Equivalence among TDVP and IVD

Alessandro Sinibaldi

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0.1 Introduction

The aim of this document is to show that the time dependent variational principle (TDVP) method and the implicit variational dynamics (IVD) method are equivalent at the first non trivial order in dt, namely $O(\delta t^2)$. Here we will consider the case of real parameters, so the McLachlan's variational principle.

Chapter 1

Time dependent variational principle

The quantity to maximize is the fidelity among $|\phi(t+\delta t)\rangle$ and $|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle$:

$$\mathcal{F}(\dot{\boldsymbol{\theta}}(t)) = \frac{|\langle\phi(t+\delta t)|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle|^2}{\langle\phi(t+\delta t)|\phi(t+\delta t)\rangle\,\langle\psi[\boldsymbol{\theta}(t+\delta t)]|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle}. \tag{1.1}$$

where:

$$|\phi(t+\delta t)\rangle = |\psi[\boldsymbol{\theta}(t)]\rangle - i\delta t\hat{H}\,|\psi[\boldsymbol{\theta}(t)]\rangle + O(\delta t^2) \tag{1.2a}$$

$$|\psi[\boldsymbol{\theta}(t+\delta t)]\rangle = |\psi[\boldsymbol{\theta}(t)]\rangle + \delta t\sum_k \dot{\theta}_k(t)\hat{O}_k(t)\,|\psi[\boldsymbol{\theta}(t)]\rangle + O(\delta t^2). \tag{1.2b}$$

$$\begin{aligned}
&|\langle\phi(t+\delta t)|\psi(t+\delta t)\rangle|^2 = |\langle\phi(t)|\,[\hat{1}+i\delta t\hat{H}][\hat{1}+\delta t\sum_k \hat{O}_k(t)\dot{p}_k(t)]\,|\psi(t)\rangle|^2 \\
&= |1+i\delta t\langle\hat{H}\rangle + \delta t\sum_k \dot{p}_k(t)\langle\hat{O}_k(t)\rangle + i\delta t^2\sum_k \dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle|^2 \\
&= \left(1+i\delta t\langle\hat{H}\rangle + \delta t\sum_k \dot{p}_k(t)\langle\hat{O}_k(t)\rangle + i\delta t^2\sum_k \dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle\right) \\
&\cdot\left(1-i\delta t\langle\hat{H}\rangle + \delta t\sum_k \dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\rangle - i\delta t^2\sum_k \dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\hat{H}\rangle\right) \\
&= 1-i\delta t\langle\hat{H}\rangle + \delta t\sum_k \dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\rangle - i\delta t^2\sum_k \dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\hat{H}\rangle \\
&+ i\delta t\langle\hat{H}\rangle + \delta t^2\langle\hat{H}\rangle^2 + i\delta t^2\langle\hat{H}\rangle\sum_k \dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\rangle + \delta t\sum_k \dot{p}_k(t)\langle\hat{O}_k(t)\rangle \\
&- i\delta t^2\langle\hat{H}\rangle\sum_k \dot{p}_k(t)\langle\hat{O}_k(t)\rangle + \delta t^2\sum_{k,k'}\langle\hat{O}_k(t)\rangle\langle\hat{O}^\dagger_{k'}(t)\rangle\dot{p}_k(t)\dot{p}^*_{k'}(t) + i\delta t^2\sum_k \dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle
\end{aligned} \tag{1.3}$$

$$\begin{aligned}
&= 1+\delta t\sum_k\left(\dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\rangle + \dot{p}_k(t)\langle\hat{O}_k(t)\rangle\right) + i\delta t^2\langle\hat{H}\rangle\sum_k\left(\langle\dot{p}^*_k(t)\hat{O}^\dagger_k(t)\rangle - \dot{p}_k(t)\langle\hat{O}_k(t)\rangle\right) \\
&+ i\delta t^2\sum_k\left(\dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle - \dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\hat{H}\rangle\right) + \delta t^2\sum_{k,k'}\langle\hat{O}_k(t)\rangle\langle\hat{O}^\dagger_{k'}(t)\rangle\dot{p}_k(t)\dot{p}^*_{k'}(t) + \delta t^2\langle\hat{H}\rangle^2
\end{aligned} \tag{1.4}$$

