Towards an improvement of the Hermitian Approximation

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1 The Exact Schrödinger-like Equation for Conditional Wave-Functions

Given a closed quantum system with N degrees of freedom described by the spatial variables $\vec{x} = (x_1, ..., x_N) \in \mathbb{R}^n$, the sate of which is given by the normalized full N dimensional wavefunction $\Psi(\vec{x}, t)$, its dynamics are governed by the time dependent Schrödinger Equation (TDSE):

$$i\hbar \frac{\partial \Psi(\vec{x}, t)}{\partial t} = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \frac{\partial^2 \Psi(\vec{x}, t)}{\partial x_k^2} + U(\vec{x}, t)\Psi(\vec{x}, t) \tag{TDSE}$$

where $U(\vec{x}, t)$ is the time dependant potential energy field that bends the wavefunction, $\{m_k\}_{k=0}^N$ are the masses of each degree of freedom, $\hbar$ is the experimentally fixed Planck constant and $i = \sqrt{-1}$. The unitary time evolution of the TDSE will allow $\forall t$: $\int_{-\infty}^{\infty} \Psi(\vec{x}, t)^\dagger \Psi(\vec{x}, t) d\vec{x} = 1$.

Given an initial point $\vec{x}(t_0) \in \mathbb{R}^N$, we can evolve a trajectory for the quantum system by interpreting the spatial variation of the phase of the full wavefunction as its velocity field (following Bohmian Mechanics). That is, defining the velocity field for the k-th dimension as:

$$v_k(\vec{x}, t) = \frac{\hbar}{m_k} \frac{\partial Phase(\Psi(\vec{x}, t))}{\partial x_k} = \frac{\hbar}{m_k} \mathbb{I}m\left(\Psi^{-1}(\vec{x}, t) \frac{\partial}{\partial x_k} \Psi(\vec{x}, t) \right)$$

Then, given the point $\vec{x}(t_0) \in \mathbb{R}^N$, the trajectory $\vec{x}(t)$ crossing it at t_0 will be uniquely defined by:

$$\frac{\mathrm{d}}{\mathrm{d}t} x_k^\beta(t) = v_k(\vec{x}(t), t) \quad \forall k \in \{1, ..., N\}$$

Given a particular Bohmian Trajectory for the system, that we will label with β, $\vec{x}^\beta(t)$, we will define for each $x_a \in \{x_k\}_{k=1}^N$ the degrees of freedom of the rest of the system as $\vec{x_b} = (x_1, ..., x_{a-1}, x_{a+1}, ..., x_N)$. Now, let us define the Conditional Wavefunction (CWF) for x_a, given the β-th Bohmian trajectory for the rest of degrees of freedom $\vec{x}_b^\beta(t)$, as:

$$\psi_a^\beta(x_a, t) := \Psi(x_a, \vec{x}_b^\beta(t), t) \tag{CWF}$$

In what follows we will show three different ways to exactly arrive to a set of Schrödinger like equations for the conditional wave-functions. We will call them in general "the exact Schrödinger like Equation for Conditional Wave-Functions" and shorten them by (CWF.SE).

1.1 Shape I: The Kinetic and Advective Correlation Potentials

Now, given the Bohmian Trajectory for the system labelled by β, $\vec{x}^\beta(t)$, for each $x_a \in \{x_k\}_{k=1}^N$ we can condition the full wavefunction in the TDSE to the trajectory for $\vec{x_b} = (x_1, ..., x_{a-1}, x_{a+1}, ..., x_N)$:

$$i\hbar \frac{\partial \Psi(\vec{x}, t)}{\partial t}\Big|_{\vec{x}_b = \vec{x}(t)_b^\beta} = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \frac{\partial^2 \Psi(\vec{x}, t)}{\partial x_k^2}\Big|_{\vec{x}_b = \vec{x}_b^\beta(t)} + U(\vec{x}, t)\Big|_{\vec{x}_b = \vec{x}(t)_b^\beta} \Psi(\vec{x}, t)\Big|_{\vec{x}_b = \vec{x}(t)_b^\beta}$$

Noting that by the chain rule:

$$\frac{\mathrm{d}\Psi(x_a, \vec{x}_b^\beta(t), t)}{\mathrm{d}t} = \frac{\partial \Psi(\vec{x}, t)}{\partial t}\Big|_{\vec{x}_b = \vec{x}(t)_b^\beta} + \sum_{\substack{k=1; \\ k \neq a}}^{N} \frac{\partial \Psi(\vec{x}, t)}{\partial x_k}\Big|_{\vec{x}_b = \vec{x}(t)_b^\beta} \dot{x}_k^\beta(t)$$

We get:

$$\begin{aligned} i\hbar \frac{\mathrm{d}\Psi(x_a, \vec{x}_b^\beta(t), t)}{\mathrm{d}t} &= -\frac{\hbar^2}{2m_a} \frac{\partial^2 \Psi(x_a, \vec{x}_b^\beta(t), t)}{\partial x_a^2} + U(x_a, \vec{x}_b^\beta(t), t)\Psi(x_a, \vec{x}_b^\beta(t), t) \\ &- \sum_{\substack{k=1; \\ k \neq a}}^{N} \frac{\hbar^2}{2m_k} \frac{\partial^2 \Psi(\vec{x}, t)}{\partial x_k^2}\Big|_{\vec{x}_b = \vec{x}_b^\beta(t)} + i\hbar \sum_{\substack{k=1; \\ k \neq a}}^{N} \frac{\partial \Psi(\vec{x}, t)}{\partial x_k}\Big|_{\vec{x}_b = \vec{x}(t)_b^\beta} \dot{x}_k^\beta(t) \end{aligned}$$

Where we see that all the terms introducing an explicit dependence from the rest of the system ($\vec{x}_b$) on x_a are gathered in the last two terms, let us define them as the Kinetic Correlation Potential (K) and the Advective Correlation Potential (A):

$$K(x_a, \vec{x}_b^{\,\beta}(t), t) = -\sum_{\substack{k=1;\\ k\neq a}}^{N} \frac{\hbar^2}{2m_k} \frac{\partial^2 \Psi(\vec{x}, t)}{\partial x_k^2}\Big|_{\vec{x}_b=\vec{x}_b^{\,\beta}(t)} \tag{K}$$

$$A(x_a, \vec{x}_b^{\,\beta}(t), t) = i\hbar \sum_{\substack{k=1;\\ k\neq a}}^{N} \frac{\partial \Psi(\vec{x}, t)}{\partial x_k}\Big|_{\vec{x}_b=\vec{x}(t)_b^{\,\beta}} \dot{x}_k^{\beta}(t) \tag{A}$$

They are both complex valued potentials that introduce the correlations (exchange and entanglement) with the rest of the degrees of freedom in the equation (even if $U(x_a, \vec{x}_b^{\,\beta}(t), t)$ also introduces some of them).

In its terms, the full TDSE can be rewritten as:

$$i\hbar \frac{\partial \psi_a^{\beta}(x_a, t)}{\partial t} = \left[-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2} + U(x_a, \vec{x}_b^{\,\beta}(t), t)\right]\psi_a^{\beta}(x_a t) + K(x_a, \vec{x}_b^{\,\beta}(t), t) + A(x_a, \vec{x}_b^{\,\beta}(t), t) \tag{CWF.SE.I}$$

We will call this the exact conditional wave-function Schrödinger like Equation (CWF.SE.I). If we could solve this for each $x_a \in \{x_k\}_{k=1}^N$ given the potential energy U, an initial shape for the full wavefunction $\Psi(\vec{x}, t_0)$ and an initial position of the trajectory $\vec{x}^{\beta}(t_0)$, then we would be evolving the exact shape of the CWF-s if we evolve the trajectory $\vec{x}^{\beta}(t)$ in a coupled fashion. Note that the ordinary differential equations ruling the trajectory can be solved even if we only knew the CWF-s! This is because each a-th velocity field is obtianed by a derivative of the same spatial variable. As such, they only depend on the CWF-s:

$$\frac{\mathrm{d}}{\mathrm{d}t}x_a^{\beta}(t) = v_a(x_a^{\beta}(t), \vec{x}_b^{\,\beta}(t), t) = \frac{\hbar}{m_k}\mathbb{I}m\left(\psi_a^{\beta}(x_a, t)^{-1}\frac{\partial}{\partial x_k}\psi_a^{\beta}(x_a, t), t\right) \quad \forall a \in \{1, ..., N\}$$

1.2 Shape II: Introducing the Born-Huang ansatz onto the K,A potentials

As the potential energy $U(\vec{x}, t)$ is a known function, for each $x_a \in \{x_k\}_{k=1}^N$ we can define the Transversal Section Eigenstates TSEig as the set of functions $\{\Phi_{x_a}^j(\vec{x}_b, t)\}_{j=0}^{\infty}$ such that:

$$\left(-\sum_{k=1;k\neq a}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2}{\partial x_k^2} + U(x_a, \vec{x}_b, t)\right)\Phi_{x_a}^j(\vec{x}_b, t) = E_{x_a}^j(t)\Phi_{x_a}^j(\vec{x}_b, t) \tag{TSEig}$$

for $j \in \{0, 1, 2, 3, ...\}$. We order the indices j such that the eigenvalues known as energies of the transversal sections fulfill: $E_{x_a}^0(t) \leq E_{x_a}^1(t) \leq E_{x_a}^2(t)$....

Note that each $\Phi_{x_a}^j(\vec{x}_b, t)$ is a different eigenstate as a function of a (the variable left aside), of where in the domain of x_a we look at and the time in which we look at ($U(x_a, \vec{x}_b, t)$ will vary in x_a and t). Thus, we compute these eigenstates for each a, x_a and t.

As the TSEig are the eigenstates of a Hermitian Operator, they can be chosen to satisfy the orthonormality condition on each transversal section Hilbert space. That is:

$$\int_{-\infty}^{\infty}\Phi_{x_a}^k(\vec{x}_b, t)^{\dagger}\Phi_{x_a}^j(\vec{x}_b, t)d\vec{x}_b = \delta_{kj} \equiv \begin{cases} 1 \; if \; k = j \\ 0 \; if \; k \neq j \end{cases} \qquad \forall t \geq t_0$$

If the potential U is known, then in principle there are plenty of numerical algorithms capable of getting these eigenstates.

Now, for each $x_a \in \{x_k\}_{k=1}^N$ as the set of TSEig $\{\Phi_{x_a}^j(\vec{x}_b,t)\}_{j=0}^\infty$ are the eigenstaes of a Hermitian operator, they will be a complete basis for the transversal section Hilbert spaces, meaning we can expand the full wavefunction in their terms as:

$$\Psi(\vec{x},t) = \sum_{j=0}^{\infty} \chi_a^j(x_a,t)\Phi_{x_a}^j(\vec{x}_b,t) \tag{BH}$$

where:

$$\chi_a^j(x_a,t) := \int_{-\infty}^{\infty} \Phi_{x_a}^j(\vec{x}_b,t)^\dagger \Psi(\vec{x},t) d\vec{x}_b \tag{chi}$$

This is the so called Born-Huang expansion (BH) of the full wave-function, while the coefficients of the expansion $\{\chi_a^j(x_a,t)\}_{j=0}^\infty$ are called the Adiabatic Coefficients (chi).

