Various forms of quantum propagation with Frozen Gaussians from variational principle.

1. Variational principle in Classical Mechanics and Coherent State notations

After Lagrangian

$$L = p\dot{q} - H(p,q) \tag{1.1}$$

and action $S = \int L\,dt$ are introduced the Hamilton's Equations can be obtained by standard variation

$$\delta S = \int \left(\delta p\,\dot{q} + \delta\dot{q}\,p - \delta p\frac{\partial H}{\partial p} - \delta q\frac{\partial H}{\partial q} \right) dt = \int \left(\delta p\left(\dot{q} - \frac{\partial H}{\partial p}\right) - \delta q\left(\dot{p} + \frac{\partial H}{\partial q}\right)\right) dt \tag{1.2}$$

which uses integration by parts $\int \left(\delta\dot{q}\,p \right) dt = -\int \left(\delta q\,\dot{p} \right) dt$

As a result the Hamiltons equations

$$\dot{q} = \frac{\partial H}{\partial p} \qquad \dot{p} = -\frac{\partial H}{\partial q} \tag{1.3}$$

Are obtained. In a similar fashion the Lagrangian can be written as

$$L = \frac{p\dot{q} - q\dot{p}}{2} - H(p,q) \tag{1.4}$$

giving the same Hamilton's Equations. Also, Lagrangian can be written in z notations $z = \frac{q+ip}{\sqrt{2}}$ $\quad z^* = \frac{q-ip}{\sqrt{2}}$

$$L = \frac{p\dot{q} - q\dot{p}}{2} - H(p,q) = \frac{i}{2}\left(\dot{z}z^* - \dot{z}^*z\right) - H(z,z^*) \tag{1.5}$$

Its variation gives

$$\delta S = \int \left[\frac{i}{2}\left(\delta\dot{z}\,z^* + \dot{z}\,\delta z^* - \delta\dot{z}^*z - \dot{z}^*\delta z \right) - \delta z^*\frac{\partial H(z,z^*)}{\partial z^*} - \delta z\frac{\partial H(z,z^*)}{\partial z} \right] dt \tag{1.6}$$

which after integration by parts

$$\int\left(\delta \dot{z}\, z^{*}\right)dt=-\int\left(-\dot{z}^{*}\delta z\right)dt \qquad \int\left(\delta \dot{z}^{*} z\right)dt=-\int\left(\dot{z}\,\delta z^{*}\right)dt \tag{1.7}$$

becomes

$$\delta S=\int\left[\delta z^{*}\left(i\dot{z}-\frac{\partial H(z,z^{*})}{\partial z^{*}}\right)-\delta z\left(i\dot{z}^{*}+\frac{\partial H(z,z^{*})}{\partial z}\right)\right]dt \tag{1.8}$$

yielding Hamilton's Equations in z-notations.

$$\dot{z}^{*}=i\frac{\partial H\left(z,z^{*}\right)}{\partial z} \qquad \text{and} \qquad \dot{z}=-i\frac{\partial H\left(z,z^{*}\right)}{\partial z^{*}} \tag{1.9}$$

Of course, they are equivalent to Lagrange equations

$$\frac{\partial L}{\partial z}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}}=0 \qquad \text{and} \qquad \frac{\partial L}{\partial z^{*}}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}^{*}}=0 \tag{1.10}$$

Indeed, for the first equation with the derivatives with respect to z one gets:

$$\frac{\partial L}{\partial z}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}}=-\left(\frac{\partial H(z,z^{*})}{\partial z}+\frac{i}{2}\dot{z}^{*}\right)-\left(\frac{i}{2}\dot{z}^{*}\right) \quad \text{hence} \quad \dot{z}^{*}=i\frac{\partial H\left(z,z^{*}\right)}{\partial z} \tag{1.11}$$

And similarly for z^{*}

2. Dynamics of a single CS from variational principle

Assume that the wave function is given by a single CS

$$|\Psi\rangle=a|z\rangle \tag{2.1}$$

Let us now work out the evolution of its position $|z(t)\rangle$ and its amplitude $a(t)$. First of all it is convenient write the operator

$$i\frac{\hat{\partial}}{\partial t}=i\frac{\vec{\partial}}{\partial t}-i\frac{\overleftarrow{\partial}}{\partial t} \tag{2.2}$$

in a more symmetric form as a sum of two parts acting on the ket $i\frac{\vec{\partial}}{\partial t}$ or on the bra $-i\frac{\bar{\partial}}{\partial t}$. Then the Lagrangian becomes:

$$L = \langle \Psi | i\frac{\hat{\partial}}{\partial t} - \hat{H} | \Psi \rangle = \frac{i}{2}\left[a^* \dot{a} - a \dot{a}^* \right] \langle z | z \rangle + \frac{i}{2}\left[z^* \dot{z} - z \dot{z}^* \right] a^* a - a^* a H_{ord}(z, z^*) \tag{2.3}$$

where $\langle z | z \rangle = 1$ and index *ord* appeared because of quantum averaging $\langle \Psi | \hat{H} | \Psi \rangle = \langle az | \hat{H} | az \rangle = a^* a \langle z | z \rangle H_{ord}(z, z^*) = a^* a H_{ord}(z, z^*)$. The Lagrangian (2.3) is a very convenient object in which classical coordinate z, z^* and quantum amplitude a, a^* enter in an absolutely similar fashion and therefore can be treated identically. Then the equations of motion are simply

$$\frac{\partial L}{\partial z} - \frac{d}{dt}\frac{\partial L}{\partial \dot{z}} = 0 \quad , \quad \frac{\partial L}{\partial z^*} - \frac{d}{dt}\frac{\partial L}{\partial \dot{z}^*} = 0 \tag{2.4}$$

and

$$\frac{\partial L}{\partial a} - \frac{d}{dt}\frac{\partial L}{\partial \dot{a}} = 0 \quad , \quad \frac{\partial L}{\partial a^*} - \frac{d}{dt}\frac{\partial L}{\partial \dot{a}^*} = 0 \tag{2.5}$$

Eqs. (2.4) and (2.5) yield correspondently

$$\frac{\partial L}{\partial z^*} - \frac{d}{dt}\frac{\partial L}{\partial \dot{z}^*} = a^* a \left[-\frac{\partial H_{ord}(z^*, z)}{\partial z^*} + i\dot{z} \right] + iz\frac{d(a^* a)}{dt} = 0 \tag{2.6}$$

$$\frac{\partial L}{\partial a^*} - \frac{d}{dt}\frac{\partial L}{\partial \dot{a}^*} = \left[i\frac{\dot{z} z^* - \dot{z}^* z}{2} - H_{ord}(z, z^*) \right] a + i\frac{da}{dt} = 0 \tag{2.7}$$

and similar equations for complex conjugates. The solution of (2.7) is

$$a = a(0)\exp(iS) \tag{2.8}$$

where

$$S = \int \left[i\frac{\dot{z}z^* - \dot{z}^* z}{2} - H_{ord}(z, z^*) \right] dt \tag{2.9}$$

The solution of (18) is simply

$$\dot{z} = -i\frac{\partial H_{ord}(z, z^*)}{\partial z^*} \tag{2.10}$$

It yeilds classical dynamics on corrected Hamiltonian $H_{ord}(z, z^*) = \langle z|\hat{H}|z\rangle$, which simply reflects the fact that the Hamiltonian should be averaged over Gaussian CS z.

The main conclusion of this section are:

(1) Classical dynamics with "reordered" potential (2.10) results from Lagrange equations based on variational principle

(2) Lagrange equations and variational principle also gives rise to the "frozen Gaussian" solution (2.8,2.9) for the amplitude.

(3) The Lagrangiane can be written such that quantum amplitudes a, a^* are treated in the same way as to the classical variables z, z^*.

(4) Even more generally the Lagrangian $\left\langle \Psi(\alpha_1^*, \alpha_2^*, \ldots) \middle| i\frac{\hat{\partial}}{\partial t} - \hat{H} \middle| \Psi(\alpha_1^*, \alpha_2^*, \ldots) \right\rangle$ and the Lagrange equations $\frac{\partial L}{\partial \alpha_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\alpha}_i} = 0$, $\frac{\partial L}{\partial \alpha_i^*} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\alpha}_i^*} = 0$ can be in principle written for any parameter of the wave function

3. Dynamics of an ensemble of CS from variational principle

Now consider a superposition of several frozen Gaussian CS

$$|\Psi\rangle = \sum a_i |z_i\rangle \tag{3.1}$$

Let us now allow a variation of amplitudes and phase space positions z. Then taking into account that

$$\langle z_i | z_j \rangle = \exp\left(z^*{}_i\, z_j - \frac{z^*{}_i\, z_i}{2} - \frac{z^*{}_j\, z_j}{2} \right) \tag{3.2}$$

and

$$\langle z_i | \frac{i}{2}\frac{\vec{\partial}}{\partial t} | z_j \rangle = \frac{i}{2}\left(\frac{\partial \langle z_i | z_j \rangle}{\partial z^*{}_j} \dot{z}^*{}_j + \frac{\partial \langle z_i | z_j \rangle}{\partial z_j} \dot{z}_j \right) = \frac{i}{2}\left(\left(z_i{}^* - \frac{z^*{}_j}{2} \right) \dot{z}_j - \frac{z_j\, \dot{z}_j{}^*}{2} \right) \langle z_i | z_j \rangle$$

(3.3)

$$\langle z_i | -\frac{i}{2}\frac{\overleftarrow{\partial}}{\partial t} | z_j \rangle = -\frac{i}{2}\left(\frac{\partial \langle z_i | z_j \rangle}{\partial z^*{}_i} \dot{z}^*{}_i + \frac{\partial \langle z_i | z_j \rangle}{\partial z_i} \dot{z}_i \right) = -\frac{i}{2}\left(\left(z_j - \frac{z_i}{2} \right) \dot{z}^*{}_i - \frac{z^*{}_i\, \dot{z}_i}{2} \right) \langle z_i | z_j \rangle$$

the Lagrangian is

$$L = \langle \Psi | i \frac{\hat{\partial}}{\partial t} - \hat{H} | \Psi \rangle = \langle \Psi | \frac{i}{2}\left(\frac{\vec{\partial}}{\partial t} - \frac{\overleftarrow{\partial}}{\partial t} \right) - \hat{H} | \Psi \rangle = \sum_{i,j} \; \{ \frac{i}{2}\left[a_i{}^* \dot{a}_j - a_j \dot{a}_i{}^* \right] \langle z_i | z_j \rangle +$$

$$\frac{i}{2}\left[\left(\left(z_i{}^* - z^*{}_j \right) \dot{z}_j + \frac{\dot{z}_j\, z^*{}_j}{2} - \frac{z_j\, \dot{z}_j{}^*}{2} \right) - \left(\left(z_j - z_i \right) \dot{z}^*{}_i + \frac{z_i\, \dot{z}^*{}_i}{2} - \frac{\dot{z}_i\, z^*{}_i}{2} \right) \right] \tag{3.4}$$

$$a_i{}^* a_j \langle z_i | z_j \rangle - a_i{}^* a_j \langle z_i | z_j \rangle H_{ord}\left(z^*{}_i, z_j \right) \}$$