$$\begin{aligned}
&\langle\psi(t+\delta t)|\psi(t+\delta t)\rangle = \langle\psi(t)|\,[\hat{1}+\delta t\sum_k \hat{O}^\dagger_k(t)\dot{p}^*_k(t)][\hat{1}+\delta t\sum_k \hat{O}_k(t)\dot{p}_k(t)]\,|\psi(t)\rangle = \\
&\qquad = 1+\delta t\sum_k\left(\dot{p}^*_k(t)\langle\hat{O}^\dagger_k(t)\rangle + \dot{p}_k(t)\langle\hat{O}_k(t)\rangle\right) + \delta t^2\sum_{k,k'}\langle\hat{O}^\dagger_k(t)\hat{O}_{k'}(t)\rangle\dot{p}^*_k(t)\dot{p}_{k'}(t)
\end{aligned} \tag{1.5}$$

Calling $|\langle\phi(t+\delta t)|\psi(t+\delta t)\rangle|^2 \equiv N$ and $\langle\psi(t+\delta t)|\psi(t+\delta t)\rangle \equiv D$, we can obtain the equation for the time evolution of $\dot{p}_j(t)$ considering:

$$\frac{\partial \mathcal{F}(\{\dot{p}_k(t), \dot{p}_k^*(t)\})}{\partial \dot{p}_j^*(t)} = 0 \implies \frac{\partial N}{\partial \dot{p}_j^*(t)} D - N \frac{\partial D}{\partial \dot{p}_j^*(t)} = 0 \tag{1.6}$$

The differentiation with respect to $\dot{p}_j(t)$ would give the equation for the time evolution of $\dot{p}_j^*(t)$. Therefore:

$$\frac{\partial N}{\partial \dot{p}_j^*(t)} = \delta t \langle \hat{O}_j^\dagger(t)\rangle + i\delta t^2 \langle \hat{H}\rangle\langle \hat{O}_j^\dagger(t)\rangle - i\delta t^2 \langle \hat{O}_j(t)^\dagger \hat{H}\rangle + \delta t^2 \sum_k \langle \hat{O}_k(t)\rangle\langle \hat{O}_j^\dagger(t)\rangle \dot{p}_k(t) \tag{1.7}$$

$$\frac{\partial D}{\partial \dot{p}_j^*(t)} = \delta t \langle \hat{O}_j^\dagger(t)\rangle + \delta t^2 \sum_k \langle \hat{O}_j^\dagger(t)\hat{O}_k(t)\rangle \dot{p}_k(t) \tag{1.8}$$

Finally:

$$\begin{aligned}\frac{\partial N}{\partial \dot{p}_j^*(t)} D - N \frac{\partial D}{\partial \dot{p}_j^*(t)} &= \delta t \langle \hat{O}_j^\dagger(t)\rangle + i\delta t^2 \langle \hat{H}\rangle\langle \hat{O}_j^\dagger(t)\rangle - i\delta t^2 \langle \hat{O}_j^\dagger(t) \hat{H}\rangle + \delta t^2 \sum_k \langle \hat{O}_k(t)\rangle\langle \hat{O}_j^\dagger(t)\rangle \dot{p}_k(t) \\ &+ \delta t^2 \langle \hat{O}_j^\dagger(t)\rangle \sum_k \Big(\dot{p}_k^*(t)\langle \hat{O}_k^\dagger(t)\rangle + \dot{p}_k(t)\langle \hat{O}_k(t)\rangle \Big) \\ &- \Big\{ \delta t \langle \hat{O}_j^\dagger(t)\rangle + \delta t^2 \sum_k \langle \hat{O}_j^\dagger(t)\hat{O}_k(t)\rangle \dot{p}_k(t) \\ &+ \delta t^2 \langle \hat{O}_j^\dagger(t)\rangle \sum_k \Big(\dot{p}_k^*(t)\langle \hat{O}_k^\dagger(t)\rangle + \dot{p}_k(t)\langle \hat{O}_k(t)\rangle \Big) \Big\} = 0\end{aligned} \tag{1.9}$$

