:

a) describe each change made (point by point) as raised in the reviewer comments AND/OR

b) provide a suitable rebuttal to each reviewer comment not addressed

When submitting your revised manuscript, please ensure that you upload the source files (e.g. LaTeX). Uploading a PDF file at this stage will create delays should your manuscript be finally accepted for publication. If your revised submission does not include the source files, we will contact you to request them.

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I look forward to receiving your revised manuscript.

Yours sincerely,

Jimena Gorfinkiel
Managing Guest Editor
Computer Physics Communications

Reviewers' comments:

Reviewer #1: The authors presented a Python code to calculate the molecular structure factor in the tunneling ionization process using the weak field approximation. Tunneling ionization, indeed, is the core of the strong-field process. Although the tunneling ionization rate can be estimated by various theories, there is no simulation code available to estimate the ionization for all the common molecules. The present code bridges the gap. I did a test run of the code. It is simple and easy to be used. I recommend the publication of the work after a minor revision.

1. Line 23-24 on page 2:
the energy of the ionizing electron -> the binding energy or orbital energy …
to avoid misleading.
1. Line 51 on page 4:
High accuracy -> the accuracy same as the SCF simulation.
Note that the present SCF is based on HF, and it is not a high-precision simulation.

In the program summary part, the authors should state on which machine the code is tested and how long it takes for a given example.

Since to run the examples, matplotlib is also needed. The authors should add this in the readme.md file.

Reviewer #2: In this work, a Python program is introduced which calculates the structure factor of molecules undergoing ionization under irradiation of intense laser light. It is based on the ionization description within the weak-field asymptotic theory (WFAT), which describes strong-field ionization as a product of functions: one function containing mainly information and parameters of the intense laser field, and a second one accounting for a molecule's structural properties. This latter factor, the molecular structure factor, is the quantity which is calculated within the herein introduced Python code. It links to another Python software package, PySCF, to calculate the molecular electronic structure and extracts from there the necessary molecular orbitals and molecular potentials.

In general, the paper is nicely written, and the proposed software seems to be robust and accurate. I also think, it may be of use for the strong-field and attosecond community, as the calculation of the molecular structure factors is often cumbersome and hard to converge. Therefore, I can in general recommend publication of the manuscript. However, in its present form, there are some minor points which I recommend addressing, and which I list in what follows:

Concerning the references, I recommend adding work of S. Patchkovskii; L.B: Madsen and K. Doblhoff-Dier on WFT and some of the applications towards strong-field ionization

Very often, the expression "multiplet molecules" occurs in the text. There is no such thing. I would suggest rephrasing to open-shell molecules.

Page 2, Introduction, it is written: "HHG is the key to the generation of extreme ultraviolet laser pulses.:" - strictly speaking are HHG no laser pulses. I would change it to "Light pulses"

Page 3, 1st paragraph, 1st sentence reads strangely, and I recommend rephrasing it "… the laser is manifested as photons in the frequency domain ..:"

Page 3, after eq.1: "Eo is the energy of the ionizing electron" -> "orbital energy"

Page 5, second line: ".. taken as the asymptotic expansion for the field strength in early stages" - unclear due to language

In chapter 2, the definition and arrangement of the angles (alpha, beta, gamma, z, y', x'') is not very clear. As this is definition of molecular orientation etc. is very important, I suggest putting a schematic picture there which might help understanding the definition of the coordinate system

Page 7, first sentence, "The structure factor … in the integral representation is given as an integral" reads odd

Eq 13 (and others): The authors use operator hats very inconsistently. Either use them throughout or leave them out.

Table 2 is not fully visible in my pdf; however, in table 2, some of the parameters are not fully clear (and are later also not properly introduced or discussed), e.g. "channel", "orient_grid_size" or "move_dip_zero", (see also my point above to the choice of the coordinate/reference system). And lmax (which sum, which eq)?

Also, the grid levels, e.g. shortly discussed on page 10 (grid levels 1,3,5,7, … "correspond to radial and angular sizes (40,194)…" is not clear. Only odd numbers? What are the numbers in brackets?

Page 11, first paragraph: why is C6H6 (benzene) labeled a "multiplet molecule"? It is closed shell singlet.

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Ordinary Attachment

StructureFactor.zip (145.25K)