Before working out the Lagrange equations it is convenient to sum up only the terms in (26) which contain index i

$$L = L_{ii} + \sum_{j \neq i} \left(L_{ij} + L_{ji} \right) \tag{3.5}$$

where L_{ii} is given by (2.3)

$$L_{ii} = i\left[\frac{a_i{}^* \dot{a}_i}{2} - \frac{a_i\, \dot{a}_i{}^*}{2} \right] + i\left[\frac{z_i{}^* \dot{z}_i}{2} - \frac{z_i\, \dot{z}_i{}^*}{2} \right] a_i{}^* a_i - a_i{}^* a_i\, H_{ord}\left(z_i, z_i{}^* \right) \tag{3.6}$$

and

$$
\begin{aligned}
&L_{ij}+L_{ji}=\\
&\sum_{j\neq i}\frac{i}{2}\left\{\left[a_i{}^*\dot{a}_j-a_j\dot{a}_i{}^*\right]\langle z_i|z_j\rangle+\left[a_j{}^*\dot{a}_i-a_i\dot{a}_j{}^*\right]\langle z_j|z_i\rangle\right\}+\\
&\sum_{j\neq i}\frac{i}{2}\left\{\left(\left(z_i{}^*-\frac{z^*{}_j}{2}\right)\dot{z}_j-\frac{z_j\dot{z}_j{}^*}{2}\right)-\left(\left(z_j-\frac{z_i}{2}\right)\dot{z}^*{}_i-\frac{\dot{z}_i z^*{}_i}{2}\right)\right\}a_i{}^*a_j\langle z_i|z_j\rangle+\\
&\sum_{j\neq i}\frac{i}{2}\left\{\left(\left(z_j{}^*-\frac{z^*{}_i}{2}\right)\dot{z}_i-\frac{z_i\dot{z}_i{}^*}{2}\right)-\left(\left(z_i-\frac{z_i}{2}\right)\dot{z}^*{}_j-\frac{\dot{z}_j z^*{}_j}{2}\right)\right\}a_j{}^*a_i\langle z_j|z_i\rangle-\\
&\sum_{j\neq i}\left\{\ a_i{}^*a_j\langle z_i|z_j\rangle H_{ord}\left(z^*{}_i,z_j\right)+a_j{}^*a_i\langle z_j|z_i\rangle H_{ord}\left(z^*{}_j,z_i\right)\right\}
\end{aligned}
\tag{3.7}
$$

The equations for amplitudes and z can be obtained as Lagrange equations (2.4), (2.5). This gives a system of linear coupled equations for N (where N is the basis set size) amplitudes a_n and M×N (where M is the number of degrees of freedom) components of N complex vectors $z_n^{(m)}$. Therefore we end up with the system of (M+1)×N coupled linear equations. (Remember that M-dimensional CS z is a product of M 1D CS)

$$|z\rangle=|z^{(1)}\rangle|z^{(2)}\rangle...|z^{(M)}\rangle \qquad (3.8))$$

The results of this section are:

(1) The full quantum Lagrangian of a system of frozen Gaussian is given by (3.7)
(2) The equations for z and their amplitudes are the Lagrange equations obtained from (3.7)
(3) This would be a full variation of the action with Lagrangian (3.7) and equivalent to those obtained by Burghardt and Woth (Chem.Phys.Lett. 4D Henon-Heiles).
(4) The experience of Burghardt and Woth shows that to obtain z requires solving (M+1)×N linear equations at every step, which is a difficult task.

In the next two sections we will consider this possible simplifications. And in the last section we will look at the "full" variational solution again.

4. Coupled Coherent States Amplitudes from variationof amplitudes only.

Let us first perform only variation with respect to amplitudes assuming that the tajectories $z_i(t)$ are known. Then

$$\frac{\partial L}{\partial a_i *} - \frac{d}{dt}\frac{\partial L}{\partial \dot{a}_i *} = \frac{\partial L_i}{\partial a_i *} - \frac{d}{dt}\frac{\partial L_i}{\partial \dot{a}_i *} = \sum_j \{ \frac{i}{2}\dot{a}_j \langle z_i | z_j \rangle +$$

$$\frac{i}{2}\left[(z_i * - z *_j)\dot{z}_j + \frac{\dot{z}_j z *_j}{2} - \frac{z_j \dot{z}_j *}{2} - (z_j - z_i)\dot{z} *_i + \frac{\dot{z}_i z *_i}{2} - \frac{z_i \dot{z} *_i}{2} \right] a_j \langle z_i | z_j \rangle -$$

$$a_j \langle z_i | z_j \rangle H_{ord}(z *_i, z_j) + \frac{i}{2}\frac{d a_j \langle z_i | z_j \rangle}{dt} \} \tag{4.1}$$

Taking into account that $\frac{d a_j \langle z_i | z_j \rangle}{dt} = \frac{d a_j}{dt}\langle z_i | z_j \rangle + a_j \frac{d\langle z_i | z_j \rangle}{dt}$ and

$$\frac{d\langle z_i | z_j \rangle}{dt} = \left[\left(z_i * - \frac{z *_j}{2} \right)\dot{z}_j - \frac{z_j \dot{z}_j *}{2} + \left(z_j - \frac{z_i}{2} \right)\dot{z} *_i - \frac{z *_i \dot{z}_i}{2} \right] \langle z_i | z_j \rangle \tag{4.2}$$

Eq.(28) becomes

$$\sum_j \; i\dot{a}_j \langle z_i | z_j \rangle - \langle z_i | z_j \rangle H_{ord}(z *_i, z_j) a_j + \tag{4.3}$$

$$i\left[(z_i * - z *_j)\dot{z}_j + \frac{\dot{z}_j z *_j}{2} - \frac{z_j \dot{z}_j *}{2} \right] \langle z_i | z_j \rangle a_j = 0$$

This is already familiar from CCS. We can now choose trajectories of z and obtain equations for amplitudes. First choose $\dot{z} = 0$ (static grid) then eq.(4.3) yields (in vector/matrix form):

$$\mathbf{\Omega}\,\dot{\mathbf{a}} = -i\,\mathbf{Ha} \tag{4.4}$$

where $\Omega_{ij} = \langle z_i | z_j \rangle$ is the overlap matrix and $H_{ij} = \langle z_i | H | z_j \rangle = \langle z_i | z_j \rangle H_{ord}(z *_i, z_j)$ is the matrix of the Hamiltonian.

Next option is to choose a time dependent z(t) (dynamical grid). At this point let us also write the amplitude as $a_j = d_j \exp(iS_j)$ where $S_j = \int \left[i\left(\frac{\dot{z}_j z^*_j}{2} - \frac{z_j \dot{z}_j^*}{2} \right) - H_{ord}(z_j^*, z_j) \right] dt$.

Then the equation (4.3) becomes

$$\sum_{j \neq i} \left[\langle z_i | z_j \rangle \dot{d}_j \exp(iS_j) + i \langle z_i | z_j \rangle \delta^2 H'_{ij} d_j \exp(iS_j) \right] = 0 \tag{4.5}$$

or in matrix form $\mathbf{\Omega} \exp(\mathbf{iS})\, \dot{\mathbf{d}} = -i\ \mathbf{\Delta^2 H'} \exp(\mathbf{iS})\, \mathbf{d}$ where

$$\Delta^2 H'_{ij} = \langle z_i | z_j \rangle \delta^2 H'_{ij} = \langle z_i | z_j \rangle \left[H_{ord}(z^*_i, z_j) - H_{ord}(z^*_j, z_j) - i(z^*_i - z^*_j)\dot{z}_j \right] \tag{4.6}$$

If now we choose $\dot{z}_j$ to be the "optimal" for single CS (i.e driven by the Eq.(3.10)) we end up with the familiar equations of the CCS theory. So the main conclusions of this section are:

(1) The CCS theory is a simplification to the full variational equations by avoiding variation of z but using simple solution for z(t), which is optimal in the approximation of single CS.
(2) The gain is huge. Instead of dealing with large (M+1)×N vectors and corresponding matrixes we get away with the vector of N amplitudes only and N×N matrixes.
(3) This however comes at a price of having less flexible wave function.

In the next few sections we will investigate other options for the choice of trajectories, such as fully variational trajectories, variations of trajectories only and also Bohmian-like trajectories.

5. Variation of z

Let us consider consider variation of z. The result is:

$$
\begin{aligned}
&\frac{\partial L}{\partial z_i *}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}_i *}=a_i * a_i\left[i\dot{z}_i-\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right]+\sum_{j\neq i} a_i * a_j\left[i\dot{z}_j-\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right]\langle z_i|z_j\rangle+i\frac{z_i}{2}\frac{d}{dt}\left(a_i^* a_i\right)+\\
&\sum_{j\neq i} a_i * a_j\left(z_j-\frac{z_i}{2}\right)\langle z_i|z_j\rangle\left\{i\left(\left(z*_i-\frac{z*_j}{2}\right)\dot{z}_j-\frac{z_j\dot{z}*_j}{2}\right)-H_{ord}\left(z*_i, z_j\right)\right\}+\\
&\sum_{j\neq i} a_i a*_j\left(\frac{z_i}{2}\right)\langle z_j|z_i\rangle\left\{i\left(\left(z_i-\frac{z_j}{2}\right)\dot{z}*_j-\frac{z*_j\dot{z}_j}{2}\right)+H_{ord}\left(z*_j, z_i\right)\right\}\\
&\sum_{j\neq i} i\left\{a_i * \dot{a}_j\left(z_j-\frac{z_i}{2}\right)\langle z_i|z_j\rangle+a_i\dot{a}*_j\left(\frac{z_i}{2}\right)\langle z_j|z_i\rangle\right\}=0
\end{aligned}
\tag{5.1}
$$

which can be rearranged as:

$$
\begin{aligned}
&\frac{\partial L}{\partial z_i *}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}_i *}=\frac{\partial L_i}{\partial z_i *}-\frac{d}{dt}\frac{\partial L_i}{\partial \dot{z}_i *}=\\
&a_i * a_i\left[i\dot{z}_i-\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right]+\sum_{j\neq i} a_i * a_j\left[i\dot{z}_j-\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right]\langle z_i|z_j\rangle+\\
&\sum_{j\neq i} a_i * a_j\left(z_j-z_i\right)\langle z_i|z_j\rangle\left\{i\left(\left(z*_i-\frac{z*_j}{2}\right)\dot{z}_j-\frac{z_j\dot{z}*_j}{2}\right)-H_{ord}\left(z*_i, z_j\right)\right\}+\\
&\sum_{j\neq i} i\left\{a_i * \dot{a}_j\left(z_j-z_i\right)\langle z_i|z_j\rangle\right\}+\\
&\left(\frac{z_i}{2}\right)\left(\sum_{j\neq i} a_i a*_j\langle z_j|z_i\rangle\left\{i\left(\left(z_i-z_j\right)\dot{z}*_j+\frac{\dot{z}*_j z_j-z*_j\dot{z}_j}{2}\right)+H_{ord}\left(z*_j, z_i\right)\right\}\right)+\\
&\left(\frac{z_i}{2}\right)\left(\sum_{j\neq i} a_i * a_j\langle z_i|z_j\rangle\left\{i\left(\left(z*_i-z*_j\right)\dot{z}_j+\frac{z*_j\dot{z}_j-z_j\dot{z}*_j}{2}\right)-H_{ord}\left(z*_i, z_j\right)\right\}\right)+\\
&\left(\frac{z_i}{2}\right)\frac{d}{dt}i\left(a_i^* a_i\right)+\left(\frac{z_i}{2}\right)\sum_{j\neq i} i\left\{a_i * \dot{a}_j\langle z_i|z_j\rangle+a_i\dot{a}*_j\langle z_j|z_i\rangle\right\}=0
\end{aligned}
\tag{5.2}
$$

or

$$\frac{\partial L}{\partial z_i *}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}_i *}=\sum_j a_i * a_j\left[i\,\dot{z}_j-\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right]\left\langle z_i \middle| z_j\right\rangle+$$
$$\sum_j a_i * a_j\left(z_j-z_i\right)\left\langle z_i \middle| z_j\right\rangle\left\{i\left(\left(z*_i-\frac{z*_j}{2}\right)\dot{z}_j-\frac{z_j\,\dot{z}*_j}{2}\right)-H_{ord}\left(z*_i,\, z_j\right)\right\}+$$
$$\sum_j i\left\{a_i * \dot{a}_j\left(z_j-z_i\right)\left\langle z_i \middle| z_j\right\rangle\right\}$$
$$\left(\frac{z_i}{2}\right)\left(\sum_j a_i a*_j\left\langle z_j \middle| z_i\right\rangle\left\{i\left(\left(z_i-z_j\right)\dot{z}*_j+\frac{\dot{z}*_j\,z_j-z*_j\,\dot{z}_j}{2}\right)+H_{ord}\left(z*_j,\, z_i\right)\right\}\right)+$$
$$\left(\frac{z_i}{2}\right)\left(\sum_j a_i * a_j\left\langle z_i \middle| z_j\right\rangle\left\{i\left(\left(z*_i-z*_j\right)\dot{z}_j+\frac{z*_j\,\dot{z}_j-z_j\,\dot{z}*_j}{2}\right)-H_{ord}\left(z*_i,\, z_j\right)\right\}\right)+$$
$$\left(\frac{z_i}{2}\right)\sum_j i\left\{a_i * \dot{a}_j\left\langle z_i \middle| z_j\right\rangle+a_i\,\dot{a}*_j\left\langle z_j \middle| z_i\right\rangle\right\}=0$$

(5.3)

This equation can be solved for the time derivatives of z together with those for the derivatives of the amplitude (4.5) and in this case will be equivalent to the approach of Burghardt and Worth. They noticed that due to highly oscillatory nature of the solution the time step must be very short.