$$\implies \boxed{i \sum_k \Big(\langle \hat{O}_j^\dagger(t)\hat{O}_k(t)\rangle - \langle \hat{O}_j^\dagger(t)\rangle\langle \hat{O}_k(t)\rangle \Big) \dot{p}_k(t) = \Big(\langle \hat{O}_j^\dagger(t)\hat{H}\rangle - \langle \hat{O}_j^\dagger(t)\rangle\langle \hat{H}\rangle \Big)} \tag{1.10}$$

Chapter 2

Implicit variational dynamics

2.1 Introduction

The main idea of this method is the same as the previous one, namely approximating the evolution of the exact state using a variational state. However, this time for the exact state we use the implicit evolution formula:

$$\begin{aligned}|\phi(t+\delta t)\rangle &= \exp(-i\delta t\hat{H})\,|\phi(t)\rangle = [\exp(i\delta t\hat{H}/2)]^{-1}\exp(-i\delta t\hat{H}/2)\,|\phi(t)\rangle \\ &\approx \left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)^{-1}\left(\hat{1}-\frac{i\delta t}{2}\hat{H}\right)|\phi(t)\rangle\end{aligned} \tag{2.1}$$

$$\implies \left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\phi(t+\delta t)\rangle \approx \left(\hat{1}-\frac{i\delta t}{2}\hat{H}\right)|\phi(t)\rangle\,. \tag{2.2}$$

Therefore, this time we want to maximize the fidelity between the states $\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\psi(t+\delta t)\rangle$ and $\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\phi(t+\delta t)\rangle$. Since we have $|\psi(t)\rangle = |\phi(t)\rangle$, this corresponds to the fidelity between the states $\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\psi(t+\delta t)\rangle$ and $\left(\hat{1}-\frac{i\delta t}{2}\hat{H}\right)|\psi(t)\rangle$, namely:

$$\begin{aligned}&\mathcal{F}\Bigg(\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\psi(t+\delta t)\rangle\,,\left(\hat{1}-\frac{i\delta t}{2}\hat{H}\right)|\psi(t)\rangle\Bigg) = \\ &= \frac{|\,\langle\psi(t)|\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\psi(t+\delta t)\rangle\,|^2}{\langle\psi(t)|\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)\left(\hat{1}-\frac{i\delta t}{2}\hat{H}\right)|\psi(t)\rangle\,\langle\psi(t+\delta t)|\left(\hat{1}-\frac{i\delta t}{2}\hat{H}\right)\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\psi(t+\delta t)\rangle}\,.\end{aligned} \tag{2.3}$$

2.2 Time evolution of the parameters

For $|\psi(t+\delta t)\rangle$, we employ the same linearization as before. The norm of $\left(\hat{1}-\frac{i\delta t}{2}\hat{H}\right)|\psi(t)\rangle$ at the denominator of (2.3) does not contain the parameters $\{\dot{p}_k(t)\}$ and, thus, can be excluded from the optimization. Let's compute the other two terms (up to order $O(\delta t^2)$):

$$\begin{aligned}&|\,\langle\psi(t)|\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)\left(\hat{1}+\frac{i\delta t}{2}\hat{H}\right)|\psi(t+\delta t)\rangle\,|^2 = |\,\langle\psi(t)|\left(\hat{1}+i\delta t\hat{H}-\frac{\delta t^2}{4}\hat{H}^2\right)|\psi(t+\delta t)\rangle\,|^2 = \\ &= |\,\langle\psi(t)|\left(\hat{1}+\delta t\sum_k \hat{O}_k(t)\dot{p}_k(t)\right)|\psi(t)\rangle + i\delta t\,\langle\psi(t)|\,\hat{H}\left(\hat{1}+\delta t\sum_k \hat{O}_k(t)\dot{p}_k(t)\right)|\psi(t)\rangle\end{aligned} \tag{2.4}$$

