Can we make the Exponential scaling in Time be Linear in Time if Parallelized Exponentially?

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1 The Objective

It is well known that the time dependent Schrödinger Equation (TDSE) that predicts the dynamics of a quantum system is a problem that scales exponentially both in space and in time for increasing dimensionality of the problem. This becomes very obvious when interpreting the wave-funtion in terms of an ensemble of tangentially interacting trajectories of the system. That is, quantum mechanical systems (experiments) depend on all their possible realizations in a way that all the possible trajectories of the system interact repulsively among them due to the quantum potential first described by David Bohm. This means that it is equivalent to think on the wavefunction of the system as an ensemble of an infinitely dense set of exactly equivalent systems forming a fluid where each copy of the system cannot cross the trajectory of any other at the same time (they cannot occupy the same point in configuration space-time) and they still have a repelling force pushing the fluid towards the most homogenenous distribution possibel given the manifold described by the potential energy term.

This clearly shows that it is impossible to evolve a single one of these trajectories without knowing the whole ensemble. This is the so called Quanutm Wholeness. This means that if we increase the dimensionality of the system, it is not enough to increase the computational complexity linearly. A single dimension more implies that in order to know about one single trajectory we now need to know as many trajectories as we needed for the previous dimensionality multiplied by all the possible positions in a new axis. The number of trajectories we would need to simultaneously compute in order to be able to even compute them (and by the way reconstruct the wave-funtion in tyheir vecinity) increases exponentially. However, it is still not clear that there is no method that could allow us evolve self-consistently in parallel at each time step enough trajectories, such that their evolution is linear in time for increasing number of dimensions (even if it scales exponentially in parallel threads that communicate at each time step).

That is, the question is, can we find a method that allows us to compute a single time step that has a fixed cost (perhaps with soem overheads for parallel communiocation) that transfers the expoenntial complexity to the parallelization? That is, it is clear, that if we try to sequentially compute the necessary number of trajectories to advance a central trajectory, we need exponentially more surrounding trajetcories, thus in the single thread's time we would require exponentially more time. Then, even if we are given as many parallel computation threads as we want, we are not able to compute all the trajectories, because they are not independent and they do influence each other. Still, if we allow a cross talk between them every time step, we could achieve an evolution for them that does not increase the complexity in sequential time (unless for the overhead). This cross talk would account for the qwuantum potential propagation. Osea esto es fundamentalemte posible si consiguiese encontrar cual es el pair-wise quantum potential discreto, que al hacer al infinito tiende a la funcion de onda continua. Si fuese asi con una integracion del sistema de edos infinito (pero cada eq simple) en paralelo actualizando los potenciales para cada uno podrias conseguir resolver cualquier problema quantum many body problem si tuvieses suficientes threads paralellos (uno por cada trayectoria evolucionada). HAbria claramente el problema del cross talk, que seria cada vez mas complicada pero bueno, en si seria eso.

Alternativamente, en vez de intentar hacer que todas las trayectorias sean por igual ecuaciones d eNewton, queiza podrias intentar darle un empujon y evolucionar fks de onda condicionadas y una trayectoria por cada conjunto. Ya que cada CWF es 1D y eso es muy facil de resolver. Si fueses capaz de aproximar la full fk de onda con estas slices en cada dimension mejor que usando las trajs en si pues mejor. Ze en si cada CWF es un ensemble de trayectorias, pero de las cuales en principio solo uan (la central) es en cada tiempo la misma. Osea la pregunta es realmente el qtm wholeness necesita trayectorias que estan super lejos? Claro, la cuestion es que no seras capaz de obtener con un solo set de cwf-s en cdad dimension (una trayectoria) evolucionada al mismo timepo el self-impulso dado por las trayectorias que lo rodean. Aka una sola cwf evolucionada en paralelo no funkiona. En todo caso muchas cwf-s evolucionadas tangentemente si, como las trayectorias. Pero esto por supuesto acabaria siendo un ensemble method tipo quantum trajectory method.

Osea la cuestion es que la velocidad e duna trayectoria de Bohm solo depende de la derivad de sus CWF-s en cada timepo! de las direcciones ortonormales (ze claro, el campo de velocidades es la derivada parcial (en las dirs cartesianas de la accion) y el qtm potential solo depende de la derivada parcial en las dirs cartesianas de la "densidad" local!). Entonces, dado un t, dada la fk onda completa, sacas condicioanndo las CWF. Ahora de las CWF tu puedes computar a donde se mueve la traj de Bohm en el sigueinte teimpo. Ahora la pregunta es, puedes si supieses toda la traj evolucionar un tiempo la CWF? Si pudieses ya estaria reuslto el problema many body. Pero la resuesta es que las ecuaciones que rigen las CWF dependen de la full wavefunction al parecer!