Before solving the equation one may notice that the last 3 sums in (5.3) are equal to zero due to eq.(4.5) so that in fully variational principle (5.3) greately simplifies and becomes:

$$\frac{\partial L}{\partial z_i *}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}_i *}=\sum_j a_i * a_j\left[i\,\dot{z}_j-\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right]\left\langle z_i \middle| z_j\right\rangle+$$
$$a_i *\sum_j\left(z_j-z_i\right)\left\langle z_i \middle| z_j\right\rangle\left\{i\,\dot{a}_j+\left(i\left(\left(z*_i-z*_j\right)\dot{z}_j+\frac{\dot{z}_j\,z*_j}{2}-\frac{z_j\,\dot{z}*_j}{2}\right)-H_{ord}\left(z*_i,\, z_j\right)\right)a_j\right\}=0$$

(5.4)

Now let us as usual write the Eq.(34) for the preexponential coefficient d_j (so that $a_i = d_i \exp(iS_i)$) instead of the amplitude a_i. Then the system of equations for $\dot{z}_i$ which follows from the Lagrange equation becomes

$$\frac{\partial L}{\partial z_i*} - \frac{d}{dt}\frac{\partial L}{\partial \dot{z}_i*} =$$

$$d_i*d_i\left[i\dot{z}_i - \frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i*}\right] + \sum_{j\neq i} d_i*d_j \exp\left(i\left(S_j - S_i\right)\right)\left[i\dot{z}_j - \frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i*}\right]\left\langle z_i \middle| z_j\right\rangle +$$
$$i\sum_{j\neq i}\left(z_j - z_i\right)\left[\left\langle z_i \middle| z_j\right\rangle \dot{d}_j\, d_i*\exp\left(i(S_j - S_i)\right) + i\left\langle z_i \middle| z_j\right\rangle \delta^2 H'_{ij} d_j d_i*\exp\left(i(S_j - S_i)\right)\right] +$$
$$i\left(\frac{z_i}{2}\right)\frac{d\left(d_i*d_i\right)}{dt} +$$
$$i\left(\frac{z_i}{2}\right)\sum_{j\neq i}\left[\left\langle z_i \middle| z_j\right\rangle \dot{d}_j\, d_i*\exp\left(i(S_j - S_i)\right) + i\left\langle z_i \middle| z_j\right\rangle \delta^2 H'_{ij} d_j d_i*\exp\left(i(S_j - S_i)\right)\right] +$$
$$i\left(\frac{z_i}{2}\right)\sum_{j\neq i}\left[\left\langle z_j \middle| z_i\right\rangle d_i\, \dot{d}*_j \exp\left(i(S_i - S_j)\right) - i\left\langle z_j \middle| z_i\right\rangle \delta^2 H'*_{ij}\, d_i d*_j \exp\left(i(S_i - S_j)\right)\right] = 0$$

(5.5)

or eventually

$$\begin{aligned}
&\sum_j d_i*d_j \exp\left(i\left(S_j - S_i\right)\right)\left[i\dot{z}_j - \frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i*}\right]\left\langle z_i \middle| z_j\right\rangle + \\
&id_i*\sum_j\left(z_j - z_i\right)\left[\left\langle z_i \middle| z_j\right\rangle \dot{d}_j \exp\left(i(S_j - S_i)\right) + i\left\langle z_i \middle| z_j\right\rangle \delta^2 H'_{ij} d_j \exp\left(i(S_j - S_i)\right)\right] + \\
&i\left(\frac{z_i}{2}\right)d_i*\sum_j\left[\left\langle z_i \middle| z_j\right\rangle \dot{d}_j \exp\left(i(S_j - S_i)\right) + i\left\langle z_i \middle| z_j\right\rangle \delta^2 H'_{ij} d_j \exp\left(i(S_j - S_i)\right)\right] + \\
&i\left(\frac{z_i}{2}\right)d_i\sum_j\left[\left\langle z_j \middle| z_i\right\rangle \dot{d}*_j \exp\left(i(S_i - S_j)\right) - i\left\langle z_j \middle| z_i\right\rangle \delta^2 H'*_{ij}\, d*_j \exp\left(i(S_i - S_j)\right)\right] = 0
\end{aligned} \tag{5.6}$$

where

$$\delta^2 H'_{ij} = \left[H_{ord}\left(z*_i, z_j\right) - H_{ord}\left(z*_j, z_j\right) - i\left(z*_i - z*_j\right)\dot{z}_j\right] \tag{5.7}$$

is given by (4.6) and

$$\delta^2 H'*_{ij} = \left[H_{ord}\left(z*_j, z_i\right) - H_{ord}\left(z*_j, z_j\right) + i\left(z_i - z_j\right)\dot{z}*_j\right] \tag{5.8}$$

The algebra needs to be checked one more time but I think it is OK now!!!

The Equations (5.6) look complicated but they simply linearly connect derivatives of z and derivatives of amplitudes./ preexponential factors. Also if variational equations (4.5) for the amplitudes are obeyed then the last two sums in (5.6) are zero. This will be considered in the section 7 in more details.

6. Coupled CS trajectories from variation of z only

Now like in the section 4 we are free to choose any time dependence of amplitudes/preesponential factors d !!!!! Let us for example choose d=const, which follow again from the optimal solution for optimal solution for single Frozen Gaussian (2.8, 2.9). Then the system of equations (5.6) becomes

$$\begin{aligned}
&\sum_j d_i^* d_j \exp\left(i\left(S_j - S_i\right)\right)\left[i\dot{z}_j - \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*}\right]\left\langle z_i \middle| z_j\right\rangle + \\
&\sum_{j\neq i}\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right) - i\left(z^*_i - z^*_j\right)\dot{z}_j\right] d_j d_i^* \exp\left(i\left(S_j - S_i\right)\right) + \\
&\left(\frac{z_i}{2}\right)\sum_{j\neq i}\left\langle z_i \middle| z_j\right\rangle\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right) - i\left(z^*_i - z^*_j\right)\dot{z}_j\right] d_j d_i^* \exp\left(i\left(S_j - S_i\right)\right) + \\
&\left(\frac{z_i}{2}\right)\sum_{j\neq i}\left\langle z_j \middle| z_i\right\rangle\left[H_{ord}\left(z^*_j, z_i\right) - H_{ord}\left(z^*_j, z_j\right) + i\left(z_i - z_j\right)\dot{z}^*_j\right] d^*_j\, d_i \exp\left(i(S_i - S_j)\right) = 0
\end{aligned}$$

(6.1)

Or to put it differently

$$i\mathbf{A}\dot{\mathbf{z}} = \mathbf{b} \tag{6.2}$$

This system gives velocities for nonclassical CS entangled trajectories, which ensure the Frozen Gaussian solution d=const. As usual if we have N CS in M dimensions we do not need to solve NM copled linear equations for the amplitudes. Instead we need to solve N coupled equations for each of the M components of the vector z, which is a much simpler task. The method of Coherent State Entangled Trajectories will be tested

The eq.(6.1) can also be written in a more “symmetric” with respect to the indexes I and j form

$$\sum_j d_i^* d_j \exp\left(i\left(S_j - S_i\right)\right)\left[i\dot{z}_j - \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*}\right]\left\langle z_i \middle| z_j\right\rangle +$$
$$\frac{1}{2}\sum_{j\neq i}\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right) - i\left(z^*_i - z^*_j\right)\dot{z}_j\right] d_j d_i^* \exp\left(i\left(S_j - S_i\right)\right) +$$
$$\left(\frac{z_j}{2}\right)\sum_{j\neq i}\left\langle z_i \middle| z_j\right\rangle\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right) - i\left(z^*_i - z^*_j\right)\dot{z}_j\right] d_j d_i^* \exp\left(i\left(S_j - S_i\right)\right) +$$
$$\left(\frac{z_i}{2}\right)\sum_{j\neq i}\left\langle z_j \middle| z_i\right\rangle\left[H_{ord}\left(z^*_j, z_i\right) - H_{ord}\left(z^*_j, z_j\right) + i\left(z_i - z_j\right)\dot{z}^*_j\right] d^*_j\, d_i \exp\left(i(S_i - S_j)\right) = 0$$
$$(6.3)$$

This approach is the closest in spirit to Bohmian mechanics. Many people liked the idea, but it has never been tried.

A nice feature of (6.3) is that it includes the elements of density matrix

7. Full variation again

Full variation will include simultaneous solution of (4.5) and (5.6). As discussed above obtaining the time derivatives of z and d would require solving (M+1)×N linear equations at every step, which is a difficult task. The equations derived here should still have an advantage before those of Burghardt and Woth in a bigger time step because highly oscillating exponent have been taken out of the equations. Notice that if solved together with Eq.(4.5) the Eq.(5.6) simplifies and becomes:

$$\sum_j d_i^* d_j \exp\left(i\left(S_j - S_i\right)\right)\left[i\dot{z}_j - \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*}\right]\left\langle z_i \middle| z_j\right\rangle +$$
$$\sum_j i d_i^*\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)\left[\dot{d}_j + i\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right) - i\left(z^*_i - z^*_j\right)\dot{z}_j\right] d_j\right]$$
$$= 0$$
$$(7.1)$$

Because according to Eq.(4.5)

$$\sum_{j\neq i}\left[\left\langle z_i \middle| z_j\right\rangle \dot{d}_j \exp\left(iS_j\right) + i\left\langle z_i \middle| z_j\right\rangle \delta^2 H'_{ij} d_j \exp\left(iS_j\right)\right] = 0 \qquad (7.2)$$

and the last two sums in Eq.(5.6) and (6.1) become zero. Remind you, that in Eq.(7.1) $\delta^2 H'_{ij} = \left[H_{ord}\left(z*_i, z_j\right) - H_{ord}\left(z*_j, z_j\right) - i\left(z*_i - z*_j\right)\dot{z}_j \right]$ (see (4.6)). The equations (7.1) and (7.2) represent a system of linear equations for the derivatives of all z and d. Previously Miklos solved it numerically in his version of variational method.