In particular, if we condition the (BH) ansatz to the trajectory $\vec{x}_b^\beta(t)$, we can get an expansion of the CWF:

$$\psi_a^\beta(x_a,t) = \Psi(x_a,\vec{x}_b^\beta(t),t) = \sum_{j=0}^{\infty} \chi_a^j(x_a,t)\Phi_{x_a}^j(\vec{x}_b^\beta(t),t)$$

We could now re-write the Kinetic and Advective Correlation potentials (K, A) in terms of this ansatz:

$$K(x_a,\vec{x}_b^\beta(t),t) = -\sum_{\substack{k=1;\\ k\neq a}}^{N}\sum_{j=0}^{\infty} \chi_a^j(x_a,t)\frac{\hbar^2}{2m_k}\frac{\partial^2\Phi_{x_a}^j(\vec{x}_b^\beta(t),t)}{\partial x_k^2}\Big|_{\vec{x}_b=\vec{x}_b^\beta(t)} \tag{K.BH}$$

$$A(x_a,\vec{x}_b^\beta(t),t) = i\hbar\sum_{\substack{k=1;\\ k\neq a}}^{N}\sum_{j=0}^{\infty} \chi_a^j(x_a,t)\frac{\partial\Phi_{x_a}^j(\vec{x}_b^\beta(t),t))}{\partial x_k}\Big|_{\vec{x}_b=\vec{x}(t)_b^\beta}\dot{x}_k^\beta(t) \tag{A.BH}$$

where we note that unlike the full wave function $\Psi(x_a,\vec{x}_b,t)$, the TSEig $\Phi_{x_a}^j(\vec{x}_b,t))$ are known, which means their numerical or analytic derivatives will also be known. Thus, we have effectively isolated the unknown out of any derivative in the shape of the chi $\chi_a^j(x_a,t)$. The point is that these coefficients still depend on the full wave-function, so we will still be unable to obtain simple expressions for the CWF-s. Still, the exact Schrödinger like Equation for the CWF-s (CWF.SE.I) can be rewritten in an alternative shape in terms of this Born-Huang ansatz by using (A.BH) and (K.BH):

$$i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t} = \left[-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2} + U(x_a,\vec{x}_b^\beta(t),t)\right]\psi_a^\beta(x_at) + K_{BH}(x_a,\vec{x}_b^\beta(t),t) + A_{BH}(x_a,\vec{x}_b^\beta(t),t) \tag{CWF.SE.II}$$

where by K_{BH} and A_{BH} we mean K and A but in their Born-Huang ansatz dependence shape given in (K.BH) and (A.BH).

The fact that the TSEig are an orthonormal set makes the norm of the expanded wavefunction to be equal to:

$$\sum_{j=0}^{\infty}\int_{-\infty}^{\infty}\chi_a^j(x_a,t)^\dagger\chi_a^j(x_a,t)dx_a = \int_{-\infty}^{\infty}\Psi(\vec{x},t)^\dagger\Psi(\vec{x},t)d\vec{x}$$

the proof is immediate. Thus, the quantity defined by $\lambda := \sum_{j=0}^\infty\int_{-\infty}^\infty\left|\chi_a^j(x_a,t)\right|^2 dx_a$ can be used as an indicator as which j is big enough as for having captured the biggest part of the sum. That is, if we truncate the sum at $j=J$ such that $\lambda \simeq 1$, then the approximation to the full expansion will be good enough. We call each integral $P_j(t) := \int_{-\infty}^\infty\left|\chi_a^j(x_a,t)\right|^2 dx_a$ the Population of the $j-th$ adiabatic level.

1.3 Shape III: Rewriting K and A in terms of the CWF - The Real Potentials G and J

Following the development in Chp.1 V 6 of [1]: In order to find a linear Schrödinger like equation for the CWF-s we are going to employ the following "trick". An arbitrary non-zero single valued complex function $f(x,t) : \mathbb{R}^2 \to \mathbb{C}$ can be imposed to be the solution of a 1D Schrödinger equation:

$$i\hbar\frac{\partial f(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 f(x,t)}{\partial x^2} + W(x,t)f(x,t)$$

if the potential term $W(x,t)$ is defined as:

$$W(x,t) := \left(i\hbar\frac{\partial f(x,t)}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2 f(x,t)}{\partial x^2}\right)\frac{1}{f(x,t)}$$

The proof is immediate. An observation that we must note is that for an arbitrary $f(x,t)$, the potential $W(x,t)$ can be complex as well! Which is not the case in the usual Schrödinger Equation. But we already assumed that K and A could be so.

Then, using this for the CWF-s $\psi_a^\beta(x_a,t)$, we will obtain an alternative to CWF.SE.I.

We must first evaluate the CWF in polar form $\psi_a^\beta(x_a,t) = r(x_a,t)e^{is(x_a,t)/\hbar}$ in the expression for $W(x_a,t)$:

$$W(x_a,t) = \left(i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t} + \frac{\hbar^2}{2m_a}\frac{\partial^2\psi_a^\beta(x_a,t)}{\partial x_a^2}\right)\frac{1}{\psi_a^\beta(x_a,t)} = \left(i\hbar\frac{\partial\left(re^{is/\hbar}\right)}{\partial t} + \frac{\hbar^2}{2m_a}\frac{\partial^2\left(re^{is/\hbar}\right)}{\partial x_a^2}\right)\frac{1}{re^{is/\hbar}}$$

using the Leibniz derivation rule several times and an inverse chain rule, rearranging we arrive at:

$$W(x_a,t) = -\frac{1}{2m_a}\left(\left(\frac{\partial s_a}{\partial x_a}\right)^2 - \frac{\hbar^2}{r_a}\frac{\partial^2 r_a}{\partial x_a^2}\right) - \frac{\partial s_a}{\partial t} + i\,\frac{\hbar}{r_a^2}\left(\frac{\partial r_a^2}{\partial t} + \frac{\partial}{\partial x_a}\left(\frac{r_a^2}{m_a}\frac{\partial s_a}{\partial x_a}\right)\right)$$

If W has that shape, $\psi_a^\beta(x_a,t)$ will be the solution of the differential equation:

$$i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_a^\beta(x_a,t)}{\partial x_a^2} + W(x_a,t)\psi_a^\beta(x_a,t)$$

which if $Im\{W\} = 0$ would look like an actual single particle SE. However, W depends on parts of the CWF itself, so the differential equation is indeed non-linear.

We can further develop the expression of W using the conditional definition of ψ_a^β. Note that $\psi_a^\beta(x_a,t) = \Psi(x_a,t;\ \vec{x}_b^\beta(t))$ and thus $s(x_a,t) = S(x_a,\vec{x}_b^\beta(t),t)$ and $r(x_a,t) = R(x_a,\vec{x}_a^\beta(t),t)$, where we have that the full wavefunction in polar form is $\Psi(\vec{x},t) = R(\vec{x},t)e^{iS(\vec{x},t)/\hbar}$. Carefully evaluating them in W and applying the chain rule, the real part of $W(x_a,t) = \mathbb{W}(x_a,t;\ \vec{x}_b^\beta(t))$ yields:

$$\mathbb{R}e\{W(x_a,t)\} = \mathbb{R}e\{\mathbb{W}(x_a,t;\vec{x}_b^\beta(t))\} =$$

$$-\frac{1}{2m_a}\left(\frac{\partial S(x_a,t;\vec{x}_b^\beta(t))}{\partial x_a}\right)^2 + \frac{\hbar^2}{2m_a R(x_a,t;\ \vec{x}_b^\beta(t))}\frac{\partial^2 R(x_a,t;\ \vec{x}_b^\beta(t))}{\partial x_a^2} - \frac{\mathrm{d}S(x_a,t,\vec{x}_b^\beta(t))}{\mathrm{d}t} =$$

$$-\frac{1}{2m_a}\left(\frac{\partial s_a(x_a,t)}{\partial x_a}\right)^2 + \frac{\hbar^2}{2m_a r_a(x_a,t)}\frac{\partial^2 r_a(x_a,t)}{\partial x_a^2} - \left(\frac{\partial S(x_a,t,\vec{x}_b)}{\partial t}\Big|_{\vec{x}_b^\beta(t)} + \sum_{k=1;\ k\neq a}^{n}\frac{\partial S(x_a,t,\vec{x}_b)}{\partial x_k}\Big|_{x_k^\beta(t)}\frac{\mathrm{d}x_k^\beta(t)}{\mathrm{d}t}\right)$$

Note how the only terms introducing some coupling with the rest of particles are the last two. They are the source of the **entanglement**, **exchange** and **correlations** with the rest of the dimensions. Now, knowing that the full wave-function follows the TDSE and thus the Quantum Hamilton-Jacobi Equation, we can evaluate the expression for $\frac{\partial S(x_a,t,\vec{x}_b)}{\partial x_k}$ in the equation above:

$$\mathbb{R}e\{W(x_a,t)\} = \; Re\{\mathbb{W}(x_a,t;\vec{x}_b^{\,\beta}(t))\} =$$

$$-\frac{1}{2m_a}\left(\frac{\partial s_a(x_a,t)}{\partial x_a}\right)^2 + \frac{\hbar^2}{2m_a r_a(x_a,t)}\frac{\partial^2 r_a(x_a,t)}{\partial x_a^2} - \sum_{k=1;\ k\neq a}^{n}\left(\frac{\partial S(x_a,t,\vec{x}_b)}{\partial x_k}\Big|_{x_k^\beta(t)}\frac{\mathrm{d}x_k^\beta(t)}{\mathrm{d}t}\right) +$$

$$+\sum_{k=1}^{n}\left[\frac{1}{2m_k}\left(\frac{\partial S}{\partial x_k}\Big|_{\vec{x}_b^{\,\beta}(t)}\right)^2 - \frac{\hbar^2}{2m_k R}\frac{\partial^2 R}{\partial x_k^2}\Big|_{\vec{x}_b^{\,\beta}(t)}\right] - U(x_a,t;\vec{x}_b^{\,\beta}(t))$$

Observe that in the last sum, the $k=a$ term is equal to the two initial terms, which cancel each other out and we are left with the final expression:

$$\mathbb{R}e\{\mathbb{W}(x_a,t;\vec{x}_b^{\,\beta}(t))\} = \sum_{k=1;\ k\neq a}^{n}\left[\frac{1}{2m_k}\left(\frac{\partial S}{\partial x_k}\Big|_{\vec{x}_b^{\,\beta}(t)}\right)^2 - \frac{\hbar^2}{2m_k R}\frac{\partial^2 R}{\partial x_k^2}\Big|_{\vec{x}_b^{\,\beta}(t)} - \frac{\partial S}{\partial x_k}\Big|_{x_k^\beta(t)}\frac{\mathrm{d}x_k^\beta(t)}{\mathrm{d}t}\right] + V(x_a,t;\vec{x}_b^{\,\beta}(t))$$

We now have defined $\mathbb{R}e(W)$ without using ψ_a^β in the same definition (necessary if we want to use the Schrödinger like equation computationally), at the cost of introducing the full wave-function to it. We see that this real part of W is composed by the classical conditional potential energy U introducing geometric constrictions between the coordinates and an additional part that stands for the quantum correlation with the rest of the system. We will call this the potential G_a:

$$G_a(x_a,t;\ \vec{x}_b^{\,\beta}(t)) := \sum_{k=1;\ k\neq a}^{n}\left[\frac{1}{2m_k}\left(\frac{\partial S}{\partial x_k}\Big|_{\vec{x}_b^{\,\beta}(t)}\right)^2 - \frac{\hbar^2}{2m_k R}\frac{\partial^2 R}{\partial x_k^2}\Big|_{\vec{x}_b^{\,\beta}(t)} - \frac{\partial S}{\partial x_k}\Big|_{x_k^\beta(t)}\frac{\mathrm{d}x_k^\beta(t)}{\mathrm{d}t}\right] \tag{G}$$