$$
\begin{aligned}
&-\frac{\delta t^2}{4}\langle\psi(t)|\,\hat{H}^2\Big(\hat{1}+\delta t\sum_k\hat{O}_k(t)\dot{p}_k(t)\Big)\,|\psi(t)\rangle\,|^2=|1+\delta t\sum_k\dot{p}_k(t)\langle\hat{O}_k(t)\rangle+i\delta t\langle\hat{H}\rangle\\
&+i\delta t^2\sum_k\dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle-\frac{\delta t^2}{4}\langle\hat{H}^2\rangle|^2=\Big(1+\delta t\sum_k\dot{p}_k(t)\langle\hat{O}_k(t)\rangle+i\delta t\langle\hat{H}\rangle\\
&i\delta t^2\sum_k\dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle-\frac{\delta t^2}{4}\langle\hat{H}^2\rangle\Big)\cdot\Big(1+\delta t\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger(t)\rangle-i\delta t\langle\hat{H}\rangle\\
&-i\delta t^2\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger\hat{H}(t)\rangle-\frac{\delta t^2}{4}\langle\hat{H}^2\rangle\Big)=1+\delta t\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger(t)\rangle-i\delta t\langle\hat{H}\rangle\\
&-i\delta t^2\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger\hat{H}(t)\rangle-\frac{\delta t^2}{4}\langle\hat{H}^2\rangle+\delta t\sum_k\dot{p}_k(t)\langle\hat{O}_k(t)\rangle\\
&\delta t^2\sum_{k,k'}\langle\hat{O}_k(t)\rangle\langle\hat{O}_{k'}^\dagger(t)\rangle\dot{p}_k(t)\dot{p}_{k'}^*(t)-i\delta t^2\langle\hat{H}\rangle\sum_k\dot{p}_k(t)\langle\hat{O}_k(t)\rangle+i\delta t\langle\hat{H}\rangle\\
&+i\delta t^2\langle\hat{H}\rangle\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger(t)\rangle+\delta t^2\langle\hat{H}\rangle^2+i\delta t^2\sum_k\dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle-\frac{\delta t^2}{4}\langle\hat{H}^2\rangle\\
&=1+\delta t\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger(t)\rangle\rangle-i\delta t^2\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger\hat{H}(t)\rangle-\frac{\delta t^2}{2}\langle\hat{H}^2\rangle\\
&+\delta t\sum_k\dot{p}_k(t)\langle\hat{O}_k(t)\rangle+\delta t^2\sum_{k,k'}\langle\hat{O}_k(t)\rangle\langle\hat{O}_{k'}^\dagger(t)\rangle\dot{p}_k(t)\dot{p}_{k'}^*(t)-i\delta t^2\langle\hat{H}\rangle\sum_k\dot{p}_k(t)\langle\hat{O}_k(t)\rangle+\\
&+i\delta t^2\langle\hat{H}\rangle\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger(t)\rangle+\delta t^2\langle\hat{H}\rangle^2+i\delta t^2\sum_k\dot{p}_k(t)\langle\hat{H}\hat{O}_k(t)\rangle
\end{aligned}
\tag{2.5}
$$

$$
\begin{aligned}
&\langle\psi(t+\delta t)|\Big(\hat{1}-\frac{i\delta t}{2}\hat{H}\Big)\Big(\hat{1}+\frac{i\delta t}{2}\hat{H}\Big)|\psi(t+\delta t)\rangle=\langle\psi(t)|\Big(\hat{1}+\delta t\sum_k\hat{O}_k^\dagger\dot{p}_k^*\Big)\\
&\Big(\hat{1}+\frac{\delta t^2}{4}\hat{H}^2\Big)\Big(\hat{1}+\delta t\sum_k\hat{O}_k\dot{p}_k\Big)|\psi(t)\rangle=\Big(1+\delta t\sum_k\dot{p}_k(t)\langle\hat{O}_k(t)\rangle+\frac{\delta t^2}{2}\langle\hat{H}^2\rangle\\
&+\delta t\sum_k\dot{p}_k^*\langle\hat{O}_k^\dagger\rangle+\delta t^2\sum_{k,k'}\langle\hat{O}_k^\dagger(t)\hat{O}_{k'}(t)\rangle\dot{p}_k^*(t)\dot{p}_{k'}(t)\Big)
\end{aligned}
\tag{2.6}
$$