Notice also that (7.1) can be formally written as

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left[i\dot{z}_j - \frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i *} \right]\left\langle z_i \middle| z_j \right\rangle + \\ i d_i * \sum_j \left(z_j - z_i\right)\left\langle z_i \middle| z_j \right\rangle \exp\left(i\left(S_j - S_i\right)\right)\left[\dot{d}_j + i\delta^2 H'_{ij} d_j \right] = 0 \tag{7.3}$$

But this is a bit misleading as it is important for us to remember that $\delta^2 H'_{ij}$ depends on $\dot{z}_j$ as we want to find all time derivatives from a system of linear equations (7.1).

8 .Approximate full variation

Let us now solve (7.2) for the amplitudes but we will make some simplifications in (7.1). First, let us disregard the second line in (7.1). We can do it because there the factor is always small $\left(z_j - z_i\right)\left\langle z_i \middle| z_j \right\rangle$. The overlap $\left\langle z_i \middle| z_j \right\rangle$ is small for remote CSs and $\left(z_j - z_i\right)$ is small for those CSs, which are close. Then (7.1) becomes

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left[-\frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i *} + i\dot{z}_j \right]\left\langle z_i \middle| z_j \right\rangle = 0 \tag{8.1}$$

or in matrix form

$$i\boldsymbol{\rho}\dot{\mathbf{z}} = \left\langle \frac{\partial H}{\partial \mathbf{z}*} \right\rangle \tag{8.2}$$

or

$$\dot{\mathbf{z}} = -i\boldsymbol{\rho}^{-1}\left\langle \frac{\partial H}{\partial \mathbf{z}*} \right\rangle = -i\left(\boldsymbol{\rho}^{-1}\left\langle \frac{\partial V}{\partial \mathbf{z}*} \right\rangle + \boldsymbol{\rho}^{-1}\left\langle \frac{\partial T}{\partial \mathbf{z}*} \right\rangle \right) \tag{8.3}$$

where

$$\boldsymbol{\rho}_{ij} = \left\langle z_i \middle| z_j \right\rangle d_i * d_j \exp\left(i\left(S_j - S_i\right)\right) \tag{8.4}$$

is the density matrix, and $\boldsymbol{\rho}^{-1}$ is the inverse density matrix. The components of the right hand side vector $\mathbf{h}$ are

$$\left\langle \frac{\partial H}{\partial \mathbf{z}^*} \right\rangle_i = \sum_j \rho_{ij} \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*} \tag{8.5}$$

In fact (43) is very familiar. If the Hamiltonian is a sum of kinetic and potential energy,

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{q}})$$

then for the real and imaginary part of (43) it becomes:

$$\begin{aligned} \dot{\mathbf{q}} &= \boldsymbol{\rho}^{-1} \frac{\langle \hat{\mathbf{p}} \rangle}{m} \\ \dot{\mathbf{p}} &= -\boldsymbol{\rho}^{-1} \langle \hat{\mathbf{F}} \rangle \end{aligned} \tag{8.6}$$

where

$$\begin{aligned} \langle \hat{\mathbf{p}} \rangle &= \left\langle \frac{\partial T}{\partial \mathbf{p}^*} \right\rangle_i = \sum_j \rho_{ij} \frac{\partial T_{ord}\left(z_i^*, z_j\right)}{\partial p_i^*} \\ \langle \hat{\mathbf{F}} \rangle &= \left\langle \frac{\partial V}{\partial \mathbf{q}^*} \right\rangle_i = \sum_j \rho_{ij} \frac{\partial V_{ord}\left(z_i^*, z_j\right)}{\partial q_i^*} \end{aligned} \tag{8.7}$$

(This needs to be checked. I am tired and have not done the algebra, but I am almost certain that (8.7) is correct). The first of the equations (8.6) is very similar to the equations for Bohmian velocity, except that it contains then inverse density matrix instead of division by local density $|\Psi|^2$. The Force changes the momentum as a parameter of each CS z. But there seem to be no Bohmian Force and Bohmian potential $\frac{\hbar^2}{2m}\frac{\Delta|\Psi|}{|\Psi|^2}$ in (8.7). Or maybe there is? We need to check this. Hopefully this recipe will be simple enough to implement as it requires dealing only with a small NxN density matrix but the trajectories will be quantum enough and close enough to the variational ones and we will not need many of them as a result.

Finally our recipe is to use the equations (8.6) or (8.2-8.3) for the trajectories together with the standard equations (7.2) for the amplitude

This can be known. Perhaps Irene Burghardt or Eric Bittner or somebody else has already tried something of that sort.
I have tried this and it does not seem to work very well. Perhaps the problem is that there is no Bohmian Force. However, it is worth looking at again. Also it can be a starting point for the next idea in the section 9.

9 Iterative full variation

One also can try use iterative method to solve the variational equations (7.1-7.2) . Write them as follows:

$$\sum_j d_i{}^* d_j \exp\left(i\left(S_j - S_i\right)\right)\left[i\dot{z}_j - \frac{\partial H_{ord}\left(z_i{}^*, z_j\right)}{\partial z_i{}^*}\right]\left\langle z_i \middle| z_j\right\rangle =$$
$$-\sum_j i d_i{}^*\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)\left[\dot{d}_j + i\left[H_{ord}\left(z^*{}_i, z_j\right) - H_{ord}\left(z^*{}_j, z_j\right) - i\left(z^*{}_i - z^*{}_j\right)\dot{z}_j\right] d_j\right] \tag{9.1}$$

Because according to Eq.(32)

$$\sum_{j\neq i}\left[\left\langle z_i \middle| z_j\right\rangle \dot{d}_j \exp\left(i(S_j - S_i)\right) + i\left\langle z_i \middle| z_j\right\rangle \delta^2 H'_{ij} d_j \exp\left(i(S_j - S_i)\right)\right] = 0 \tag{9.2}$$

or

$$\sum_j d_i{}^* d_j \exp\left(i\left(S_j - S_i\right)\right)\left\langle z_i \middle| z_j\right\rangle\left[i\dot{z}_j\right] =$$
$$\sum_j d_i{}^* d_j \exp\left(i\left(S_j - S_i\right)\right)\left[\frac{\partial H_{ord}\left(z_i{}^*, z_j\right)}{\partial z_i{}^*}\right]\left\langle z_i \middle| z_j\right\rangle$$
$$-\sum_j i\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)\left[d_i{}^*\dot{d}_j + i\left[H_{ord}\left(z^*{}_i, z_j\right) - H_{ord}\left(z^*{}_j, z_j\right) - i\left(z^*{}_i - z^*{}_j\right)\dot{z}_j\right] d_i{}^* d_j\right] \tag{9.3}$$

First neglect the right hand side in (9.1) (or the last line of the right hand side in (9.3)) and find Bohmilan-like $\dot{\mathbf{z}}$ given by equations (8.6) from the previous section. Then find $\dot{\mathbf{d}}$ from (9.1). Substitute $\dot{\mathbf{z}}$ and $\dot{\mathbf{d}}$ to the right hand side of (9.1) or (9.3) and find new $\dot{\mathbf{z}}$. Then find $\dot{\mathbf{d}}$ again and so on so forth. This may converge. If it does then we get a great method to do variational dynamics cheaply. It will be based on Bohmian like trajectories, which will suit CHAMPS and Darryl will like it.

Let us have more details about iterations. Let us rewrite (9.3) as follows:

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left(1-\left|z_i - z_j\right|^2\right)\left\langle z_i \middle| z_j\right\rangle\left[i\dot{z}_j\right]=$$

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left[\frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*} - \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_j^*}\left|z_i - z_j\right|^2\right]\left\langle z_i \middle| z_j\right\rangle$$

$$+\sum_j \left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right) - \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_j^*}\left(z^*_i - z^*_j\right)\right] d_i * d_j$$

$$-\sum_j i\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)\left[d_i * \dot{d}_j\right]$$

Here I moved all terms with $\dot{z}$ to the left and added and subtracted $\frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_j^*}\left|z_i - z_j\right|^2$ on the right. Here is the algebra

Step 1

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left\langle z_i \middle| z_j\right\rangle\left(1-\left|z_j - z_i\right|^2\right)\left[i\dot{z}_j\right]=$$

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left[\frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*}\right]\left\langle z_i \middle| z_j\right\rangle$$

$$-\sum_j i\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)\left[d_i * \dot{d}_j + i\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right)\right] d_i * d_j\right]$$

Step 2

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left\langle z_i \middle| z_j\right\rangle\left(1-\left|z_j - z_i\right|^2\right)\left[i\dot{z}_j\right]=$$

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left[\frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*}\right]\left\langle z_i \middle| z_j\right\rangle$$

$$-\sum_j i\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)$$

$$\left[d_i * \dot{d}_j + i\left[H_{ord}\left(z^*_i, z_j\right) - H_{ord}\left(z^*_j, z_j\right) + \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*}\left(z^*_j - z^*_i\right) - \frac{\partial H_{ord}\left(z_i^*, z_j\right)}{\partial z_i^*}\left(z^*_j - z^*_i\right)\right] d_i * d_j\right]$$

Step 3

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left\langle z_i \middle| z_j\right\rangle\left(1-\left|z_j - z_i\right|^2\right)\left[i\dot{z}_j\right] =$$

$$\sum_j d_i * d_j \exp\left(i\left(S_j - S_i\right)\right)\left(1-\left|z_j - z_i\right|^2\right)\left[\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right]\left\langle z_i \middle| z_j\right\rangle$$

$$-\sum_j i\left(z_j - z_i\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right)$$

$$\left[d_i * \dot{d}_j + i\left[H_{ord}\left(z *_i, z_j\right) - H_{ord}\left(z *_j, z_j\right) + \frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\left(z *_j - z *_i\right)\right] d_i * d_j\right]$$

Step 4. Then, finally we obtain:

$$\boxed{\begin{aligned}
&\sum_j \rho_{ij}^{(2)}\left[i\dot{z}_j\right] = \\
&\sum_j \rho_{ij}^{(2)}\left[\frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\right] \\
&\qquad + \sum_j \rho_{ij}\left(z_j - z_i\right)\left[H_{ord}\left(z *_i, z_j\right) - H_{ord}\left(z *_j, z_j\right) + \frac{\partial H_{ord}\left(z_i *, z_j\right)}{\partial z_i *}\left(z *_j - z *_i\right)\right] \\
&\qquad\quad + \sum_j i\omega_{ij}\left(z_j - z_i\right)\left[d_i * \dot{d}_j\right]
\end{aligned}} \tag{9.4}$$

$$\begin{aligned}
\omega_{ij} &= \left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right) \\
\rho_{ij} &= \left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right) d_i * d_j = \omega_{ij}\, d_i * d_j \\
\rho_{ij}^{(2)} &= \left(1-\left|z_j - z_i\right|^2\right)\left\langle z_i \middle| z_j\right\rangle \exp\left(i\left(S_j - S_i\right)\right) d_i * d_j = \left(1-\left|z_j - z_i\right|^2\right)\rho_{ij}
\end{aligned} \tag{9.5}$$

We probably can use (9.4) and (9.5) for iteration scheme:

1) Disregard the last term in the right hand side, which includes $\dot{d}$. Alternatively you can try to use use CCS for $\dot{d}$ instead of zero. And solve (9.4)
2) Then find $\dot{d}$ from (9.2)
3) Repeat

The sums on the right hand side should be analyzed. Perhaps we can disregard some of them. For example the second one is of the cubic order with respect to the absolute value

of $z_j - z_i$? Or perhaps if we do everything in the continuum z, i.e with the integral instead of the finite sum. Then perhaps we could prove that this term is zero? This might be because it includes *$(z_i$-$z_j)$* which gives zero in complex contour integration $\oint$.
???