Performing the same development for the imaginary part of W, that is, evaluating the definition of CWF in $\mathbb{I}m\{W(x_a,t)\}$ and applying the chain rule:

$$Im\{W(x_a,t)\} = Im\{\mathbb{W}(x_a,t;\vec{x}_b^{\,\beta}(t))\} =$$

$$\frac{\hbar}{2R^2}\Big|_{\vec{x}_b^{\,\beta}(t)}\left(\frac{\partial R(x_a,t;\vec{x}_b^{\,\beta}(t))^2}{\partial t} + \frac{\partial}{\partial x_a}\left(\frac{R^2}{m_a}\frac{\partial S(x_a,t;\vec{x}_b^{\,\beta}(t))}{\partial x_a}\right)\right) =$$

$$\frac{\hbar}{2R^2}\Big|_{\vec{x}_b^{\,\beta}(t)}\left(\frac{\partial R(x_a,t,\vec{x}_b)^2}{\partial t}\Big|_{\vec{x}_b^{\,\beta}(t)} + \sum_{k=1;\ k\neq a}^{n}\frac{\partial R^2}{\partial x_k}\Big|_{\vec{x}_b^{\,\beta}(t)}\frac{\mathrm{d}x_k^\beta(t)}{\mathrm{d}t} + \frac{\partial}{\partial x_a}\left(\frac{R^2}{m_a}\frac{\partial S(x_a,t;\vec{x}_b^{\,\beta}(t))}{\partial x_a}\right)\right)$$

As the whole wave-function follows the TDSE, we have an expression for the N-particle continuity equation, which evaluating at $\frac{\partial R(x_a,t,\vec{x}_b)^2}{\partial t}$ and noting there is a cancellation of the $k=a$ term (as happened with the real case), we arrive at an expression independent of ψ_a^β for the imaginary part. We will define the potential energy term $J_a(x_a,t;\vec{x}_b^{\,\beta}(t)) := \mathbb{I}m\{\mathbb{W}(x_a,t;\vec{x}_b^{\,\beta}(t))\}$.

$$J_a(x_a,t;\vec{x}_b^{\,\beta}(t)) := \frac{\hbar}{2R^2}\Big|_{\vec{x}_b^{\,\beta}(t)}\sum_{k=1;\ k\neq a}^{n}\left[\frac{\partial R^2}{\partial x_k}\Big|_{\vec{x}_b^{\,\beta}(t)}\frac{\mathrm{d}x_k^\beta(t)}{\mathrm{d}t} - \frac{1}{m_k}\frac{\partial}{\partial x_k}\left(R^2\frac{\partial S}{\partial x_k}\right)\Big|_{\vec{x}_b^{\,\beta}(t)}\right] \tag{J}$$

With all, we have that the complex potential is decomposed in the following potential terms:

$$W(x_a,t) = \mathbb{W}(x_a,t;\vec{x}_b^{\,\beta}(t)) = U(x_a,t;\vec{x}_b^{\,\beta}(t)) + G_a(x_a,t;\vec{x}_b^{\,\beta}(t)) + i\ J_a(x_a,t;\vec{x}_b^{\,\beta}(t))$$

In a nutshell, we have decomposed the N dimensional TDSE into an exact system of N coupled Schrödinger-like Equations for the CWF-s. For each $a \in \{1..n\}$:

$$i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t} = \left[\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2} + U(x_a,t;\vec{x}_b^{\,\beta}(t)) + G_a(x_a,t;\vec{x}_b^{\,\beta}(t)) + i\ J_a(x_a,t;\vec{x}_b^{\,\beta}(t))\right]\psi_a^\beta(x_a,t) \tag{CWF.SE.III}$$

$$\frac{\mathrm{d}x_a(t)}{\mathrm{d}t} = v_a(x_a,t) = \frac{1}{m_a}\frac{\partial s_a(x_a,t)}{\partial x_a}$$

2 The Approximation 1.0

Until here everything was theoretically correct, no approximations were assumed at any point. However, we have seen that the exact Schrödinger like equations for the CWF-s (in their three shapes) are not useful to surpass the many-body problem because in all three cases, there were terms that depended on the full wavefunction $\Psi(\vec{x},t)$ instead of only the CWF-s for a given trajectory β:

- In the case of CWF.SE.I, K and A depended on derivatives of Ψ on $\vec{x}_b$.
- In the case of CWF.SE.II the computation of the χ_a^j coefficients depended on an overlap integral between Ψ and the transversal section eigenstates.
- In the case of CWF.SE.III both G and J depended on derivatives of the magnitude and phase of Ψ on $\vec{x}_b$.

Therefore, it seems clear that if we want to introduce approximations at the theoretical level that can help us educatedly surpass the many body problem, it is the shape of $\Psi(\vec{x},t)$ used to compute K and A, the χ_a^j or G and J, that should be educatedly guessed.

In particular, if we look back to the (CWF.SE.I) and .II we can notice that if we achieve to write $\Psi(\vec{x},t)$ as proportional to the CWF $\psi_a^\beta(x_a,t)$, then the differential equations would take a linear look, which would allow us to use very convenient numerical resolution techniques like the Crank Nicholson method.

The simplest approximation we will use is to assume the full wave-function has the shape of a normalized factorizable product of functions that depend on a single spatial variable:

$$\Psi(\vec{x},t) \simeq \frac{f_1(x_1,t)\cdots f_N(x_N,t)}{\sqrt{n_1(t)\cdots n_N(t)}}$$

with $n_k(t) := \int_\infty^\infty f_k(x_k,t)^\dagger f_k(x_k,t)dx_k$. If we apply the definition of CWF:

$$\Psi(x_a,\vec{x}_b^\beta(t),t) = \psi_a^\beta(x_a,t) \simeq \frac{f_1(x_1^\beta(t),t)\cdots f_{a-1}(x_{a-1}^\beta(t),t)f_a(x_a,t)f_{a+1}(x_{a+1}^\beta(t),t)f_N(x_N^\beta(t),t)}{\sqrt{n_1(t)\cdots n_N(t)}}$$

$$\implies f_a(x_a,t) = \frac{\psi_a^\beta(x_a,t)\sqrt{n_1(t)\cdots n_N(t)}}{\prod_{\substack{k=1;\\ k\neq a}}^N f_k(x_k^\beta(t))}$$

Evaluating it for every $a \in \{1,...,N\}$, we can see that the approximation is actually the same as:

$$\Psi(\vec{x},t) \simeq \frac{\left(\sqrt{n_1(t)\cdots n_N(t)}\right)^N \prod_{a=1}^N \psi_a^\beta(x_a,t)}{\sqrt{n_1(t)\cdots n_N(t)}\left(\prod_{k=1}^N f_k(x_k^\beta(t))\right)^{N-1}} = \prod_{a=1}^N \psi_a^\beta(x_a,t)\cdot\left(\frac{\sqrt{n_1(t)\cdots n_N(t)}}{f_1(x_1^\beta(t),t)\cdots f_N(x_N^\beta(t),t)}\right)^{N-1}$$

Where we can identify the one over the approximation evaluated in the trajectory and thus we get a simple expression for the approximation we are doing, in terms of the CWF-s:

$$\Psi(\vec{x},t) = \frac{\psi_1^\beta(x_1,t)\cdots\psi_N^\beta(x_N,t)}{(\Psi(\vec{x}^\beta(t),t))^{N-1}} \qquad \text{(CWF.Prod)}$$

Therefore, the approximation we are doing is to assume that the full wavefunction is roughly equal to the product of the CWF-s divided by the value of the full wave-funciton Ψ evaluated in each time in the position of the trajectory in the configuration space (a complex time varying dividing factor). One could argue that the value of the full wavefunction on the trajectory is unknown unless we know the whole wavefunction. However, we actually have N different approximations for it, as in theory $\Psi(\vec{x}^\beta(t),t) = \psi_1^\beta(x_1^\beta(t),t) = \cdots = \psi_N^\beta(x_N^\beta(t),t)$, if we recall the definition (CWF). Therefore, we could use as its best approximation the average of the N estimations we have, one per approximate CWF.

2.1 Algorithm 1.0 - The Hermitian Approximation

2.1.1 Using CWF.SE.I: the Raw K and A

If we now introduce (CWF.Prod) in the expressions for (K) and (A), we will get an approximation for them, that we will call $W_K^{(a)}\psi_a^\beta(x_a,t)$ and $W_A^{(a)}\psi_a^\beta(x_a,t)$:

$$K(x_a,\vec{x}_b^\beta(t),t) \simeq -\left(\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2\psi_k^\beta(x_k,t)}{\partial x_k^2}\Big|_{x_k^\beta(t)}\cdot\frac{\prod_{\substack{s=1\\s\neq a,k}}^{N}\psi_s^\beta(x_s^\beta(t),t)}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}}\right)\psi_a^\beta(x_a,t) = W_K^{(a)}(\vec{x}_b^\beta(t),t)\psi_a^\beta(x_a,t)$$

$$A(x_a,\vec{x}_b^\beta(t),t) \simeq i\hbar\left(\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\partial\psi_k^\beta(x_k,t)}{\partial x_k}\Big|_{x_k^\beta(t)}\cdot\dot{x}_k^\beta(t)\cdot\frac{\prod_{\substack{s=1\\s\neq a,k}}^{N}\psi_s^\beta(x_s^\beta(t),t)}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}}\right)\psi_a^\beta(x_a,t) = W_A^{(a)}(\vec{x}_b^\beta(t),t)\psi_a^\beta(x_a,t)$$

Where we have defined (note that the product could be simplified using the approximation (CWF.Prod)):

$$W_K^{(a)}(\vec{x}_b^\beta(t),t) = -\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2\psi_k^\beta(x_k,t)}{\partial x_k^2}\Big|_{x_k^\beta(t)}\cdot\frac{\Psi(\vec{x}^\beta(t),t))}{\psi_a^\beta(x_a^\beta(t),t)\psi_k^\beta(x_k^\beta(t),t)}$$

$$W_A^{(a)}(\vec{x}_b^\beta(t),t) = i\hbar\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\partial\psi_k^\beta(x_k,t)}{\partial x_k}\Big|_{x_k^\beta(t)}\cdot\dot{x}_k^\beta(t)\cdot\frac{\Psi(\vec{x}^\beta(t),t))}{\psi_a^\beta(x_a^\beta(t),t)\psi_k^\beta(x_k^\beta(t),t)}$$

With them, the (CWF.SE.I) would be left with a linear differential equation shape, such that we could now evolve the following N coupled linear equations in order to obtain the set of CWF-s $\{\psi_a^\beta(x_at)\}_{a=1}^N$ and the trajectory $\vec{x}^\beta(t)$ given their initial conditions:

$$i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t} = \left[-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2} + U(x_a,\vec{x}_b^\beta(t),t) + W_K^{(a)}(\vec{x}_b^\beta(t),t) + W_A^{(a)}(\vec{x}_b^\beta(t),t)\right]\psi_a^\beta(x_at)$$