Disclaimer, all the present work will be made for 3 dims but is clearly generalizable to N.

2 Expanding the Full Wavefunction in energy eigenstates

2.1 General Time Dependent Potentials

Given the TDSE in N dimensions, with $x := \vec{x} = (x_1, ..., x_N) \in \mathbb{R}^N$:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(\sum_{j=1}^{N} \hat{T}_{x_j} + U(x,t) \right) \psi(x,t) \tag{1}$$

with $\hat{T}_{x_j} := \frac{\hbar^2}{2m_j} \frac{\partial^2}{\partial x j^2}$ and $\hbar$ the Planck constant. We consider the Hamiltonian operator in spatial representation:

$$\hat{H}(x,t) := \sum_{j=1}^{N} \hat{T}_{x_j} + U(x,t) \tag{2}$$

We can in general find the eigenstates of this operator for each time as the set of functions $\{\phi_k(x,t)\}_{k=0}^{\infty}$ with associated eigenvalues $E^j(t)$ (ordered from lower to higher together with the index j) such that:

$$\hat{H}(x,t)\phi_k(x,t) = E^j(t)\phi_k(x,t) \tag{3}$$

If we know that the quantum system is restricted to be proportional to one of these eigenstates at all times, then the wavefunction will have a shape $\psi(x,t) = c_k(t)\phi^k(x,t)$ and the TDSE will define which will the constant $c_k(t)$ be:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \Rightarrow i\hbar \frac{\partial (c_k(t)\phi^k(x,t))}{\partial t} = c_k(t)E^k(t)\phi(x,t) \tag{4}$$

$$\Rightarrow i\hbar \phi^k(x,t) \frac{\partial c_k(t)}{\partial t} = c_k(t)E^k(t)\phi(x,t) - i\hbar c_k(t) \frac{\partial \phi^k(x,t)}{\partial t}$$

Knowing that the state $\phi^k(x,t)$ is normalized $\int_{-\infty}^{\infty} \phi^{k\dagger}\phi^k(x,t)\phi^k(x,t)dx = 1$, we can multiply both sides of the equation by $\phi^{k\dagger}$ and integrate them in all x dimensions to get the dynamical equation ruling the coefficient $c_k(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t} c_k(t) = -\left(\frac{i}{\hbar} E^k(t) + W^k(t) \right) c_k(t) \tag{5}$$

with:

$$W^k(t) := \int_{-\infty}^{\infty} \phi^{k\dagger} \frac{\partial \phi^k(x,t)}{\partial t} dx \tag{6}$$

Leaving:

$$c_k(t) = c_k(t_0)\ e^{-\int_{-\infty}^{\infty} \left(\frac{i}{\hbar} E^k(t) + W^k(t) \right) dt} \tag{7}$$

Thus meaning that $\forall t > t_0$:

$$\psi(x,t) = c_k(t_0)\ e^{-\int_{-\infty}^{\infty} \left(\frac{i}{\hbar} E^k(t) + W^k(t) \right) dt} \phi^k(x,t)$$

It can be proven that the eigenstates $\phi_k(x,t)$ form a complete orthonormal basis of the Hilbert space of the system for each of the considered times. As such, any wavefunction can be written as a linear combination of them:

$$\Psi(x,t) = \sum_j c_j(t)\phi_j(x,t) \tag{8}$$

This means that any wavefunction solution to the TDSE can be represented as such. Thus, we could impose this shape in the TDSE and look for the time evolution of the coefficients $c_j(t)$. If we

have the knowledge of the wavefunction at a certain initial time t_0 as $\psi(x,t_0)$, we could first get the coefficients $c(t_0)$ using the fact that:

$$c_k(t) = \int_{-\infty}^{\infty} \phi^{k\dagger}(x,t)\psi(x,t)dx \tag{9}$$

Then, we could get the rest of the times for $\psi(x,t)$ by:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \Rightarrow \sum_k i\hbar\frac{\partial(c_k(t)\phi^k(x,t))}{\partial t} = \sum_k c_k(t)E^k(t)\phi(x,t) \tag{10}$$

$$\Rightarrow \sum_k i\hbar\phi^k(x,t)\frac{\partial c_k(t)}{\partial t} = \sum_k c_k(t)E^k(t)\phi^k(x,t) - i\hbar c_k(t)\frac{\partial\phi^k(x,t)}{\partial t}$$