Let us keep going: One more step: Let us add and subtract $\sum_j \rho_{ij}^{(2)} \left[\frac{\partial H_{ord}\left(z_j*, z_j\right)}{\partial z_j*} \right]$

$$
\begin{aligned}
&\sum_j \rho_{ij}^{(2)} \left[i \dot{z}_j \right] = \\
&\sum_j \rho_{ij}^{(2)} \left[\frac{\partial H_{ord}\left(z_j*, z_j\right)}{\partial z_j*} \right] + \sum_j \rho_{ij}^{(2)} \left[\frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i*} - \frac{\partial H_{ord}\left(z_j*, z_j\right)}{\partial z_j*} \right] \\
&\quad + \sum_j \rho_{ij}\left(z_j - z_i\right)\left[H_{ord}\left(z*_i, z_j\right) - H_{ord}\left(z*_j, z_j\right) + \frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i*}\left(z*_j - z*_i\right) \right] \\
&\quad + \sum_j i\omega_{ij}\left(z_j - z_i\right)\left[d_i * \dot{d}_j \right]
\end{aligned}
$$

In this form

$$
\sum_j \rho_{ij}^{(2)} \left[i \dot{z}_j \right] = \sum_j \rho_{ij}^{(2)} \left[\frac{\partial H_{ord}\left(z_j*, z_j\right)}{\partial z_j*} \right]
$$

Yeilds the CCS solution. And the rest is quantum contribution, which is

$$
\begin{aligned}
&\sum_j \rho_{ij}^{(2)} \left[i \dot{z}_j \right] - \sum_j \rho_{ij}^{(2)} \left[\frac{\partial H_{ord}\left(z_j*, z_j\right)}{\partial z_j*} \right] = \\
&\sum_j \rho_{ij}\left(1 - \left(z_j - z_i\right)\left(z_j* - z_i*\right)\right)\left[\frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i*} - \frac{\partial H_{ord}\left(z_j*, z_j\right)}{\partial z_j*} \right] \\
&\quad + \sum_j \rho_{ij}\left(z_j - z_i\right)\left[H_{ord}\left(z*_i, z_j\right) + \frac{\partial H_{ord}\left(z_i*, z_j\right)}{\partial z_i*}\left(z*_j - z*_i\right) - H_{ord}\left(z*_j, z_j\right) \right] \\
&\quad + \sum_j i\omega_{ij}\left(z_j - z_i\right)\left[d_i * \dot{d}_j \right]
\end{aligned}
$$

Or

$$\sum_j \rho_{ij}^{(2)}\left[i\dot{z}_j\right]-\sum_j \rho_{ij}^{(2)}\left[\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\right]=$$

$$\sum_j \rho_{ij}\left[\frac{\partial H_{ord}\left(z_i^*,z_j\right)}{\partial z_i^*}-\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\right]$$

$$+\sum_j \rho_{ij}\left(z_j-z_i\right)\left[H_{ord}\left(z^*_i,z_j\right)+\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\left(z^*_j-z^*_i\right)-H_{ord}\left(z^*_j,z_j\right)\right]$$

$$+\sum_j i\omega_{ij}\left(z_j-z_i\right)\left[d_i^*\dot{d}_j\right]$$

Then finally:

$$\boxed{\begin{aligned}
&\sum_j \rho_{ij}^{(2)}\left[i\dot{z}_j-\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\right]=\\
&=\sum_j \rho_{ij}\left[\frac{\partial H_{ord}\left(z_i^*,z_j\right)}{\partial z_i^*}-\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\right]\\
&\quad+\sum_j \rho_{ij}\left(z_j-z_i\right)\left[H_{ord}\left(z^*_i,z_j\right)-\left(H_{ord}\left(z^*_j,z_j\right)+\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\left(z^*_i-z^*_j\right)\right)\right]\\
&\quad+\sum_j i\omega_{ij}\left(z_j-z_i\right)\left[d_i^*\dot{d}_j\right]=\\
&=\sum_j \rho_{ij}\left[\frac{\partial H_{ord}\left(z_i^*,z_j\right)}{\partial z_i^*}-\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\right]\\
&\quad+\sum_j \rho_{ij}\left(z_j-z_i\right)\left[H_{ord}\left(z^*_i,z_j\right)-\left(H_{ord}\left(z^*_j,z_j\right)+\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\left(z^*_i-z^*_j\right)\right)\right]\\
&\quad+i\sum_j \rho_{ij}\left(z_j-z_i\right)\frac{\dot{d}_j}{d_j}
\end{aligned}}$$

(9.6)

Is it better than (9.4) ? The advantage is that the left there is written as a correction to CCS. So the right hand side gives quantum contribution. Can we simplify it even further? The leading order of second sum on the right hand side is cubic with respect to the absolute value of z_j-z_i . How about the first sum on the right hand side? Can we write it like this?

$$\sum_j \rho_{ij}\left[\frac{\partial H_{ord}\left(z_i^*,z_j\right)}{\partial z_i^*}-\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}\right]=$$

$$=\sum_j \rho_{ij}\left[\frac{\partial H_{ord}\left(z_i^*,z_j\right)}{\partial z_i^*}-\left(\frac{\partial H_{ord}\left(z_j^*,z_j\right)}{\partial z_j^*}+\frac{\partial^2 H_{ord}\left(z_j^*,z_j\right)}{\partial^2 z_j^*}\left(z_i^*-z_j^*\right)\right)\right]+$$

$$+\sum_j \rho_{ij}\left[\frac{\partial^2 H_{ord}\left(z_j^*,z_j\right)}{\partial^2 z_j^*}\left(z_i^*-z_j^*\right)\right]$$

The first sum on the right is quadratic with respect to $z_j^*-z_i^*$ and its absolute value. Can it be used? Can we prove that some sums are zero? Or at least perhaps we can neglect some of the sums?

10. A Technical note on matrix regularization.

When solving systems of linear equations matrixes have to be regularized as their small eigen values may cause problems. An n×n matrix **A** with a set of n eigen values $\lambda^{(1)}\ldots\lambda^{(n)}$ and eigen vectors $\boldsymbol{v}^{(1)}\ldots\boldsymbol{v}^{(n)}$ can be presented in the form:

$$\mathbf{A}=\begin{bmatrix} v_1^{(1)} & v_1^{(2)} & v_1^{(3)} & \ldots & v_1^{(n)} \\ v_2^{(1)} & v_2^{(2)} & v_2^{(3)} & \ldots & v_2^{(n)} \\ v_3^{(1)} & v_3^{(2)} & v_3^{(3)} & \ldots & v_3^{(n)} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ v_n^{(1)} & v_n^{(2)} & v_n^{(3)} & \ldots & v_n^{(n)} \end{bmatrix}\begin{bmatrix} \lambda^{(1)} & 0 & 0 & \ldots & 0 \\ 0 & \lambda^{(2)} & 0 & \ldots & 0 \\ 0 & 0 & \lambda^{(3)} & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & \lambda^{(n)} \end{bmatrix}\begin{bmatrix} v_1^{(1)*} & v_2^{(1)*} & v_3^{(1)*} & \ldots & v_n^{(1)*} \\ v_1^{(2)*} & v_2^{(2)*} & v_3^{(2)*} & \ldots & v_n^{(2)*} \\ v_1^{(3)*} & v_2^{(3)*} & v_3^{(3)*} & \ldots & v_n^{(3)*} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ v_1^{(n)*} & v_2^{(n)*} & v_3^{(n)*} & \ldots & v_n^{(n)*} \end{bmatrix}$$

Its inverse is simply given as

$$\mathbf{A}^{-1}=\begin{bmatrix} v_1^{(1)} & v_1^{(2)} & v_1^{(3)} & \ldots & v_1^{(n)} \\ v_2^{(1)} & v_2^{(2)} & v_2^{(3)} & \ldots & v_2^{(n)} \\ v_3^{(1)} & v_3^{(2)} & v_3^{(3)} & \ldots & v_3^{(n)} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ v_n^{(1)} & v_n^{(2)} & v_n^{(3)} & \ldots & v_n^{(n)} \end{bmatrix}\begin{bmatrix} 1/\lambda^{(1)} & 0 & 0 & \ldots & 0 \\ 0 & 1/\lambda^{(2)} & 0 & \ldots & 0 \\ 0 & 0 & 1/\lambda^{(3)} & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & 1/\lambda^{(n)} \end{bmatrix}\begin{bmatrix} v_1^{(1)*} & v_2^{(1)*} & v_3^{(1)*} & \ldots & v_n^{(1)*} \\ v_1^{(2)*} & v_2^{(2)*} & v_3^{(2)*} & \ldots & v_n^{(2)*} \\ v_1^{(3)*} & v_2^{(3)*} & v_3^{(3)*} & \ldots & v_n^{(3)*} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ v_1^{(n)*} & v_2^{(n)*} & v_3^{(n)*} & \ldots & v_n^{(n)*} \end{bmatrix}$$

Small eigen values may cause a numerical problem because for them $1/\lambda$ can be huge but they are usually unphysical and can be thrown away. Then the matrix and its inverse become:

$$\mathbf{A}=\begin{bmatrix} v_1^{(1)} & \dots & v_1^{(k)} \\ v_2^{(1)} & \dots & v_1^{(k)} \\ v_3^{(1)} & \dots & v_1^{(k)} \\ \dots & \dots & \dots \\ v_n^{(1)} & \dots & v_1^{(k)} \end{bmatrix}\begin{bmatrix} \lambda^{(1)} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & \lambda^{(k)} \end{bmatrix}\begin{bmatrix} v_1^{(1)*} & v_2^{(1)*} & v_3^{(1)*} & \dots & v_n^{(1)*} \\ \dots & \dots & \dots & \dots & \dots \\ v_1^{(k)*} & v_2^{(k)*} & v_3^{(k)*} & \dots & v_n^{(k)*} \end{bmatrix}$$

and

$$\mathbf{A}^{-1}=\begin{bmatrix} v_1^{(1)} & \dots & v_1^{(k)} \\ v_2^{(1)} & \dots & v_1^{(k)} \\ v_3^{(1)} & \dots & v_1^{(k)} \\ \dots & \dots & \dots \\ v_n^{(1)} & \dots & v_1^{(k)} \end{bmatrix}\begin{bmatrix} 1/\lambda^{(1)} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & 1/\lambda^{(k)} \end{bmatrix}\begin{bmatrix} v_1^{(1)*} & v_2^{(1)*} & v_3^{(1)*} & \dots & v_n^{(1)*} \\ \dots & \dots & \dots & \dots & \dots \\ v_1^{(k)*} & v_2^{(k)*} & v_3^{(k)*} & \dots & v_n^{(k)*} \end{bmatrix}$$

where k is the number of kept eigen values. This should be implemented. It is more expensive, but it may work. Then the elements of the matrix and its inverse become:

$$\left(\mathbf{A}\right)_{ij}=\sum_{\lambda_k>\varepsilon} v_i^{(k)}\lambda^{(k)}v_j^{(k)*}$$

$$\left(\mathbf{A}^{-1}\right)_{ij}=\sum_{\lambda_k>\varepsilon}\frac{v_i^{(k)}v_j^{(k)*}}{\lambda^{(k)}}$$

This should be very easy to code and to use.

THIS IS A BIT OF A DELIRIUM!! IF YOU ARE NOT DMITRY, DO NOT READ IT.