However, it turns out that the approximation (which may be correct if the full wave-function is really factorizable), leads to a shape for the complex correlation potentials that is purely time dependant. It is well known that this only introduces a time dependant global phase to the solution CWF-s relative to solving the same set of equations with $K\equiv 0$ and $A\equiv 0$. Thus, as the trajectories are evolved using the derivative of the phase, and as the probability distribution is given by the magnitude squared of the wavefunction, non of these quantities are changed by a global phase shift, meaning that the same solution can be obtained by only preserving the correlations introduced by the classical potential U. Leting $K\equiv 0\equiv A$. That is, using the so called **Hermitian Approximation** $\forall x_a\in\{x_k\}_{k=1}^N$:

$$i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t} = \left[-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2} + U(x_a,\vec{x}_b^\beta(t),t)\right]\psi_a^\beta(x_at) \tag{Herm}$$

2.1.2 Using CWF.SE.II: the Born-Huang K.BH and A.BH

If we introduce this approximate shape for $\Psi(\vec{x},t)$ onto the computation of the coefficients $\chi_a^j(x_a,t)$ for the Born-Huang expansion of the approximate shape of the full wave-function:

$$\chi_a^j(x_a,t) = \int_{-\infty}^{\infty}\Phi_{x_a}^j(\vec{x}_b,t)^\dagger\Psi(\vec{x},t)d\vec{x}_b \simeq \left[\frac{1}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}}\prod_{\substack{k=1;\\k\neq a}}^{N}\int_{-\infty}^{\infty}\Phi_{x_a}^j(\vec{x}_b,t)^\dagger\psi_k^\beta(x_k,t)dx_k\right]\psi_a^\beta(x_at)$$

Where if we define the factors:

$$\mathscr{U}_a^j(x_a,t) := \frac{1}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}} \prod_{\substack{k=1;\\ k\neq a}}^{N} \int_{-\infty}^{\infty} \Phi_{x_a}^j(\vec{x}_b,t)^\dagger \psi_k^\beta(x_k,t)dx_k \tag{Uj}$$

Then, we are left with the χ_a^j adiabatic coefficients of the expansion for the CWF.Prod:

$$\chi_a^j(x_a,t) = \mathscr{U}_a^j(x_a,t)\psi_a^\beta(x_a t)$$

One could see these χ_a^j coefficients as an approximation of the χ_a^j coefficients that the true full wavefunction $\Psi(\vec{x},t)$ would yield. However, even if this is indeed true, it would be an error to forget that they are actually the exact coefficients of the expansion for CWF.Prod! If in a second step, this CWF.Prod is then a good approximation for the exact full wavefunction or not, then that is another thing. This means that we should never forget that these χ_a^j mean:

$$\sum_{j=0}^{\infty} \chi_a^j(x_a,t)\Phi_{x_a}^j(\vec{x}_b,t) = \sum_{j=0}^{\infty} \Phi_{x_a}^j(\vec{x}_b,t) \left[\frac{1}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}} \prod_{\substack{k=1;\\ k\neq a}}^{N} \int_{-\infty}^{\infty} \Phi_{x_a}^j(\vec{x}_b,t)^\dagger \psi_k^\beta(x_k,t)dx_k \right] \psi_a^\beta(x_a t) =$$

$$= \sum_{j=0}^{\infty} \Phi_{x_a}^j(\vec{x}_b,t) \int_{-\infty}^{\infty} \Phi_{x_a}^j(\vec{x}_b,t)^\dagger \left[\frac{\psi_1^\beta(x_1,t)\cdots\psi_N^\beta(x_N,t)}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}} \right] d\vec{x} = \frac{\psi_1^\beta(x_1,t)\cdots\psi_N^\beta(x_N,t)}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}}$$

where we have used that we are adding up all the infinite projections of the factorized product on each orthonormal eigenstate times the same eigenstate. By definition of orthonormal basis, this must add up to the original function: the factorizable product (its the so called **completeness relation**).

This means that, if we introduce these χ_a^j into the computation of K.BH and A.BH for the CWF.SE.II, we get the following approximations for them:

$$K(x_a,\vec{x}_b^\beta(t),t) \simeq -\sum_{\substack{k=1;\\ k\neq a}}^{N} \sum_{j=0}^{\infty} \mathscr{U}_a^j(x_a,t)\psi_a^\beta(x_a t) \frac{\hbar^2}{2m_k} \frac{\partial^2 \Phi_{x_a}^j(\vec{x}_b,t)}{\partial x_k^2}\Big|_{\vec{x}_b=\vec{x}_b^\beta(t)} =: W_K^{(a)}(x_a,\vec{x}_b^\beta(t),t)\psi_a^\beta(x_a t)$$

$$A(x_a,\vec{x}_b^\beta(t),t) \simeq i\hbar \sum_{\substack{k=1;\\ k\neq a}}^{N} \sum_{j=0}^{\infty} \mathscr{U}_a^j(x_a,t)\psi_a^\beta(x_a t) \frac{\partial \Phi_{x_a}^j(\vec{x}_b,t))}{\partial x_k}\Big|_{\vec{x}_b=\vec{x}(t)_b^\beta} \dot{x}_k^\beta(t) =: W_K^{(a)}(x_a,\vec{x}_b^\beta(t),t)\psi_a^\beta(x_a t)$$

where we have defined the terms $W_K^{(a)}(x_a,\vec{x}_b^\beta(t),t)$ and $W_A^{(a)}(x_a,\vec{x}_b^\beta(t),t)$ by taking out the common factor CWF. We know the eigenstes and we know the terms $\mathscr{U}_a^j$ at each time, becasue we can evolve all the N CWF-s simultaneously. With this, CWF.SE.II adopts a linear look:

$$i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t} = \left[-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2} + U(x_a,\vec{x}_b^\beta(t),t) + W_K^{(a)}(x_a,\vec{x}_b^\beta(t),t) + W_A^{(a)}(x_a,\vec{x}_b^\beta(t),t) \right] \psi_a^\beta(x_a t)$$

Unlike in the previous case, it now looks like the approximation is giving us something additional to the Hermitian Approximation, because now $W_K^{(a)}$ and $W_A^{(a)}$ depend on x_a per each $j-th$ term in the sum. Therefore, it looks like we should be able to obtain some correlation and entanglement we could not observe with the bare Hermitian Approximation.

However, this is **not** true. If we really use the infinite j terms in the Born-Huang expansion, we have just seen above that we recover the approximation of the product of CWF-s. Thus, if in the

expressions for $W_K^{(a)}$ and $W_A^{(a)}$ we revert the operations, we will get to see that they are exactly the same as the $W_K^{(a)}$ and $W_A^{(a)}$ we got in the previous section, that were purely time dependant. For example:

$$W_K^{(a)}(x_a,\vec{x}_b^{\,\beta}(t),t)\psi_a^\beta(x_at) =$$

$$-\sum_{\substack{k=1;\\k\neq a}}^{N}\sum_{j=0}^{\infty}\mathscr{U}_a^j(x_a,t)\frac{\hbar^2}{2m_k}\frac{\partial^2\Phi_{x_a}^j(\vec{x}_b,t)}{\partial x_k^2}\Big|_{\vec{x}_b=\vec{x}_b^{\,\beta}(t)}\psi_a^\beta(x_at) = -\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2}{\partial x_k^2}\left[\sum_{j=0}^{\infty}\mathscr{U}_a^j(x_a,t)\psi_a^\beta(x_at)\Phi_{x_a}^j(\vec{x}_b,t)\right]\Big|_{\vec{x}_b=\vec{x}_b^{\,\beta}(t)}$$

$$= -\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2}{\partial x_k^2}\frac{\psi_1^\beta(x_1,t)\cdots\psi_N^\beta(x_N,t)}{\left(\Psi(\vec{x}^{\,\beta}(t),t)\right)^{N-1}}\Big|_{\vec{x}_b^{\,\beta}(t)} = -\left(\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2\psi_k^\beta(x_k,t)}{\partial x_k^2}\Big|_{x_k^\beta(t)}\frac{\prod_{\substack{s=1\\s\neq a,k}}^{N}\psi_s^\beta(x_s^\beta(t),t)}{\left(\Psi(\vec{x}^{\,\beta}(t),t)\right)^{N-1}}\right)\psi_a^\beta(x_a,t)$$

$$= W_K^{(a)}(\vec{x}_b^{\,\beta}(t),t)\psi_a^\beta(x_at)$$

Therefore, we end up in the same conclusion: purely time dependant complex potentials lead to the Hermitian approximation. So, it looked like we had gained new insight, but we have not. Or have we? Let us emphasize that the recovering of the Hermitian approximation is only true when we use all the necessary j to complete the expansion. However, if we truncate the expansion in a small enough j, then we will indeed have that $W_K^{(a)}$ and $W_A^{(a)}$ are dependant on x_a through the parametrization of the eigenstates $\Phi_{x_a}^j(\vec{x}_b^{\,\beta}(t),t)$)! Paradoxically, using a less precise expansion can lead to something that could capture some entanglement! This will be precisely the approximation we will work with after the next section.

2.1.3 Using CWF.SE.III: the Raw G and J

Looking at the equations CWF.SE.I and CWF.SE.III, we notice that the relation between the Kinetic and Advective Correlation potentials and the G,J real potentials is that:

$$G_a(x_a,\vec{x}_b^{\,\beta}(t),t) = \mathbb{R}e\left\{\frac{K(x_a,\vec{x}_b^{\,\beta}(t),t)+A(x_a,\vec{x}_b^{\,\beta}(t),t)}{\psi_a^\beta(x_at)}\right\} \tag{G(KA))}$$

$$J_a(x_a,\vec{x}_b^{\,\beta}(t),t) = \mathbb{I}m\left\{\frac{K(x_a,\vec{x}_b^{\,\beta}(t),t)+A(x_a,\vec{x}_b^{\,\beta}(t),t)}{\psi_a^\beta(x_at)}\right\} \tag{J(KA))}$$

We therefore see that if the CWF product approximation CWF.Prod made both K and A be a purely time dependant term times the CWF $\psi_a^\beta(x_a,t)$ (remember $K(x_a,\vec{x}_b^{\,\beta}(t),t)\simeq W_K^{(a)}(\vec{x}_b^{\,\beta}(t),t)\psi_a^\beta(x_a,t)$ and so for A), then this approximation will yield purely time dependent G_a and J_a, which in fact will be:

$$\begin{cases} G_a(x_a,\vec{x}_b^{\,\beta}(t),t)\simeq\mathbb{R}e\left\{W_K^{(a)}(\vec{x}_b^{\,\beta}(t),t)+W_A^{(a)}(\vec{x}_b^{\,\beta}(t),t)\right\}\\ J_a(x_a,\vec{x}_b^{\,\beta}(t),t)\simeq\mathbb{I}m\left\{W_K^{(a)}(\vec{x}_b^{\,\beta}(t),t)+W_A^{(a)}(\vec{x}_b^{\,\beta}(t),t)\right\}\end{cases}$$

The conclusion is once again the same, looking back to (CWF.SE.III), if G_a and J_a are purely time dependent, they will only introduce a global phase to the solution and thus we will obtain the same probability densities for the CWF-s and the same trajectories as simply using the Hermitian Approximation Herm.