Calling $|\langle\psi(t)|\Big(\hat{1}+\frac{i\delta t}{2}\hat{H}\Big)\Big(\hat{1}+\frac{i\delta t}{2}\hat{H}\Big)|\psi(t+\delta t)\rangle|^2\equiv N$ and $\langle\psi(t+\delta t)|\Big(\hat{1}-\frac{i\delta t}{2}\hat{H}\Big)\Big(\hat{1}+\frac{i\delta t}{2}\hat{H}\Big)|\psi(t+\delta t)\rangle\equiv D$, as before, we compute:

$$
\frac{\partial N}{\partial\dot{p}_j^*}=\delta t\langle\hat{O}_j^\dagger(t)\rangle-i\delta t^2\langle\hat{O}_j^\dagger(t)\hat{H}\rangle+\delta t^2\sum_k\langle\hat{O}_k(t)\rangle\langle\hat{O}_j^\dagger(t)\rangle\dot{p}_k(t)+i\delta t^2\langle\hat{H}\rangle\langle\hat{O}_j^\dagger(t)\rangle \tag{2.7}
$$

$$
\frac{\partial D}{\partial\dot{p}_j^*}=\delta t\langle\hat{O}_j^\dagger(t)\rangle+\delta t^2\sum_k\langle\hat{O}_j^\dagger(t)\hat{O}_k(t)\rangle\dot{p}_k(t) \tag{2.8}
$$

Finally:

$$
\begin{aligned}
&\frac{\partial N}{\partial\dot{p}_j^*}D-\frac{\partial D}{\partial\dot{p}_j^*}N=\delta t\langle\hat{O}_j^\dagger(t)\rangle-i\delta t^2\langle\hat{O}_j^\dagger(t)\hat{H}\rangle+\delta t^2\sum_k\langle\hat{O}_k(t)\rangle\langle\hat{O}_j^\dagger(t)\rangle\dot{p}_k(t)+i\delta t^2\langle\hat{H}\rangle\langle\hat{O}_j^\dagger(t)\rangle\\
&+\delta t^2\langle\hat{O}_j^\dagger(t)\rangle\sum_k\dot{p}_k^*(t)\langle\hat{O}_k^\dagger(t)\rangle-\Big\{\delta t\langle\hat{O}_j^\dagger(t)\rangle+\delta t^2\sum_k\langle\hat{O}_j^\dagger(t)\hat{O}_k(t)\rangle\dot{p}_k(t)
\end{aligned}
\tag{2.9}
$$

$$+ \delta t^2 \langle \hat{O}_j^\dagger(t) \rangle \sum_k \dot{p}_k^*(t) \langle \hat{O}_k^\dagger(t) \rangle + \delta t^2 \langle \hat{O}_j^\dagger(t) \rangle \sum_k \dot{p}_k(t) \langle \hat{O}_k(t) \rangle \Bigg\} = 0 \tag{2.10}$$

$$\implies \boxed{i \sum_k \Bigg(\langle \hat{O}_j^\dagger(t) \hat{O}_k(t) \rangle - \langle \hat{O}_j^\dagger(t) \rangle \langle \hat{O}_k(t) \rangle \Bigg) \dot{p}_k(t) = \Bigg(\langle \hat{O}_j^\dagger(t) \hat{H} \rangle - \langle \hat{O}_j^\dagger(t) \rangle \langle \hat{H} \rangle \Bigg)} \tag{2.11}$$

We obtained the same equation for the time evolution of $\{\dot{p}_k(t)\}$ as in chapter 1.