11. New form of variational equations related to quantum Liouville's equation and density matrix

Quantum Lagrangian for variational principle can be written in the form:

$$L=\vec{L}=\left\langle \Psi \right| i\frac{\vec{\partial}}{\partial t}-\hat{H}\left|\Psi\right\rangle \tag{11.1}$$

or in complex conjugate form:

$$L^{+}=\overleftarrow{L}=\left\langle \Psi \right| -i\frac{\overleftarrow{\partial}}{\partial t}-\hat{H}\left|\Psi\right\rangle \tag{11.2}$$

or in symmetrized form

$$L_{sym} = \frac{L+L^{+}}{2} = \frac{\vec{L}+\overleftarrow{L}}{2} = \langle \Psi | \frac{i}{2}\left(\frac{\vec{\partial}}{\partial t} - \frac{\overleftarrow{\partial}}{\partial t} \right) - \hat{H} | \Psi \rangle$$

(11.3)

One can use either of these Lagrangians and perhaps also the antisymmetric form

$$L_{sym} = \frac{L-L^{+}}{2} = \frac{\vec{L}-\overleftarrow{L}}{2} = \frac{1}{2}\langle \Psi | i\left(\frac{\vec{\partial}}{\partial t} + \frac{\overleftarrow{\partial}}{\partial t} \right) - \left(\vec{\hat{H}} - \overleftarrow{\hat{H}} \right) | \Psi \rangle$$

(11.4)

which can be written as

$$L_{sym} = \frac{1}{2} tr\left(i\dot{\hat{\rho}} - \left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H} \right) \right) \tag{11.5}$$

If, for example the wave function is given as a superposition of orthonormal basis functions $|\varphi_m\rangle$.

$$|\Psi\rangle = \sum_m a_m |\varphi_m\rangle \tag{11.6}$$

then

$$L = \quad i\sum_{n,m} a_n{}^* \langle \varphi_n | \varphi_m \rangle \dot{a}_m - \sum_{nm} \langle \varphi_n | \hat{H} | \varphi_m \rangle a_m a_n{}^* \tag{11.7}$$

$$\overleftarrow{L} = -i\sum_{n,m} \dot{a}_m{}^* \langle \varphi_m | \varphi_n \rangle a_n - \sum_{nm} a_n a_m{}^* \langle \varphi_m | \hat{H} | \varphi_n \rangle \tag{11.8}$$

Then subtracting and using $\langle \varphi_m | \varphi_n \rangle = \delta_{mn}$ we get

$$\begin{aligned} 2L_{asymm} &= L - L^* = \\ &= i\sum_n \left(\dot{a}_n{}^* a_n + a_n{}^* \dot{a}_n \right) - \sum_{nm} \left[\langle \varphi_n | \hat{H} | \varphi_m \rangle a_m a_n{}^* - a_n a_m{}^* \langle \varphi_m | \hat{H} | \varphi_n \rangle \right] = \\ &= tr\left(i\dot{\hat{\rho}} - (\hat{H}\hat{\rho} - \hat{\rho}\hat{H}) \right) \end{aligned} \tag{11.9}$$

Interestingly the asymmetric form of the Lagrangian L_{asymm} is simply given by the trace of the Quantum Liouville equation. Its variation with respect to all parameters must be equal to zero

$$\delta L_{asym} = \quad \frac{\delta\vec{L} - \delta\overleftarrow{L}}{2} = 0 \tag{11.10}$$

simply because

$$\delta\vec{L} = 0 \quad , \qquad \delta\overleftarrow{L} = 0 \tag{11.11}$$

Let us try to do variation of the difference $L_{asymm} = L - L^*$ and see what we get. Let us do the variation over $a_k{}^*$ for example. Then

$$\frac{\partial L_{asymm}}{\partial a_n *}-\frac{d}{dt}\frac{\partial L_{asymm}}{\partial \dot{a}_n *}=-i\dot{a}_n+i\dot{a}_n+\frac{\partial}{\partial a_n *}\left[\sum_{nm}\left[\langle\varphi_n|\hat{H}|\varphi_m\rangle a_m a_n *-a_m * a_n\langle\varphi_m|\hat{H}|\varphi_n\rangle\right]\right]=$$
$$=-i\dot{a}_n+i\dot{a}_n+\frac{\partial}{\partial a_n *}\left[\sum_{nm}\langle\varphi_n|\hat{H}|\varphi_m\rangle a_m a_n *\right]-\frac{\partial}{\partial a_n *}\left[\sum_{nm}\langle\varphi_n|\hat{H}|\varphi_m\rangle a_m a_n *\right]=$$
$$\sum_n\left(-i\dot{a}_n+i\dot{a}_n\right)+\sum_m\langle\varphi_n|\hat{H}|\varphi_m\rangle a_m-\sum_m a_n\langle\varphi_n|\hat{H}|\varphi_n\rangle=$$
$$\left[-i\dot{a}_k+\sum_m\langle\varphi_k|\hat{H}|\varphi_m\rangle a_m\right]+\left[i\dot{a}_k-\sum_n a_n\langle\varphi_k|\hat{H}|\varphi_n\rangle\right]=0+0 \tag{11.12}$$

We have got the known equations for the amplitudes.

We can also get the Liouville equation for the density matrix not only for orthogonal basis set (1.6) but also for a basis set of nonorthogonal Gaussians in which the wave function is given as:

$$|\Psi\rangle=\sum_m a_m|z_m\rangle=|\Psi\rangle=\sum_m d_m e^{iS_m}|z_m\rangle \tag{11.13}$$

I am not going to do variation, but simply will write the equations for the density matrix in the basis of Gaussian Coherent States which I already know. The density matrix operator we can write as

$$\hat{\rho}=\sum_{i,j}|\zeta_i\rangle\rho_{ij}\langle\zeta_j|=\sum_{i,j}|z_i\rangle e^{iS_i}\rho_{ij}e^{-iS_j}\langle z_j|=\sum_{i,j}|z_i\rangle B_{ij}\langle z_j| \tag{11.14}$$

where

$$\begin{aligned}|\zeta_i\rangle&=|z_i\rangle e^{iS_i}\\ \langle\zeta_j|&=e^{-iS_j}\langle z_j|\end{aligned} \tag{11.15}$$

so that $\rho_{ij}=d_i d_j *$. For the wave function propagation we do not get anything new here of course. But one can also think about (11.14) as a generic operator, not just density matrix and this is where density matrix propagation can be really important. Then the equations for the density matrix elements (i.e. quantum Liouville equation in Coherent State representation), are as follows.

$$\boxed{\frac{d\hat{\boldsymbol{\rho}}}{dt}=-i\left(\hat{\boldsymbol{\Omega}}^{-1}\ \boldsymbol{\delta}^2\hat{\mathbf{H}}'*\hat{\boldsymbol{\rho}}-\hat{\boldsymbol{\rho}}\ \boldsymbol{\delta}^2\hat{\mathbf{H}}\ \hat{\boldsymbol{\Omega}}^{-1}\right)} \tag{11.16}$$

We get the matrixes $\boldsymbol{\delta}^2\hat{\mathbf{H}}$ and $\boldsymbol{\delta}^2\hat{\mathbf{H}}'*$ just like those in the CCS method (see review Chem.Phys. 304 (2004) 103), where these two matrixes appear when we propagate amplitudes C and D in CCS. The overlap matrix in (11.16) includes actions

$$\hat{\boldsymbol{\Omega}}_{ij} = \langle \zeta_i | \zeta_j \rangle = \langle z_i | z_j \rangle e^{i(S_j - S_i)} \tag{11.17}$$

The matrixes $\boldsymbol{\delta}^2\hat{\mathbf{H}}$ and $\boldsymbol{\delta}^2\hat{\mathbf{H}}'*$ are given as follows:

$$i\frac{\overleftarrow{d}\hat{\boldsymbol{\Omega}}_{ij}}{dt} + \hat{\mathbf{H}}_{ij} = \left(H_{ij}\left(z_i^*, z_j\right) - H_{ii}\left(z_i^*, z_i\right) + i\dot{z}_i^*(z_j - z_i)\right)\langle \zeta_i | \zeta_j \rangle = \boldsymbol{\delta}^2\hat{\mathbf{H}}_{ij} \tag{11.18}$$

$$\hat{\mathbf{H}}_{ij} - i\frac{\vec{d}\hat{\boldsymbol{\Omega}}_{ij}}{dt} = \left(H_{ij}\left(z_i^*, z_j\right) - H_{jj}\left(z_j^*, z_j\right) - i\dot{z}_j(z_i^* - z_j^*)\right)\langle \zeta_i | \zeta_j \rangle = \boldsymbol{\delta}^2\hat{\mathbf{H}}'*_{ij} \tag{11.19}$$

See the write-up on density matrix, its properties, forms and propagation. It should be possible to obtain the equation (11.17) from variational principle, but I got them simply by substitution to the Schrödinger equation (or quantum Liouville equation). Any type of trajectories can be used in the equations (11.17). But if we use CCS trajectories $i\dot{z}_j = \dfrac{\partial H_{jj}\left(z_j^*, z_j\right)}{\partial z_j^*}$ then these matrixes are always small and have zero diagonal. Not so many modifications of the standard CCS code will be required! Only replace vector by matrix !!!

It would be interesting to get variational trajectories for the Lagrangian L_{asymm}

$$L_{asymm}=\frac{\vec{L}-\overleftarrow{L}}{2}=tr\left(i\dot{\hat{\rho}}-\left(\hat{H}\hat{\rho}-\hat{\rho}\hat{H}\right)\right)=$$

$$=i\sum_{n,m}\frac{d}{dt}\left(a_n{}^*\langle z_n|z_m\rangle a_m\right)-\sum_{nm}\left[\langle z_n|\hat{H}|z_m\rangle a_m a_n{}^*-a_m{}^*a_n\langle z_m|\hat{H}|z_n\rangle\right]=$$

$$=i\sum_{n,m}\langle z_n|z_m\rangle\frac{d}{dt}\left(a_n{}^*a_m\right)+i\sum_{n,m}a_n{}^*a_m\frac{d}{dt}\langle z_n|z_m\rangle-\sum_{nm}\left[\langle z_n|\hat{H}|z_m\rangle a_n{}^*a_m-a_m{}^*a_n\langle z_m|\hat{H}|z_n\rangle\right]=$$

$$\begin{aligned}&=i\sum_{n,m}\langle z_n|z_m\rangle\left(\dot{a}_n{}^*a_m+a_n{}^*\dot{a}_m\right)+\\&i\sum_{n,m}\langle z_n|z_m\rangle\left(a_n{}^*a_m\right)\left(\dot{z}_n{}^*z_m+z_n{}^*\dot{z}_m-\left(\frac{\dot{z}_n{}^*z_n}{2}+\frac{z_n{}^*\dot{z}_n}{2}\right)-\left(\frac{\dot{z}_m{}^*z_m}{2}+\frac{z_m{}^*\dot{z}_m}{2}\right)\right)-\\&-\sum_{nm}\left[\langle z_n|z_m\rangle H\left(z_n{}^*,z_m\right)a_n{}^*a_m-a_m{}^*a_n\langle z_m|z_n\rangle H\left(z_m{}^*,z_n\right)\right]\end{aligned}$$

$$\begin{aligned}&=i\sum_{n,m}\langle z_n|z_m\rangle\frac{d}{dt}\left(e^{iS_m}\rho_{mn}e^{-iS_n}\right)+\\&+\ i\sum_{n,m}\langle z_n|z_m\rangle e^{iS_m}\rho_{mn}e^{-iS_n}\left(\dot{z}_n{}^*z_m+z_n{}^*\dot{z}_m-\left(\frac{\dot{z}_n{}^*z_n}{2}+\frac{z_n{}^*\dot{z}_n}{2}\right)-\left(\frac{\dot{z}_m{}^*z_m}{2}+\frac{z_m{}^*\dot{z}_m}{2}\right)\right)-\\&-\sum_{nm}\left[\langle z_n|\hat{H}|z_m\rangle e^{iS_m}\rho_{mn}e^{-iS_n}-e^{-iS_m}\rho_{nm}e^{iS_n}\langle z_m|\hat{H}|z_n\rangle\right]\end{aligned}$$