This same result could have been obtained by making a Taylor expansion of G_a and J_a around the trajectory at each time and truncating them leaving only the zero-th order terms:

$$\begin{cases} G(x_a,\vec{x}_b^{\,\beta}(t),t) = G(x_a^\beta(t),\vec{x}_b^{\,\beta}(t),t)+\frac{\partial G(x_a,\vec{x}_b^{\,\beta}(t),t)}{\partial x_a}\Big|_{x_a^\beta(t)}\left(x_a-x_a^\beta(t)\right)+...\\ J(x_a,\vec{x}_b^{\,\beta}(t),t) = J(x_a^\beta(t),\vec{x}_b^{\,\beta}(t),t)+\frac{\partial J(x_a,\vec{x}_b^{\,\beta}(t),t)}{\partial x_a}\Big|_{x_a^\beta(t)}\left(x_a-x_a^\beta(t)\right)+...\end{cases}$$

3 The Approximation 2.0

3.1 Algorithm 2.0 - The Paradoxical Approximation

We have seen that if we use all the j terms (or at least enough of them) in the Born-Huang expansion of the (CWF.Prod) approximation, we recover the (CWF.Prod) approximation of the full wave-function, which leads to the Hermitian approximation and fails to capture entanglement between the dimensions. However, we also realized that interesting enough, even if all the terms added up $\sum_{j=0}^{\infty}\chi_a^j(x_a,t)\Phi_{x_a}^j(\vec{x}_b,t)$ result in the factorized product of CWF-s, each term in the Born-Huang expansion, each $\chi_a^j(x_a,t)\Phi_{x_a}^j(\vec{x}_b,t)$, in themselves are for a general potential not factorizable in separate spatial variables! Even if the $\chi_a^j(x_a,t)$ are computed with the (CWF.Prod) shape. And precisely it was the fact that we were imposing the shape of the full wavefunction $\Psi(\vec{x},t)$ to be factorizable that resulted in the approximate Advective and Kinetic Correlation Potentials to be purely time dependant. Therefore, if paradoxically, we use less adiabatic terms than those necessary to complete the expansion of (CWF.Prod), say J, then the effective approximation we will be using on the full-wavefunction will be non-factorizable:

$$\Psi(\vec{x},t)=\sum_{j=0}^{J}\chi_a^j(x_a,t)\Phi_{x_a}^j(\vec{x}_b,t) \tag{Aprox.Trunc}$$

Note that J must be small enough as to avoid the sum being a good enough approximation of the infinite sum. In order to quantify this, we could dynamically choose J to avoid the norm λ of the approximation defined in Section 1.2 to be bigger than a certain tolerance. This is because else the truncated sum will end up being a good enough approximation of the product of CWF-s and thus will loose its appeal.

The bad thing about this approximation is that one knows nothing about to which degree the approximation is closer to the true solution CWF than the Hermitian approximation. The idea is that if the Aprox.Trunc is close enough to the shape of the true full wavefunction, then it could work. Each particular potential will require to be reviewed in particular, in order to judge if this approximation for the regions where there is non-factorisability really makes sense or not. We will visit an example where it turns out to yield better results than the Hermitian approximation.

3.1.1 Using CWF.SE.II

The only difference between using (Aprox.Trunc) or (CWF.Prod) when it comes to the approximate expression for (CWF.SE.II) is that the sum over j will not go until $j=\infty$, but until $j=J$ fixed according to the criterium stated above. Thus, we would have the same definition for (Uj):

$$\mathscr{U}_a^j(x_a,t):=\frac{1}{\left(\Psi(\vec{x}^\beta(t),t)\right)^{N-1}}\prod_{\substack{k=1;\\k\neq a}}^{N}\int_{-\infty}^{\infty}\Phi_{x_a}^j(\vec{x}_b,t)^\dagger\psi_k^\beta(x_k,t)dx_k$$

Such that $\chi_a^j(x_a,t)=\mathscr{U}_a^j(t)\psi_a^\beta(x_at)$ and thus:

$$K(x_a,\vec{x}_b^\beta(t),t)\simeq-\sum_{\substack{k=1;\\k\neq a}}^{N}\sum_{j=0}^{J}\mathscr{U}_a^j(x_a,t)\frac{\hbar^2}{2m_k}\frac{\partial^2\Phi_{x_a}^j(\vec{x}_b,t)}{\partial x_k^2}\Big|_{\vec{x}_b=\vec{x}_b^\beta(t)}\psi_a^\beta(x_at)=:W_K^{(a)}(x_a,\vec{x}_b^\beta(t),t)\psi_a^\beta(x_at)$$

$$A(x_a,\vec{x}_b^\beta(t),t)\simeq i\hbar\sum_{\substack{k=1;\\k\neq a}}^{N}\sum_{j=0}^{J}\mathscr{U}_a^j(x_a,t)\frac{\partial\Phi_{x_a}^j(\vec{x}_b,t))}{\partial x_k}\Big|_{\vec{x}_b=\vec{x}(t)_b^\beta}\dot{x}_k^\beta(t)\psi_a^\beta(x_at)=:W_K^{(a)}(x_a,\vec{x}_b^\beta(t),t)\psi_a^\beta(x_at)$$

where we see the only difference with respecto to the approximations we made for K and A in the previous algorithm, is that now the sum in j stops at J. With this, CWF.SE.II adopts a linear look that will now **not** be equivalent to the Hermitian approximation, as W_K and W_A will now be x_a dependent:

$$i\hbar\frac{\partial\psi_a^\beta(x_a,t)}{\partial t}=\left[-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2}+U(x_a,\vec{x}_b^\beta(t),t)+W_K^{(a)}(x_a,\vec{x}_b^\beta(t),t)+W_A^{(a)}(x_a,\vec{x}_b^\beta(t),t)\right]\psi_a^\beta(x_at)$$

Again, this will work as long as J is small enough. However, we do not have still any theoretically reliable proof that the approximations we are using for W_K and W_A are better than simply not using them. If they deviate a lot from the true shape they should have, then we might be making a bigger error than simply neglecting them!

3.1.2 Using CWF.SE.III

When it comes to the G and J formalism, recalling the relation these real potentials had with the kinetic and advective correlation potentials that we manifested in equations (G(KA)) and (J(KA)), we can immediately see the approximations we are doing for them:

$$G_a(x_a,\vec{x}_b^\beta(t),t)\simeq\mathbb{R}e\left\{-\sum_{j=0}^{J}\mathscr{U}_a^j(x_a,t)\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2\Phi_{x_a}^j(\vec{x}_b,t)}{\partial x_k^2}\Big|_{\vec{x}_b=\vec{x}_b^\beta(t)}+i\hbar\frac{\partial\Phi_{x_a}^j(\vec{x}_b,t))}{\partial x_k}\Big|_{\vec{x}_b=\vec{x}(t)_b^\beta}\dot{x}_k^\beta(t)\right\}$$

$$J_a(x_a,\vec{x}_b^\beta(t),t)\simeq\mathbb{I}m\left\{-\sum_{j=0}^{J}\mathscr{U}_a^j(x_a,t)\sum_{\substack{k=1;\\k\neq a}}^{N}\frac{\hbar^2}{2m_k}\frac{\partial^2\Phi_{x_a}^j(\vec{x}_b,t)}{\partial x_k^2}\Big|_{\vec{x}_b=\vec{x}_b^\beta(t)}+i\hbar\frac{\partial\Phi_{x_a}^j(\vec{x}_b,t))}{\partial x_k}\Big|_{\vec{x}_b=\vec{x}(t)_b^\beta}\dot{x}_k^\beta(t)\right\}$$

Perhaps one could study the goodness of the approximation by looking at how close these expressions are to what we would expect from first or second order terms in the Taylor expansions around the trajectory that we introduced at the end of Section 2.1.3.

3.1.3 Example where the approach works: The Single Slit Transmission

The algorithm was implemented in a simple yet interesting 2D system (we will call them $x\equiv x_1$ and $y\equiv x_2$) where the Hermitian approximation fails dramatically to capture the physics: the transmission of a wave-packet through a bottleneck with infinite potential energy walls. This situation could model a sudden narrowing of the electron channel of a 2D electronic device. We will identify the direction x with the *transport direction* of the electron and the direction y with the *transversal direction*.

Given a zero potential energy in the space taking in the direction y a length $L(x)$ as a function of the position in x and an infinite potential elsewhere:

$$U(x,y,t)=\begin{cases}0\\-\infty & y\notin(-L(x)/2,L(x)/2)\end{cases}$$

it is trivial to obtain the TSEig set in y for this set-up, because on the one hand, the potential is stationary (the eigenstaes will be time independent). On the other hand, each transversal section is nothing else but the "1d particle in an infinite potential box", confined in a box of length $L(x)$. As the infinite potential means there must not be probability density in those regions, it will be a boundary

condition that the wave-function is zero at the edges of the box, which yields sinusoidal transversal eigenstates:

$$\Phi_x^j(y) = \begin{cases} \sqrt{\frac{2}{L(x)}} sin\left(\frac{j\pi(y+L(x)/2)}{L(x)}\right) & if\ y \in (-L(x)/2, L(x)/2) \\ 0 \quad else \end{cases}$$

with eigenenergies $E^j(x) = \frac{j^2\pi^2\hbar^2}{2m_y L(x)^2}$ for $j \in \{0, 1, 2, 3.., J\}$.

We could make a similar treatment for the other direction, x, however, for simplicity in this first example we will consider that in x the particle is "free", even if this is not true, and apply to the evolution of its complementary CWF $\psi_y^\beta(y,t)$ the Hermitian approximation. Only the CWF in x, that is $\psi_x^\beta(x,t)$, will be evolved using the approximation of Section 3.1.1.[1].

The fun point about this problem is that if both CWF-s are evolved with the Hermitian algorithm, then the CWF in the transport direction x will see no potential energy barrier anywhere while $y^\beta(t) \in (-L(x)/2, L(x)/2)$ because in that case $U(x; y^\beta(t)) = 0$ and the only possible correlation that the Hermitian approximation can capture is through the conditioned potential energy. Therefore, the CWF $\psi_x^\beta(x,t)$ will evolve as if it was in a free potential irrespective of the initial momentum and the width of the slit $L_{min} := min_x(L(x))$. However, this same setting was studied in a recent work by Devashish P. *et al* [3] using the full Schrödinger Equation TDSE and the Born-Huang expansion and found that a "virtual" potential energy barrier emerged from the quantum geometrical correlation between the spatial degrees of freedom. Such that if the initial kinetic energy of the wave-packet transported through the narrowing channel was smaller than the energy eigenstates of the transversal sections TSEig then the wavepacket was reflected (only slightly transmitted) as if there was a true potential energy barrier in the slit. Then the rest of eigenenergies of the transversal sections played additonal roles in the dynamics of this transmission. Therefore, it this simple setting seems a perfect benchmark to identify algorithms that perform better than the basic HErmitian approximation. In principle, any improvement approximating the 1 beyond the Hermitian approximation should prove to be capable of capturing this "virtual" energy barrier. As we will see soon, Algorithm 2.0 is precisely capable of doing this.

