Subject:	Re: Fwd: your recent paper
From:	"Jian Liu" <jianliupku@pku.edu.cn> Jan 21, 2020 2:05:03 PM
To:	millerwh@berkeley.edu

Dear Bill,

It is great to hear from you! My father and brother will spend the Spring Festival holidays with me and Yirang in Beijing. Yirang got in the kindergarden in last September. He is learning a lot now. Being a father is a new stage of life.

Reply to Q1: The trace over the electronic state DOF in quantum mechanics is replaced by the integral in the mapping phase space with the constraint that the total population is 1 [i.e., Eq. (28)]. The initial sampling of the electronic state DOF is described in Appendix A [i.e., Eqs. (A4) and (A5)], which is equal to a uniform distribution in the phase space with the constraint that the total population is 1 [i.e., Eq. (28)]. That is, the initial sampling is from the trace over the electronic state DOF.

If one freezes the nuclear DOF, use the Meyer-Miller model as the example.
The constraint that the total population is 1 [i.e., Eq. (28)] is
Sum_over_n states [x_n^2 + p_n^2] = 1

The normalization procedure in Appendix A is to ensure the following conditions
1) In quantum mechanics, one has Tr [|1><1|] = 1. In CMMs, it is equal to
Integral_Over_ x and p _ with the constraint [integrand = x1^2 + p1^2] = 1
2) In quantum mechanics, one has Tr [|1><1| |1><1|] = 1 . In CMMs, it is equal to
Integral_Over_ x and p _ with the constraint [integrand = (x1^2 + p1^2)*(x1^2 + p1^2)] = 1
3) In quantum mechanics, one has Tr [|1><1| |2><2|] = 0 . In CMMs, it is equal to
Integral_Over_ x and p _ with the constraint [integrand = (x1^2 + p1^2)*(x2^2 + p2^2)] = 0
4) In quantum mechanics, one has Tr [|1><1| |1><2|] = 0 and Tr [|1><1| |2><1|] = 0. In CMMs, it is equal to
Integral_Over_ x and p _ with the constraint [integrand = (x1^2 + p1^2)*(x1*x2 + p1*p2)] = 0

There is no Wigner distribution or window function for the electronic DOF. The initial electronic state is treated as a physical oberservable rather than the density operator. The QM trace is replaced by the integral in the constrainted surface.

Reply to Q2: If CMM1 (classical Li-Miller mapping model) and CMM2 (classical Meyer-Miller mapping model) are treated exactly in the same fashion, they lead to the same results. If not, they can produce different results. In fact, Li-Miller mapping Hamiltonian and Meyer-Miller mapping Hamiltonian are not the same. The former was proposed by you and Bin Li in 2012 originally for mapping the second-quantized many-electron Hamiltonian. What we showed in JCP 145, 204105 (2016) is that both Li-Miller and Meyer-Miller mapping models can be derived from a unified framework for mapping a multi-state Hamiltonian.

Jeremy Richardson recently had a manuscript on arXiv.
https://arxiv.org/abs/1912.10906
What they did is in practice an extension from our work in JCP 151, 024105 (2019).
Add the zero-point energy to the electronic DOF, then use the constraint
Sum_over_n states [x_n^2 + p_n^2 - gama] = 1
with the Meyer-Miller mapping model.

Please feel free to contact me in case of any more questions or comments. It is very encouraging that the field pioneered by you has been so active.

All the best
Jian

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主题: your recent paper

Dear Jian,

You may be getting ready to celebrate the New Year, while I'mfinally catching up on some things that have been 'on my plate' for a while.Things have been pretty wild here at homeas Emily and family are now in my house with me for a few months while theirsin Oakland is undergoing an extensive addition.

I wanted to send you some thoughts/questions regarding yourrecent paper JCP 151, 024105:

1. It looks like forboth CMM1 and CMM2 you set gamma == 0 in the Hamiltonian (and thus in the eqnsof motion) and are of course then not using the SQC model to define the initialand final ‘window functions’, i.e., to define initial and final electronicstates.This is certainly OK; we did itas the simplest thing we could think of, and tying the ZPE parameter in theHamiltonian to histogram windows simply minimized the number of empirical parameters.But then it is not clear to me what youchoose for the initial conditions for the electronic DOF,and define the final probability, Pm(t), in Eq29.Do you use the Wigner fcn of thefinal states, as LSC-IVR?It looksthough that you do not use this for the initial state Pn(0) (since you statethat you impose Eq 28 for the initial populations, which would not be true withthe LSC-IVR initial conditions).

E.g., With gamma = 0, and requiring the sum Pn(0) = 1, thisalmost sounds like Ehrenfest initial conditions; is this correct?

Thus it would help clarify things to state EXPLICITLY whatthe initial conditions for the initial electronic state are, and the final ‘windowfcns’ for the final states.

2.It is remarkablethat the results from your CMM1 and CMM2 models seem to be effectivelyindistinguishable!Is that always thecase?

Sorry you’re not hear to talk directly with you about allthis, so email will have to do!

With best wishes for 2020!

Bill

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