

Subject:	Re: Sunday night in Lyon	
From:	"Jian Liu" <jianliupku@pku.edu.cn>	Jan 21, 2020 8:46:31 PM
To:	"jeremy richardson" <rjeremy@ethz.ch>	

Hi Jeremy,

I got to know your recent manuscript on arXiv.

<https://arxiv.org/abs/1912.10906>

I presented a talk on our earlier work JCP 151, 024105 (2019) in the CECAM workshop and even mentioned it when you and your student particularly asked me for a discussion on our mapping models in Lyon.

In Appendix A of the paper we have already shown the case for the general multi-state system with the constraint $\text{Sum_over_all states } [x_n^2 + p_n^2] = 1$

and derived how to do the integral over the electronic state DOF with the constraint for the correlation function.

In the second last paragraph in Conclusions, we also suggested

"The new viewpoint in CMMs can also have implication for nonadiabatic dynamics with semiclassical/quasiclassical mapping models in the Cartesian phase space since the pioneering work by Meyer and Miller"

What you did is in practice an extension from our work. Add the zero-point energy to the electronic DOF, then use the constraint

$\text{Sum_over_all states } [x_n^2 + p_n^2 - \text{gama}] = 1$

with the Meyer-Miller mapping model.

What you worked related to Q/P/W in this manuscript and to your previous work is certainly interesting, providing another angle for the problem. It is close to a unified approach for our work which we are going to write on. It is quite encouraging to see your progress. I also wish to mention some of this when our work is totally ignored in your manuscript.

All the best

Jian

> -----Original Messages-----

> From: "Jeremy Richardson" <rjeremy@ethz.ch>

> Sent Time: 2019-06-14 22:26:14 (Friday)

> To: "CURCHOD, BASILE" <basile.f.curchod@durham.ac.uk>, "Federica Agostini" <federica.agostini@u-psud.fr>, "Aaron Kelly" <aaron.kelly@dal.ca>, "Mariana

> Rossi" <rossi@fhi-berlin.mpg.de>, guillermo.albareda@mpsd.mpg.de, "Ceriotti Michele" <michele.ceriotti@epfl.ch>, "Jian Liu" <jianliupku@pku.edu.cn>

> Cc:

> Subject: Sunday night in Lyon

>

> Are any of you (or anyone else at the conference) going to be arriving

> in Lyon on Sunday and fancy meeting up for dinner? I'll be there from

> 7:30 ish and am staying at Apparteo Jean Jaures. Let me know and see

> you soon.

> Jeremy

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