Applying these TSEig to the potentials $W_K^{(x)}$ and $W_K^{(x)}$, we get:

$$W_K^{(x)}(x, y^\beta(t), t) = -\sum_{j=0}^{J} \mathscr{U}_x^j(x,t) \frac{\hbar^2}{2m_y} \frac{\partial^2 \Phi_x^j(y,y)}{\partial y^2}\Big|_{y^\beta(t)} = -\sum_{j=0}^{J} \mathscr{U}_x^j(x,t) \frac{\hbar^2}{2m_y} \left(\frac{j\pi}{L(x)}\right)^2 \left(-\sqrt{\frac{2}{L}} sin\left(\frac{j\pi(y+L(x)/2)}{L(x)}\right)\right)$$

$$= \sum_{j=0}^{J} \mathscr{U}_x^j(x,t) \frac{\hbar^2}{2m_y} \left(\frac{j\pi}{L(x)}\right)^2 \Phi_x^j(y^\beta(t))$$

$$W_A^{(x)}(x, y^\beta(t), t) = \sum_{j=0}^{J} \mathscr{U}_x^j(x,t) i\hbar\dot{y}^\beta(t) \frac{\partial \Phi_x^j(y,y)}{\partial y}\Big|_{y^\beta(t)} = \sum_{j=0}^{J} \mathscr{U}_x^j(x,t) i\hbar\dot{y}^\beta(t) \frac{j\pi}{L(x)} \sqrt{\frac{2}{L(x)}} cos\left(\frac{j\pi(y^\beta(t)+L(x)/2}{L(x)}\right)$$

Where the effect of the second potential energy terms are not that clear, but the real part of the first clearly show the introduction of a potential energy in the transport direction that is directly proportional to the narrowness of the slit. Not only that, but it also seems like we could recover the adiabatic coefficient language used in Ref.[3], but now applied to the Bohmian interpretation.

[1]Remember that the kinetic and advective correlation potentials depend on the knowledge of the complementary direction, that is why, knowing the TSEig in y allows their approximation for the CWF in x.

4 Reconstructing the Full Wave-Function from CWF-s

Apart from the ontological interest that these algorithms could have, where only one Bohmian trajectory and its associated CWF-s are evolved at each run, the observed results in quantum mechanics still are randomly found among the ensemble of possible trajectories. As such, the ensemble measurements are the most interesting for orthodox quantum mentality and perhaps quantum information and computation, as we cannot get rid of the probabilistic nature of the observation. Therefore, it seems clear that if the many-body problem can be educatedly surpassed in the computation of individual Bohmian trajectories and CWF-s as defined in (CWF), we should try to take advantage from it to approach an approximate solution for the full wavefunction (which in reality contains information about all the possible trajectories and associated CWF-s). But how to do this?

Let us review what is the information we have, once an approximate solution to any of the shapes of the (CWF.SE) is found, and see if we can build something from there:

(a) Given a bounded time domain $t \in [t_0, t_f]$, we know $\Psi(\vec{x}, t = t_0)$, the full wave-function at the first time, and $U(\vec{x}, t)$ $\forall t[t_0, t_f]$, all of which were given a priori by the user or the problem we are facing.

(b) We can choose M initial positions in configuration space $\{\vec{x}^\beta(t_0)\}_{\beta=1}^M$ sampling them as independent observations from the initial wave-function, using its interpretation as probability density $\rho(\vec{x}, t_0) = \Psi(\vec{x}, t_0)^\dagger \Psi(\vec{x}, t_0)$. Using each of the M trajectories, we can define the set of N conditional wave-functions (CWF) related to each as:

$$\left\{ \left\{ \psi_a^\beta(x_a, t_0) \equiv \Psi(x_a, \vec{x}_b^\beta(t_0), t_0) \right\}_{a=1}^N \right\}_{\beta=1}^M$$

(c) If we are to use the Born-Huang ansatz, we will have calculated numerically or analytically the transversal section eigenstates $\left\{ \left\{ \Phi_a^j(\vec{x}_b, t) \right\}_{j=0}^{J_a} \right\}_{a=1}^N$, following equation (TSEig).

All (a), (b) and (c) will be as exact as finite precision arithmetics and numerical eigensolver allow us. In principle no theoretical approximations on them.

(d) Using an approximation to one of the shapes of (CWF.SE), we will have an approximation of the following functions:

- The M trajectories: $\{\vec{x}^\beta(t)\}_{\beta=1}^M \quad t \in [t_0, t_f]$
- The MN CWF-s: $\left\{ \left\{ \psi_a^\beta(x_a, t) \right\}_{a=1}^N \right\}_{\beta=1}^M \quad t \in [t_0, t_f]$
- In case the Born-Huang expansion was used, the adiabatic coefficients:

$$\left\{ \left\{ \{\chi_a^j(x_a, t)\}_{a=1}^N \right\}_{j=0}^{J_a} \right\}_{\beta=1}^M \quad t \in [t_0, t_f]$$

So the question at this point is: isn't there any way to unify all this information that each trajectory provides us? Should we really only use the resulting Bohmian trajectories as source of information, or can we use the information in the approximated CWF-s?

4.1 Using the CWF definition

In reality, each conditional wave-function is a slice of the full wavefunction, meaning that if we had enough CWF-s (if M was big enough and the trajectories were evenly enough sampled), we would

effectively be also approximating the full wave-function. Even if the CWF-s are approximations of the true CWF-s, the value predicted around the trajectory which in theory should be coincident between the CWF-s, that is:

$$\Psi(\vec{x}^{\beta}(t),t) = \psi_1^{\beta}(x_1^{\beta}(t),t) = \cdots = \psi_N^{\beta}(x_N^{\beta}(t),t)$$

may be expected to be one of the most accurate parts of the predicted CWF. This perhaps could be consequence of the fact that for instance the Hermitian approximation is compatible with a zeroth order Taylor expansion around the trajectory for G and J. If this assumption was true, then the set of CWF-s and their associated trajectories would provide us with a dynamical grid over which we are evolving the full wavefunction. The problem with this approach would be that the number of grid points in $\mathbb{R}^N$, over which we are evolving the full wave-function would be equal to the number of trajectories evolved M, which unfortunately would need to be geometrically bigger to obtain a good enough resolution with increasing dimensions, which would therefore be avoiding us to solve the many body problem anyway. It could be argued that at least this way, the many body problem that scales exponentially in time would be now translated into an exponential scaling only in space (memory), because the evolution of each trajectory is actually independent and thus may be done in parallel.

Anyhow, there are several options to directly use the information we have to obtain an approximation of the full wave-function at each point $\vec{x}$

4.1.1 Use only the trajectories and the values of the CWF-s on them

If we considered the trajectories $\{\vec{x}^{\beta}(t)\}_{\beta=1}^{M}$ and for each of them, the set of approximations $\{\psi^{\beta}(x_a^{\beta}(t),t)\}_{a=1}^{N}$ for $\Psi(\vec{x}^{\beta}(t),t)$, we could use as a net approximation for it, the average:

$$\Psi_{approx}(\vec{x}^{\beta}(t),t) = \frac{1}{N}\sum_{a=1}^{N}\psi_a^{\beta}(x_a^{\beta}(t),t)$$

where the CWF-s are approximations too. Thus, the value of the full wavefunction would have been predicted successfully for the moving points $\{\vec{x}^{\beta}(t)\}_{\beta=1}^{M}$. Then if we were interested to know the value of $\Psi(\vec{x},t)$ in any other $(\vec{x},t)$ pair, we could apply a simple k-Nearest Neighbourgh (KNN) algorithm:

1. Compute the distance in configuration space between the point of interest $(\vec{x},t)$ and all the points $\{(\vec{x}^{\beta}(t),t)\}_{\beta=1}^{M}$. Order them by distance.
2. Choose a k (say 7) and assign a value $\Psi(\vec{x},t)$ equal to the average value of Ψ over the k closest points in the known set, weighted by the inverse of the distance from the point of interest to them.

By an assumption of continuity, the algorithm should work fine with enough points M.

An alternative could be to make an interpolation of the points using a polynomial with a sufficient degree p:

$$f(\vec{x},\vec{w}) = w_0 + x_1 w_{11} + \cdots + x_N w_{1N} + \cdots + x_1^p w_{p1} + \cdots + x_N^p w_{pN}$$

where the complex weights w_{ij} would be fitted using a gradient descent with regularization or the normal equations with regularization (to avoid Runge-like phenomena).

Yet another alternative would be to build an $\mathbb{R}^N$ histogram to reflect the proportion of trajectories in each bin, which should reflect by definition the probability density $R^2(\vec{x},t)$, the modulous squared of the wavefunction. Then the phase $S(\vec{x},t)$ could be recovered by integrating the velocity fields that the trajectory velocities generate, following their Bohmian interpretation.

Still another alternative, conceptually close to the previous option would be to center gaussian functions in each trajectory and sum all the gaussians. Then if normalized, a pretty good approximation for the probability density R^2 could be obtained. The same could be done for the velocity fields.

For each of the N velocity fields $v_a(\vec{x},t)$, we have the values on the trajectories. Thus, we could also center gaussians on those speeds, add them all and integrate them to approximate the phase S.

All of these options relay on the assumption of continuity and none of them would require any heavy additional computation. In fact, even if these approximations might result in a poor approximation for the full wave-function, it could now be used to compute new approximations for the correaltion potentials K, A and G, J, which would pressumably yield a better approximation for the trajectories and the CWF-s.

So it is clear that one of the things we are approximating is actually the probability associated with each trajectory in each different time as $|\Psi(\vec{x}^\beta(t),t)|^2 := \Psi(\vec{x}^\beta(t),t)^\dagger\Psi(\vec{x}^\beta(t),t)$ or rather the normalized sum of gaussians or the histogram (note that probability is not conserved along the trajectories due to the shape of the continuity equation). Let us call this probability $\rho(\vec{x},t)$. If we had some time varying (or constant) quantity $E^\beta(t)$ associated with each trajectory, we could try to get its true value by doing an average weighted by the probability of the trajectory:

$$E(t) = \frac{\sum_{\beta=1}^{M}\rho(\vec{x}^\beta(t),t)E^\beta(t)}{\sum_{\beta=1}^{M}\rho(\vec{x}^\beta(t),t)}$$

As an example, if we compute the adiabatic coefficients $\chi_a^j(x_a,t)$ per trajectory, we can get an estimation of the marginalized probability density of each variable $\rho_a(x_a,t)$ doing $\sum_{j=0}^{J_a}|\chi_a^j(x_a,t)|^2$. We could unify all the marginalized densities predicted by each trajectory using the weighted sum of their probabilities:

$$\rho(x_a,t) = \frac{\sum_{\beta=1}^{M}\rho(\vec{x}^\beta(t),t)\rho_a^\beta(x_a,t)(t)}{\sum_{\beta=1}^{M}\rho(\vec{x}^\beta(t),t)}$$

4.1.2 Using the whole CWF-s and trajectories

In reality, the CWF-s for a single R^N trajectory are not only giving us the value of the full wavefunction over the trajectory, but also along the N orthogonal directions each spatial variable represents, centred in the trajectory. The N CWF-s are by definition the (only) slices of the "pilot-wave" that directly affect the actual piloted $\mathbb{R}^N$ particle(s). That is, as it is shown in Figure **??**, there are N 1D slices of the full wavefunction that we know per trajectory $\vec{x}^\beta(t)$. Mathematically, knowing the N CWF-s of the M trajectories is the same as knowing $\Psi(\vec{x},t)$ restricted at each time t to the set of NM lines parallel to the axes of $\mathbb{R}^N$:

$$\Gamma := \bigcup_{\beta=1}^{M}\left\{\vec{\gamma}_1^\beta(s;t) = \Big(s, x_2^\beta(t)..., x_N^\beta(t)\Big)\bigcup \ ... \ \bigcup\vec{\gamma}_N^\beta(s;t) = \Big(x_1^\beta(t),...,x_{N-1}^\beta(t),s\Big); \quad s\in\mathbb{R}\right\}$$

Therefore, we already know an approximation (as good as the approximation of the CWF-s is) of the set of points $\{\{\Psi(\vec{\gamma}_a^\beta(s;t),t)\}_{a=1}^N\}_{\beta=1}^M$ for $s\in\mathbb{R}$. Therefore, assuming the quality of the approximation does not get worse if we get away from the driven trajectory by the CWF-s, we can apply rather:

Option 1 : The k-Nearest Neighbour idea, just that now instead of only having M points in $\mathbb{R}^N$ with known Ψ value at each time, we know the value of Ψ at any point in the 1D affine manifolds $\Gamma = \{\{\vec{\gamma}_a^\beta(s;t)\}_{a=1}^N\}_{\beta=1}^M$ which are certainly way more points than M. Thus, in order to get the value of Ψ at any point $(\vec{x},t)$, one could take the k closest points among the 1D affine manifolds to it and compute the average Ψ weighted by the inverse of the distance.