(11.20)

Eq.(11.20) relies on the fact that previously in (11.14) we have written density matrix as

$$\begin{aligned}\hat{\rho}&=\sum_{m,n}|\zeta_m\rangle\rho_{mn}\langle\zeta_n|=\sum_{m,n}|z_m\rangle e^{iS_m}\rho_{mn}e^{-iS_n}\langle z_n|=\sum_{m,n}|z_m\rangle B_{mn}\langle z_n|=\\&=\sum_{m,n}|z_m\rangle a_m a_n{}^*\langle z_n|=\sum_{m,n}|z_m\rangle e^{iS_m}d_m d_n{}^*e^{-iS_n}\langle z_n|\end{aligned}\qquad(11.21)$$

and therefore

$$\rho_{mn}=a_m a_n{}^*\qquad(11.22)$$

Now let us do the variation of L_{asymm} but before doing it let us do some algebra on the Lagrangian and try to simplify it.

$$L_{asymm}=i\sum_{n,m}\langle z_n|z_m\rangle\frac{d}{dt}\left(\rho_{mn}e^{i(S_m-S_n)}\right)+$$
$$i\sum_{n,m}\langle z_n|z_m\rangle\rho_{mn}e^{i(S_m-S_n)}\left(\dot z_n{}^*z_m+z_n{}^*\dot z_m-\left(\frac{\dot z_n{}^*z_n}{2}+\frac{z_n{}^*\dot z_n}{2}\right)-\left(\frac{\dot z_m{}^*z_m}{2}+\frac{z_m{}^*\dot z_m}{2}\right)\right)-$$
$$-\sum_{nm}\left[\langle z_n|z_m\rangle H(z_n{}^*,z_m)\rho_{mn}e^{i(S_m-S_n)}-\rho_{nm}e^{i(S_n-S_m)}\langle z_m|z_n\rangle H(z_m{}^*,z_n)\right]=$$

$$=i\sum_{n,m}\langle z_n|z_m\rangle\dot\rho_{mn}e^{i(S_m-S_n)}+$$
$$+i\sum_{n,m}\langle z_n|z_m\rangle\rho_{mn}e^{i(S_m-S_n)}\left(i\left(\frac{i}{2}\left(\dot z_m z_m{}^*-\dot z_m{}^*z_m\right)-H(z_m{}^*,z_m)\right)-i\left(\frac{i}{2}\left(\dot z_n z_n{}^*-\dot z_n{}^*z_n\right)-H(z_n{}^*,z_n)\right)\right)+$$
$$i\sum_{n,m}\langle z_n|z_m\rangle\rho_{mn}e^{i(S_m-S_n)}\left(\dot z_n{}^*z_m+z_n{}^*\dot z_m-\left(\frac{\dot z_n{}^*z_n}{2}+\frac{z_n{}^*\dot z_n}{2}\right)-\left(\frac{\dot z_m{}^*z_m}{2}+\frac{z_m{}^*\dot z_m}{2}\right)\right)-$$
$$-\sum_{nm}\left[\langle z_n|z_m\rangle H(z_n{}^*,z_m)\rho_{mn}e^{i(S_m-S_n)}-\rho_{nm}e^{i(S_n-S_m)}\langle z_m|z_n\rangle H(z_m{}^*,z_n)\right]=$$

$$=i\sum_{n,m}\langle z_n|z_m\rangle\dot\rho_{mn}e^{i(S_m-S_n)}+$$
$$+i\sum_{n,m}\langle z_n|z_m\rangle\rho_{mn}e^{i(S_m-S_n)}\left(-\frac{1}{2}\left(\dot z_m z_m{}^*-\dot z_m{}^*z_m\right)+\frac{1}{2}\left(\dot z_n z_n{}^*-\dot z_n{}^*z_n\right)\right)+$$
$$+i\sum_{n,m}\langle z_n|z_m\rangle\rho_{mn}e^{i(S_m-S_n)}\left(\dot z_n{}^*z_m+z_n{}^*\dot z_m-\left(\frac{\dot z_n{}^*z_n}{2}+\frac{z_n{}^*\dot z_n}{2}\right)-\left(\frac{\dot z_m{}^*z_m}{2}+\frac{z_m{}^*\dot z_m}{2}\right)\right)-$$
$$-\sum_{nm}\begin{bmatrix}\langle z_n|z_m\rangle H(z_n{}^*,z_m)\rho_{mn}e^{i(S_m-S_n)}-\langle z_n|z_m\rangle H(z_m{}^*,z_m)\rho_{mn}e^{i(S_m-S_n)}+\\+\langle z_n|z_m\rangle H(z_n{}^*,z_n)\rho_{mn}e^{i(S_m-S_n)}-\rho_{nm}e^{i(S_n-S_m)}\langle z_m|z_n\rangle H(z_m{}^*,z_n)+\end{bmatrix}=$$

$$=i\sum_{n,m}\langle z_n|z_m\rangle\dot\rho_{mn}e^{i(S_m-S_n)}+$$
$$+i\sum_{n,m}\langle z_n|z_m\rangle\rho_{mn}e^{i(S_m-S_n)}\left(\dot z_n{}^*z_m+z_n{}^*\dot z_m-z_m{}^*\dot z_m-\dot z_n{}^*z_n\right)-$$
$$-\sum_{nm}\left[\langle z_n|z_m\rangle H(z_n{}^*,z_m)\rho_{mn}e^{i(S_m-S_n)}-\langle z_n|z_m\rangle H(z_m{}^*,z_m)\rho_{mn}e^{i(S_m-S_n)}\right]$$
$$-\sum_{nm}\left[\langle z_n|z_m\rangle H(z_n{}^*,z_n)\rho_{mn}e^{i(S_m-S_n)}-\rho_{nm}e^{i(S_n-S_m)}\langle z_m|z_n\rangle H(z_m{}^*,z_n)+\right]=$$

$$
\begin{aligned}
&= i\sum_{n,m}\langle z_n | z_m\rangle \dot{\rho}_{mn} e^{i(S_m - S_n)} + \\
&+ i\sum_{n,m}\langle z_n | z_m\rangle \rho_{mn} e^{i(S_m - S_n)}\left(\dot{z}_n * (z_m - z_n) + (z_n * - z_m *)\dot{z}_m\right) - \\
&- \sum_{nm}\left[\langle z_n | z_m\rangle H\left(z_n *, z_m\right)\rho_{mn} e^{i(S_m - S_n)} - \langle z_n | z_m\rangle H\left(z_m *, z_m\right)\rho_{mn} e^{i(S_m - S_n)}\right] \\
&- \sum_{nm}\left[\langle z_n | z_m\rangle H\left(z_n *, z_n\right)\rho_{mn} e^{i(S_m - S_n)} - \langle z_n | z_m\rangle H\left(z_n *, z_m\right)\rho_{mn} e^{i(S_m - S_n)}\right] =
\end{aligned}
$$

We have used (11.16) to cancel out a bunch of sums which contain $\left(\frac{z_m}{2}\right)$ and get rid of them. Finally, we get an expression for the Lagrangian. Several equivalent expressions to be precise.

$$
\begin{array}{|l|}
\hline
L_{symm} = i\sum_{n,m}\langle z_n|z_m\rangle \dot{\rho}_{mn} e^{i(S_m-S_n)} + \\
-\sum_{nm}\langle z_n|z_m\rangle\left[H(z_n^*,z_m)-H(z_m^*,z_m)-i((z_n^*-z_m^*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)} \\
+\sum_{nm}\langle z_m|z_n\rangle\left[H(z_m^*,z_n)-H(z_m^*,z_m)+i(\dot{z}_m^*(z_n-z_m))\right]\rho_{nm}e^{i(S_n-S_m)} \\
\\
=\frac{i}{2}\sum_{n,m}\langle z_n|z_m\rangle \dot{\rho}_{mn} e^{i(S_m-S_n)} + \frac{i}{2}\sum_{n,m}\langle z_m|z_n\rangle \dot{\rho}_{nm} e^{i(S_n-S_m)} + \\
-\sum_{nm}\langle z_n|z_m\rangle\left[H(z_n^*,z_m)-H(z_m^*,z_m)-i((z_n^*-z_m^*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)} \\
+\sum_{nm}\langle z_m|z_n\rangle\left[H(z_m^*,z_n)-H(z_m^*,z_m)+i(\dot{z}_m^*(z_n-z_m))\right]\rho_{nm}e^{i(S_n-S_m)} \\
\\
=\frac{i}{2}\sum_{n,m}\langle z_n|z_m\rangle \dot{\rho}_{mn} e^{i(S_m-S_n)} + \frac{i}{2}\sum_{n,m}\langle z_m|z_n\rangle \dot{\rho}_{nm} e^{i(S_n-S_m)} + \\
-\sum_{nm}\langle z_n|z_m\rangle\left[H(z_n^*,z_m)-H(z_m^*,z_m)-i((z_n^*-z_m^*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)} \\
+\sum_{nm}\langle z_n|z_m\rangle\left[H(z_n^*,z_m)-H(z_n^*,z_n)+i(\dot{z}_n^*(z_m-z_n))\right]\rho_{mn}e^{i(S_m-S_n)} \\
\\
= i\sum_{n,m}\langle z_n|z_m\rangle \dot{\rho}_{mn} e^{i(S_m-S_n)} + \\
-\sum_{nm}\langle z_n|z_m\rangle\left[H(z_n^*,z_m)-H(z_m^*,z_m)-i((z_n^*-z_m^*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)} \\
+\sum_{nm}\langle z_n|z_m\rangle\left[H(z_n^*,z_m)-H(z_n^*,z_n)+i(\dot{z}_n^*(z_m-z_n))\right]\rho_{mn}e^{i(S_m-S_n)} \\
\hline
\end{array}
\tag{11.23}
$$

All these expressions are equivalent. But which of them is the most convenient?