Option 2 : Following the same idea, now that we have way more than M points with their respective values, we could make a regularized polynomial interpolation of degree p at each time to obtain an approximation of the wavefunciton at any point. Even if it seems like, this would not be that computationally costly thanks to the fact we could use the normal equations instead of a gradient descend.

The great appeal of these ideas is that they are very computationally cheap compared with the following ones.

4.2 Using the CWF definition+Using the CWF-s as basis functions

Additionaly, we could combine the ideas explained in the previous section with the ideas we will discuss in the following to approach a yet even more interesting idea than those in the last section and a computationaly cheaper one than those in the next section. When we said we could make a polynomial interpolation of degree p on the points over the manifold bundle Γ, we were implicitly trying to write the full wavefunction in atruncated basis of polynomial functions. Why not use the fact that possibly tensor products of the CWF-s will be closer to the full wave-function than polynomials? That is, if we define a linear combination of the tensor products:

$$\Psi(\vec{x},t) \simeq f(\vec{x},t;\vec{C}(t)) = \sum_{\beta=1}^{M} C_\beta(t)\psi_1^\beta(x_1,t)\cdots\psi_N^\beta(x_N,t)$$

Then we will be able to fit the complex coefficients $C_\beta(t)$ to the value that minimizes at each time the cost:

$$\mathfrak{L}(\vec{C}(t)) = \sum_{\vec{x}\in\Gamma} |f(\vec{x},t) - \Psi(\vec{x},t)|^2$$

where we know the approximate values of Ψ over Γ from the CWF definition. This minimization could be easily done using a gradient descent algorithm for example.

In fact, as we suggest in the next section, we could not only use the sum of the products o a same trajectory, but also the products of CWF-s of different trajectories in order to have more "basis" functions (even if they will most likely not be orthogonal).

The difference between this approach and the following one is that in this case we are relying on the fact that the approximations of the CWF-s are close enough to the true CWF-s (and thus to the full wave-function's sections). In the case of the next section, we will forget about what the CWF-s are by definition, and just use their product as basis functions hoping they might be closer to the full Ψ than a random set of functions (like we have also assumed here), however, the fitting will be given by the full TDSE instead of the already computed CWF-s. Of course, this will require a good deal more of computations.

4.3 Using the CWF-s as basis functions: Fit the best possible Full Wavefunction

In this section we will play with an idea introduced by *Albareda G. et al* in Ref [4].

Instead of directly using individual CWF-s, we could gather the information that all of them contain fitting them the best way possible to the exact N dimensional TDSE. We dispose per each of the N spatial dimension x_a, of M different conditional wave-functions $\psi_a^\beta(x_a,t)$ (due to the M trajectories). Thus, we could consider the linear combination of the tensor products of each trajectory's CWF set as an approximation to the full wavefunction. The obvious case would be to only use products of CWF-s evolved with the same trajectory β:

$$\Psi(\vec{x},t) \simeq \sum_{\beta=1}^{M} C_\beta(t)\psi_1^\beta(x_1,t)\cdots\psi_N^\beta(x_N,t) \quad for\ some\ C_\beta(t)\in\mathbb{C}\ to\ be\ fitted$$

after all, if these approximate CWF-s were computed using Algorithm 1.0 or 2.0, in both cases the approximation we were using was that the full wave-function was a product of the CWF-s. We would now be extending the capacity of the ansatz to take non-factorizable shapes, as in principle, if we used

enough $\mathbb{R}^N \times \mathbb{R} :\to \mathbb{C}$ linearly independent functions, we could end up approximating any function, even if the basis functions were a simple tensor product. The thing is that, we expect that these M terms will be close enough to the full wavefuncton as to provide a better fit than a random set of M functions of a given basis. Then the question would be, how do we choose the coefficients $C_\beta(t)$?

Before going there, notice that with only doing this sum we might be wasting resources that we already have in hands: the more functions we use in the expansion, the better it will be, and yes, computing more trajectories (increasing M) could do it, but notice that we need not. We could actually use not only the combination $\psi_1^\beta(x_1,t)\cdots\psi_N^\beta(x_N,t)$ but also any $\psi_1^{\beta_1}(x_1,t)\cdots\psi_N^{\beta_N}(x_N,t)$ with any combination $\beta_1,...,\beta_N \in \{1,...,M\}$ (mix CWF-s of different trajectories -CWF of dimension 1 of trajectory 3 times CWF of dimension 2 of trajectory 4 etc.-). Letting:

$$\Psi(\vec{x},t) \simeq \sum_{s=1}^{M^N} C_s(t)\psi_1^{\sigma_s^{(1)}}(x_1,t)\cdots\psi_N^{\sigma_s^{(N)}}(x_N,t) \tag{CWF.LinComb}$$

where the set $\{\sigma_s^{(1)},...,\sigma_s^{(N)}\}_{s=1}^{M^N}$ is the set of all possible combinations of N elements that take values in $(1,2,...,M)$. It is true that these tensor products (among which there are also all the previous ones) might now not be that close to the full wave-function individually, but perhaps the extra effort to find more coefficients $C_s(t)$ is worth it. Still, this should be tested. After all, the fun thing about doing this is that thanks to the fact that the tensor products are close to the true TDSE evolution a smaller M can be used providing a better quality than say, a set of M eigenstates of the system Hamiltonian. Thus, if these M^N combinations introduce equally "desviado" terms, then only using the M might be better.

In any of these cases though, how can we find the closest fit for this linear sum to the full wave-function? Well, the ones that the best fit to the full TDSE allow! If we introduce the CWF.LinComb in the TDSE:

$$i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t} = \sum_{k=1}^{N}\hat{T}_k\Psi(\vec{x},t) + U(\vec{x},t)\Psi(\vec{x},t)$$

with $\hat{T}_k \equiv -\frac{\hbar^2}{2m_k}\frac{\partial^2}{\partial x_k^2}$:

$$i\hbar\frac{\partial}{\partial t}\left(C_s(t)\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right) = \sum_{k=1}^{N}\hat{T}_k\left(C_s(t)\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right) + UC_s(t)\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)$$

where there is an implicit sum of $s \in \{1,...M^N\}$ on both sides. By the Leibiniz rule, the *lhs* leads to:

$$i\hbar\left(\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\frac{\mathrm{d}}{\mathrm{d}t}C_s(t) + C_s(t)\sum_{k=1}^{N}\frac{\partial}{\partial t}\psi_k^{\sigma_s^{(k)}}(x_k,t)\cdot\prod_{a=1;a\neq k}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right)$$

and we see that in the rhs:

$$\hat{T}_k\left(C_s(t)\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right) = C_s(t)\sum_{k=1}^{N}\prod_{a=1;a\neq k}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\cdot\hat{T}_k\psi_k^{\sigma_s^{(k)}}(x_k,t)$$

Now, as for any of the possible approximations we have suggested, we know that the CWF-s $\psi_k^\beta(x_k,t)$ were obtained as a solution to:

$$i\hbar\frac{\partial\psi_k^\beta(x_k,t)}{\partial t} = \hat{T}_k\psi_k^\beta(x_k,t) + U(x_k,\vec{x}_b^\beta(t),t)\psi_k^\beta(x_k,t) + W^{(k)}(x_k,\vec{x}_b^\beta(t),t)\psi_k^\beta(x_k,t)$$

where $W^{(k)}(x_k,\vec{x}_b(t),t)$ is the approximation of $G_k(x_k,\vec{x}_b^\beta(t),t) + iJ_k(x_k,\vec{x}_b^\beta(t),t)$ or alternatively of $(K_k(x_k,\vec{x}_b^\beta(t),t) + A_k(x_k,\vec{x}_b^\beta(t),t))/\psi_k^\beta(x_k,t)$; a complex potential particular to the β-th trajectory

and the k-th degree of freedom. Then, we can evaluate $i\hbar\frac{\partial\psi_k^{\beta}(x_k,t)}{\partial t}$ in the lhs of the previous equation and we will see that the terms of $\sum_{k=1}^{N}\hat{T}_k\psi_k^{\sigma_s^{(a)}}(x_k,t)$ will cancel each other, leaving:

$$\sum_{s=1}^{M^N}\left[i\hbar\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right]\frac{\mathrm{d}}{\mathrm{d}t}C_s(t)=\sum_{s=1}^{M^N}C_s(t)\left[U(\vec{x},t)\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right.$$

$$\left.-\sum_{k=1}^{N}U(x_k,\vec{x}_b^{\sigma}(t),t)\psi_k^{\sigma_s^{(k)}}(x_k,t)\prod_{a=1;a\neq k}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)-\sum_{k=1}^{N}W^{(k)}(x_k,\vec{x}_b^{\sigma}(t),t)\psi_k^{\sigma_s^{(k)}}(x_k,t)\prod_{a=1;a\neq k}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right]$$

Defining $V^{(k)}(\vec{x},t):=U(\vec{x},t)+W^{(k)}(\vec{x},t)$, then we are left with a rather compact expression ruling the time evolution of the coefficients in the linear expansion:

$$\sum_{s=1}^{M^N}\left[i\hbar\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right]\frac{\mathrm{d}}{\mathrm{d}t}C_s(t)= \tag{PDE.c}$$

$$\sum_{s=1}^{M^N}\left[\left(U(\vec{x},t)+\sum_{k=1}^{N}V^{(k)}(x_k,\vec{x}_b^{\sigma_s^{(k)}}(t),t)\right)\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right]C_s(t)$$

As all U,V and the CWF-s $\psi_a^{\sigma_s^{(a)}}(x_a,t)$ are known, we just have the coefficients that are unknown. We can get rid of the spatial dependance in $\vec{x}$ and thus be left with simple ordinary differential equations (ODEs) for the $C_s(t)$ if for instance, we multiply the rhs and lhs by $\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)^{\dagger}$ for any of the $s\in\{1,...,M^N\}$. For each possible s we will get one ODE for the set $\{C_s(t)\}_{s=1}^{M^N}$. As we have M^N coefficients $C_s(t)$ and we can do this trick for that many times, we will get a system of M^N ODEs with M^N unknown functions. Let us see their shape. Let each side of WWk be multiplied by $\prod_{a=1}^{N}\psi_a^{\sigma_\eta^{(a)}}(x_a,t)^{\dagger}$ for a certain trajectory combiantion $\eta\in\{1,...,M^N\}$ and integrate each side in the whole domain (which will in principle be $\mathbb{R}^N$):

$$\sum_{s=1}^{M^N}\left[i\hbar\prod_{a=1}^{N}\int_{-\infty}^{\infty}\psi_a^{\sigma_\eta^{(a)}}(x_a,t)^{\dagger}\psi_a^{\sigma_s^{(a)}}(x_a,t)dx_a\right]\frac{\mathrm{d}}{\mathrm{d}t}C_s(t)=$$

$$\sum_{s=1}^{M^N}\left[\int_{-\infty}^{\infty}U(\vec{x},t)\prod_{a=1}^{N}\psi_a^{\sigma_\eta^{(a)}}(x_a,t)^{\dagger}\psi_a^{\sigma_s^{(a)}}(x_a,t)dx_a+\right.$$

$$\left.+\sum_{k=1}^{N}\int_{-\infty}^{\infty}V^{(k)}(x_k,\vec{x}_b^{\sigma_s^{(k)}}(t),t)\prod_{a=1}^{N}\psi_a^{\sigma_\eta^{(a)}}(x_a,t)^{\dagger}\psi_a^{\sigma_s^{(a)}}(x_a,t)dx_a\right]C_s(t)$$

Now, if we denote:

$$\langle f(x_1,...,x_r,t)|g(x_1,...,x_r,t)\rangle:=\int_{-\infty}^{\infty}f^{\dagger}g\;dx_1\cdots dx_r$$

Then the above expression is equivalent to:

$$\sum_{s=1}^{M^N}\left[i\hbar\prod_{a=1}^{N}\left\langle\psi_a^{\sigma_\eta^{(a)}}(x_a,t)\middle|\psi_a^{\sigma_s^{(a)}}(x_a,t)\right\rangle\right]\frac{\mathrm{d}}{\mathrm{d}t}C_s(t)=$$

$$\sum_{s=1}^{M^N}\left[\left\langle\prod_{a=1}^{N}\psi_a^{\sigma_\eta^{(a)}}(x_a,t)\middle|U(\vec{x},t)\prod_{a=1}^{N}\psi_a^{\sigma_s^{(a)}}(x_a,t)\right\rangle+\right.$$

$$\left.+\sum_{k=1}^{N}\left\langle\psi_k^{\sigma_\eta^{(k)}}(x_k,t)\middle|V^{(k)}(x_k,\vec{x}_b^{\sigma_s^{(k)}}(t),t)\psi_k^{\sigma_s^{(k)}}(x_k,t)\right\rangle\prod_{a=1;a\neq k}^{N}\left\langle\psi_a^{\sigma_\eta^{(a)}}(x_a,t)\middle|\psi_a^{\sigma_s^{(a)}}(x_a,t)\right\rangle\right]C_s(t)$$

Thus, defining the 2-tensors that we can numerically compute as we have already computed the necessary functions for $\eta, s \in \{1, ..., M^N\}$:

$$\mathbb{M}_{\eta s} := \prod_{a=1}^{N} \left\langle \psi_a^{\sigma_\eta^{(a)}}(x_a, t) \middle| \psi_a^{\sigma_s^{(a)}}(x_a, t) \right\rangle \tag{M}$$

$$\mathbb{W}_{\eta s} := \left\langle \prod_{a=1}^{N} \psi_a^{\sigma_\eta^{(a)}}(x_a, t) \middle| U(\vec{x}, t) \prod_{a=1}^{N} \psi_a^{\sigma_s^{(a)}}(x_a, t) \right\rangle \tag{WW}$$

$$\mathbb{W}^{(k)}_{\eta s} := \left\langle \psi_k^{\sigma_\eta^{(k)}}(x_k, t) \middle| V^{(k)}(x_k, \vec{x}_b^{\sigma_s^{(k)}}(t), t) \psi_k^{\sigma_s^{(k)}}(x_k, t) \right\rangle \prod_{a=1; a\neq k}^{N} \left\langle \psi_a^{\sigma_\eta^{(a)}}(x_a, t) \middle| \psi_a^{\sigma_s^{(a)}}(x_a, t) \right\rangle \tag{WWk}$$

Then, we see that the ODE system we must solve for the $C_s(t)$ is the set:

$$\sum_{s=1}^{M^N} i\hbar \mathbb{M}_{\eta s} \frac{\mathrm{d}}{\mathrm{d}t} C_s(t) = \sum_{s=1}^{M^N} \left(\mathbb{W}_{\eta s} + \sum_{k=1}^{N} \mathbb{W}^{(k)}_{\eta s} \right) C_s(t) \quad for\ \eta, s \in \{1, ..., M^N\}$$

which is equivalent to the matrix-vector equation:

$$i\hbar \mathbb{M}(t) \frac{\mathrm{d}}{\mathrm{d}t} \vec{C}(t) = \left(\mathbb{W}(t) + \sum_{k=1}^{N} \mathbb{W}^{(k)}(t) \right) \vec{C}(t) \tag{M}$$

with $\mathbb{M}, \mathbb{W}, \mathbb{W}^{(k)} \in \mathcal{M}_{M^N \times M^N}(\mathbb{C})$ and $\vec{C} \in \mathbb{C}^{M^N}$.

Again, note that all the elements of those matrices can readily be computed integrating the results obtained when evolving the CWF-s for the different initial trajectory positions. Then, if per each time step we invert $\mathbb{M}$ or use some sort of LU decomposition, we can integrate the set of ODE-s using a Runge-Kutta4 method or any ODE solver. Once we know the coefficients $\{C_s(t)\}_{s=1}^{M^N}$, we can compute the sum $\Psi(\vec{x}, t) \simeq \sum_{s=1}^{M^N} C_s(t) \psi_1^{\sigma_s^{(1)}}(x_1, t) \cdots \psi_N^{\sigma_s^{(N)}}(x_N, t)$ and forget about the CWF-s and the matrices. This approximation of the full wavefunction, could perhaps be now used in order to compute new shapes for K and A or G and J, and repeat the whole process, to get presumably a yet more accurate full wavefunction!

5 Suggestion for a self-consistent Composed Algorithm

Given all the present discussion, one could suggest the following idea: the main problem in the various alternative shapes of (CWF) is that they depend on our knowledge of the full wave-function. Now, we have seen that, using the Hermitian approximation or the second algorithm (thus assuming the full wave-function is a factorizable product or a gross simplification), we can build approximate CWF-s, with which we can generate the best possible approximation of the full wave-function using WWk and the CWF.LinComb. Sure, if we use more trajectories, the expansion CWF.LinComb will give the full wave-function more flexibility in the fit, but: Why not to use this reconstruction as ansatz to approximate the potentials K and A or G and J, in order to build new approximations for the CWF-s, and construct presumably an even better approximation for the full wavefunction, and reiterate till we are happy with the result? In principle, as we are introducing information about the exact TDSE each time, the full wavefunction should tend towards the exact solution, as each time the CWF-s will be closer to the true ones. Well, this is still to be proved but as a first thought it makes sense.

Throughout all the discussion we continuously considered CWF-s of a single free variable, however, we could choose to partition the system in a coarser grain. The only change would be to do $x_a \longrightarrow \vec{x}_a$ in all the developments, where $\vec{x}_a$ would represent a set of degrees of freedom and $a \in \{1, ..n\}$, where n would represent the number of partitions of the N degrees of freedom.

5.1 Algorithm Steps: Draft

Step 0 Ask the user $\Psi(\vec{x}, t = t_0)$, $U(\vec{x}, t)$ and other simulation parameters like M (number of trajectories to compute), $j - tolerances$ or $\{J_a\}_{a=1}^N$, last time iteration t_f etc.

Step 1 If necessary, compute the transversal section eigenstates (TSEig) of $U(\vec{x}, t)$ given by $\{\{\Phi^j_{x_a}(x_a, t)\}_{j=1}^{J_a}\}_{a=1}^N$. *Massively parallelizable.*

Step 2 Sample M initial points $\{\vec{x}^\beta(t_0)\}_{\beta=1}^M$ from $|\Psi(\vec{x}, t_0)|$. Evolve the set of N CWF-s for each β-th trajectory *in parallel*, using any of the approximations to (CWF.SE). In each time iteration of each trajectory, the N dimension CWF-s can be independently computed *in parallel*. There is only a Barrier there to make the cross talk through the configuration space trajectory.

We get M sets of N CWF-s: $\{\{\psi^\beta_a(x_a, t)\}_{a=1}^N\}_{\beta=1}^M$ together with the trajectiories $\{\vec{x}^\beta(t)\}_{\beta=1}^M$.

Step 3 Once we have the M sets of N CWF-s and the approximated correlation potentials W^k for each of the CWF-s saved in memory, we can compute the overlap integrals *in parallel* $\mathbb{M}_{\eta s}, \mathbb{W}_{\eta s}, \mathbb{W}^{(k)}_{\eta s}$.

Step 4 Invert $\mathbb{M}$ and evolve the $\vec{C}(t)$. It is readily thought to be vectorized and thus *parallelized*.

Step 5 Once obtained the full wavefunciton approximation $\Psi(\vec{x}, t) = \sum_{s=1}^{M^N} C_s(t) \prod_{a=1}^N \psi_a^{\sigma_s^{(a)}}(x_a, t)$. Clean all the memory buffers and compute using the reconstructed full wavefunction better approximations for the correlation potentials K and A or G and J.

Step 6 If tolerance achieved then finish. Else go back to Step 2.

5.2 Parallelization Strategy: Draft

If we ignore message pass overheads and memory latencies and we had as many processing units as necessary, the whole computation (Step 2-5) would require in sequential time:

(1) The time a single (worst case) solution finding of $\left(-\sum_{k=1;k\neq a}^N \frac{\hbar^2}{2m_k}\frac{\partial^2}{\partial x_k^2} + U(x_a, \vec{x}_b, t)\right)\Phi^j_{x_a}(\vec{x}_b, t) = E^j_{x_a}(t)\Phi^j_{x_a}(\vec{x}_b, t)$ could take for a single j and single x_a. The rest could be computed in parallel

(perhaps not the j-s, that will depend on the eigensolver employed). Ofcourse the computation time of a single one is at least proportional to N.

(2) The time a single CWF evolution in one dimension takes. In principle step 2 does not depend on the dimension N. One should add perhaps a sm,all overhead for the cross talk between the CWF-s of a same trajectory after each time iteration.

(3) The time to compute all the overlap integrals $\mathbb{M}_{\eta s}, \mathbb{W}_{\eta s}, \mathbb{W}^{(k)}_{\eta s}$. They can all be computed in parallel. Actually they could be computed while the CWF-s and the correlation potentials are outputted, in a second thread. In principle this should not depend on M.

(4) The time to invert $\mathbb{M}$ and to evolve the ODE system for the $C_s(t)$.

It looks like overall it does not scale that much with N.

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