Let us try some and do variation with respect to z in a way similar to how this variation has been done for the symmetric Lagrangian L_{symm} above in the eq(5.1). We get

$$
\begin{aligned}
L = &\frac{i}{2}\sum_{n,m}\langle z_n|z_m\rangle \dot{\rho}_{mn} e^{i(S_m-S_n)} + \frac{i}{2}\sum_{n,m}\langle z_m|z_n\rangle \dot{\rho}_{nm} e^{i(S_n-S_m)} + \\
&-\sum_{nm}\langle z_n|z_m\rangle\left[H(z_n^*,z_m)-H(z_m^*,z_m)-i((z_n^*-z_m^*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)} \\
&+\sum_{nm}\langle z_m|z_n\rangle\left[H(z_m^*,z_n)-H(z_m^*,z_m)+i(\dot{z}_m^*(z_n-z_m))\right]\rho_{nm}e^{i(S_n-S_m)}
\end{aligned}
\tag{11.24}
$$

$$\frac{\partial L}{\partial z_m*}-\frac{d}{dt}\frac{\partial L}{\partial \dot{z}_m*}=\frac{i}{2}\sum_n\langle z_n|z_m\rangle\left(-\frac{z_m}{2}\right)\dot{\rho}_{mn}e^{i(S_m-S_n)}+\frac{i}{2}\sum_n\langle z_m|z_n\rangle\left(z_n-\frac{z_m}{2}\right)\dot{\rho}_{nm}e^{i(S_n-S_m)}+$$

$$-\sum_n\langle z_n|z_m\rangle\left(-\frac{z_m}{2}\right)\left[H(z_n*,z_m)-H(z_m*,z_m)-i((z_n*-z_m*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)}$$

$$-\sum_n\langle z_n|z_m\rangle\left[-\frac{\partial}{\partial z_m*}H(z_m*,z_m)+i\dot{z}_m\ \ ((z_n*-z_m*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)}$$

$$+\sum_n\langle z_m|z_n\rangle\left(z_n-\frac{z_m}{2}\right)\left[H(z_m*,z_n)-H(z_m*,z_m)+i(\dot{z}_m*(z_n-z_m))\right]\rho_{nm}e^{i(S_n-S_m)}$$

$$+\sum_n\langle z_m|z_n\rangle\left[\frac{\partial}{\partial z_m*}H(z_m*,z_n)-\frac{\partial}{\partial z_m*}H(z_m*,z_m)-i(\dot{z}_n-\dot{z}_m)\right]\rho_{nm}e^{i(S_n-S_m)}=$$

$$=\frac{i}{2}\sum_n\langle z_m|z_n\rangle(z_n-z_m)\dot{\rho}_{nm}e^{i(S_n-S_m)}-\frac{i}{2}\sum_n\langle z_n|z_m\rangle\left(\frac{z_m}{2}\right)\dot{\rho}_{mn}e^{i(S_m-S_n)}+\frac{i}{2}\sum_n\langle z_m|z_n\rangle\left(\frac{z_m}{2}\right)_{nm}\dot{\rho}_{nm}e^{i(S_n-S_m)}$$

$$-\sum_n\langle z_n|z_m\rangle\left(-\frac{z_m}{2}\right)\left[H(z_n*,z_m)-H(z_m*,z_m)-i((z_n*-z_m*)\dot{z}_m)\right]\rho_{mn}e^{i(S_m-S_n)}$$

$$+\sum_n\langle z_m|z_n\rangle\left(\frac{z_m}{2}\right)\left[H(z_m*,z_n)-H(z_m*,z_m)+i(\dot{z}_m*(z_n-z_m))\right]\rho_{nm}e^{i(S_n-S_m)}$$

$$+\sum_n\langle z_m|z_n\rangle(z_n-z_m)\left[H(z_m*,z_n)-H(z_m*,z_m)+i(\dot{z}_m*(z_n-z_m))\right]\rho_{nm}e^{i(S_n-S_m)}$$

$$-\sum_n\langle z_n|z_m\rangle\left[-\frac{\partial}{\partial z_m*}H(z_m*,z_m)+i\dot{z}_m\ \ \right]\rho_{mn}e^{i(S_m-S_n)}+$$

$$+\sum_n\langle z_m|z_n\rangle\left[\frac{\partial}{\partial z_m*}H(z_m*,z_n)-\frac{\partial}{\partial z_m*}H(z_m*,z_m)-i(\dot{z}_n-\dot{z}_m)\right]\rho_{nm}e^{i(S_n-S_m)}=$$

$$=\frac{i}{2}\sum_n\langle z_m|z_n\rangle(z_n-z_m)\dot{\rho}_{nm}e^{i(S_n-S_m)}+$$

$$+\sum_n\langle z_m|z_n\rangle(z_n-z_m)\left[H(z_m*,z_n)-H(z_m*,z_m)+i(\dot{z}_m*(z_n-z_m))\right]\rho_{nm}e^{i(S_n-S_m)}$$

$$-\sum_n\langle z_n|z_m\rangle\left[-\frac{\partial}{\partial z_m*}H(z_m*,z_m)+i\dot{z}_m\ \ \right]\rho_{mn}e^{i(S_m-S_n)}+$$

$$+\sum_n\langle z_m|z_n\rangle\left[\frac{\partial}{\partial z_m*}H(z_m*,z_n)-\frac{\partial}{\partial z_m*}H(z_m*,z_m)-i(\dot{z}_n-\dot{z}_m)\right]\rho_{nm}e^{i(S_n-S_m)}=0$$

(11.25)

Finally:

$$\boxed{\begin{aligned}&\sum_n\left[-\frac{\partial}{\partial z_m{}^*}H\left(z_m{}^*,z_m\right)+i\dot{z}_m\right]\left[\left\langle z_m|z_n\right\rangle\rho_{nm}e^{i\left(S_n-S_m\right)}-\left\langle z_n|z_m\right\rangle\rho_{mn}e^{i\left(S_m-S_n\right)}\right]+\\&+\frac{i}{2}\sum_n\left\langle z_m|z_n\right\rangle\left(z_n-z_m\right)\dot{\rho}_{nm}e^{i\left(S_n-S_m\right)}+\\&+\sum_n\left\langle z_m|z_n\right\rangle\left(z_n-z_m\right)\left[H\left(z_m{}^*,z_n\right)-H\left(z_m{}^*,z_m\right)+i\dot{z}_m{}^*\left(z_n-z_m\right)\right]\rho_{nm}e^{i\left(S_n-S_m\right)}=\\&=0\end{aligned}}$$

(11.26)

The first line is classical but the rest represents all kind of quantum effects.

CHECK ALL THIS !!! Also check whether other forms give the same set of equations. They should.

THIS IS ALL BASED ON THE DENCITY MATRIX THIS IS WHAT WE WANT BECAUE DENSITY MATRIX IS A BETTER BEHAVING AND MORE GENERIC OBJECT THAN WAVE FUNCTION..!

VARIATION WITH RESPECT TO Z GIVES THE TRAJECTORIES EXPRESSED THROUGH DENCITY MATRIX AND THE EQUATIONS FOR THE DENCITY MATRIX ELEMENTS ALONG THE TRAJECTORY ARE KNOWN ABOVE!!!

With density matrix it can be more stable numerically and also it can be used for operators other than density matrix.

MORE DELIRIUM

SEE (3.4)

$$L=\left\langle \Psi \right| i\frac{\hat{\partial}}{\partial t}-\hat{H}\left| \Psi \right\rangle =\left\langle \Psi \right| \frac{i}{2}\left(\frac{\vec{\partial}}{\partial t}-\frac{\overleftarrow{\partial}}{\partial t}\right)-\hat{H}\left| \Psi \right\rangle =\sum_{i,j}\ \{\ \frac{i}{2}\left[a_i*\dot{a}_j-a_{\ j}\dot{a}_i*\right]\left\langle z_i \middle| z_j\right\rangle +$$

$$\frac{i}{2}\left[\left(\left(z_i*-z*_j\right)\dot{z}_j+\frac{\dot{z}_j\, z*_j}{2}-\frac{z_j\, \dot{z}_j*}{2}\right)-\left(\left(z_j-z_i\right)\dot{z*}_i+\frac{z_i\, \dot{z*}_i}{2}-\frac{\dot{z}_i\, z*_i}{2}\right)\right]$$

$$a_i*a_j\left\langle z_i \middle| z_j\right\rangle -a_i*a_j\left\langle z_i \middle| z_j\right\rangle H_{ord}\left(z*_i,z_j\right)\ \}=$$

$$\sum_{i,j}\ \{\ \frac{i}{2}\left[d_i*\dot{d}_j\, e^{iS_j-iS_i}-d_{\ j}\dot{d}_i*e^{iS_j-iS_i}\right]\left\langle z_i \middle| z_j\right\rangle$$

$$+\frac{i}{2}\left[a_i*a_j\left(i\left(i\left(\frac{\dot{z}_j\, z*_j}{2}-\frac{z_j\, \dot{z}_j*}{2}\right)-H\left(z_j*,z_j\right)+i\left(\frac{\dot{z}_i\, z*_i}{2}-\frac{z_i\, \dot{z}_i*}{2}\right)-H\left(z_i*,z_i\right)\right)\right)\right]\left\langle z_i \middle| z_j\right\rangle +$$

$$\frac{i}{2}\left[\left(\left(z_i*-z*_j\right)\dot{z}_j+\left(\frac{\dot{z}_j\, z*_j}{2}-\frac{z_j\, \dot{z}_j*}{2}\right)\right)-\left(\left(z_j-z_i\right)\dot{z*}_i-\left(\frac{\dot{z}_i\, z*_i}{2}-\frac{z_i\, \dot{z*}_i}{2}\right)\right)\right]$$

$$a_i*a_j\left\langle z_i \middle| z_j\right\rangle -a_i*a_j\left\langle z_i \middle| z_j\right\rangle H_{ord}\left(z*_i,z_j\right)\ \}=$$

$$=$$

$$\sum_{i,j}\ \{\ \frac{i}{2}\left[d_i * \dot{d}_j\, e^{iS_j - iS_i} - d_{\ j}\dot{d}_i * e^{iS_j - iS_i}\right]\langle z_i | z_j\rangle$$

$$\frac{i}{2}\left[\left(\left(z_i * - z*_j\right)\dot{z}_j\right) - \left(\left(z_j - z_i\right)\dot{z*}_i\right) + i\left(-H\left(z_j *, z_j\right) - H\left(z_i *, z_i\right)\right)\right] a_i * a_j \langle z_i | z_j\rangle$$

$$-a_i * a_j \langle z_i | z_j\rangle H_{ord}\left(z*_i, z_j\right)\ \} =$$

$$\sum_{i,j}\ \ \frac{i}{2}\left[d_i * \dot{d}_j\, e^{iS_j - iS_i} - d_{\ j}\dot{d}_i * e^{iS_j - iS_i}\right]\langle z_i | z_j\rangle +$$

$$+\sum_{i,j}\ \left[\frac{i}{2}\left(z_i * - z*_j\right)\dot{z}_j\left(\ \right) - \frac{i}{2} iH\left(z_j *, z_j\right) - \frac{1}{2} H_{ord}\left(z*_i, z_j\right)\right] a_i * a_j \langle z_i | z_j\rangle +$$

$$+\sum_{i,j}\ \left[-\frac{i}{2}\left(\left(z_j - z_i\right)\dot{z*}_i\right) - i\frac{i}{2}\left(H\left(z_i *, z_i\right)\right) - \frac{1}{2} H_{ord}\left(z*_i, z_j\right)\right] a_i * a_j \langle z_i | z_j\rangle =$$

$$=$$

$$\sum_{i,j}\ \ \frac{i}{2}\left[d_i * \dot{d}_j\, e^{iS_j - iS_i} - d_{\ j}\dot{d}_i * e^{iS_j - iS_i}\right]\langle z_i | z_j\rangle +$$

$$+\frac{1}{2}\sum_{i,j}\ \left[i\left(z_i * - z*_j\right)\dot{z}_j + H\left(z_j *, z_j\right) - H_{ord}\left(z*_i, z_j\right)\right] a_i * a_j \langle z_i | z_j\rangle +$$

$$+\frac{1}{2}\sum_{i,j}\ \left[-i\left(z_j - z_i\right)\dot{z*}_i + H\left(z_i *, z_i\right) - H_{ord}\left(z*_i, z_j\right)\right] a_i * a_j \langle z_i | z_j\rangle$$

From (7.2) we know that:

$$\sum_{j \neq i}\left[\langle z_i | z_j\rangle \dot{d}_{\ j} \exp\left(iS_j\right) + i\langle z_i | z_j\rangle \delta^2 H'_{ij} d_{\ j} \exp\left(iS_j\right)\right] = 0$$

where $\delta^2 H'_{ij} = \left[H_{ord}\left(z*_i, z_j\right) - H_{ord}\left(z*_j, z_j\right) - i\left(z*_i - z*_j\right)\dot{z}_j\right]$

CAN WE USE IT ? NOW I AM TAKING A BREACK WITH VARIATIONAL PRINCIPLE AND GO TO WIGNER AGAIN.