Multiplying everything by $\phi^{j\dagger}(x,t)$ and integrating on x, using the orthonormality condition $\int \phi^{j\dagger}\phi^k dx = \delta_{jk}$ (note that hereafter all the integrals will be in all $\mathbb{R}^N$ so we will omit the upper and lower bounds):

$$\frac{\mathrm{d}}{\mathrm{d}t}c_j(t) = -\frac{i}{\hbar}E^j(t)c_j(t) + \sum_k W^{jk}(t)c_k(t) \tag{11}$$

where we define the coupling terms between the eigenstates:

$$W^{jk}(t) := \int_{-\infty}^{\infty} \phi^{j\dagger}\frac{\partial\phi^k(x,t)}{\partial t}dx \tag{12}$$

Which is a system of as many linear and coupled ordinary differential equations as energy eigenstates we consider. In principle infinite for arbitrarity, but in practice we could truncate them at a certain maximum J if we had ad hoc reasons for each given potential energy $U(x,t)$ and initial wavefunction $\psi(x,t_0)$ (the two degrees of freedom aside from the dimensionality of the system).

These last equations tell us that the magnitude of the projection of the system in each eigenstate $c_j(t)$ will be transferred in time from state to state in a proportional fashion to the projection on each $c_k(t)$ and the coupling coefficient W^{jk}.

2.2 Adiabatically Time Dependent Potentials

If we have that the potential energy is so slowly varying in time that the eigenstates vary very smoothly in time for each x, then $\frac{\partial\phi^k(x,t)}{\partial t} \simeq 0$. We will call this potential adiabatic. In such a case, we see that the terms $W^{jk} \simeq 0$, leaving a system of uncoupled ordinary differential equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}c_j(t) = -\frac{i}{\hbar}E^j(t)c_j(t) \tag{13}$$

Which can be solved in general to be:

$$c_j(t) = c_j(t_0)\ e^{-\frac{i}{\hbar}\int E^j(t)dt} \tag{14}$$

This would leave us with a general solution of the wavefunction:

$$\psi(x,t) = \sum_j c_j(t_0)e^{-\frac{i}{\hbar}\int E^j(t)dt}\phi(x,t) \tag{15}$$

with $c_j(t_0) = \int \phi^{j\ \dagger}(x,t_0)\Psi(x,t_0)dx$.

This would imply that the magnitude of the projections in each of the eigenstates would remain constant at all times. This magnitude (its square) is called the population of that eigenstate:

$$|c_j(t)|^2 = |c_j(t_0)e^{-\frac{i}{\hbar}\int E^j(t)dt}|^2 = |c_j(t_0)|^2 \quad \forall t > t_0$$

2.3 Time Independent Potentials

If we have that the potential energy is time independent $\frac{\partial U(x,t)}{\partial t} = 0$ then we have that the eigenstates and eigenvalues do not depend in time as they will be solutions to a time independent equation:

$$\hat{H}(x)\phi_k(x) = E^j\phi_k(x) \tag{16}$$

As such, equation (10) woould be reduced to:

$$\sum_k i\hbar\phi^k(x)\frac{\partial c_k(t)}{\partial t} = \sum_k c_k(t)E^k\phi^k(x) \tag{17}$$

which can be multiplied by each eigenstate and integrated in all $\mathbb{R}^N$ to get an uncoupled system of equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}c_j(t) = -\frac{i}{\hbar}E^j c_j(t) \tag{18}$$

Yielding:

$$c_j(t) = c_j(t_0)\ e^{-\frac{i}{\hbar}E^j(t-t_0)} \tag{19}$$

And thus leaving a general time evolution for the full wavefunction as:

$$\psi(x,t) = \sum_j c_j(t_0)e^{-\frac{i}{\hbar}E^j(t-t_0)}\phi(x) \tag{20}$$

with $c_j(t_0) = \int \phi^{j\ \dagger}(x)\Psi(x,t_0)dx$.

Thus, given a certain initial wavefunction, and its projections into each eigenstate, the populations of each state are maintained constant at all times.

2.4 Comments on this Method

Clearly, if we knew the eigenstates of the full hamiltonian $\hat{H}$, we could for the time independent or adiabatic case of the potential compute the time evolution of any initial wavefunction at any future time by simply computing the initial projections on each eigenstate $c_j(t_0) = \int \phi^{j\ \dagger}(x,t)\Psi(x,t_0)dx$. This method would only require computing as many integrals as necessary (say J) to achieve a given norm tolerance $\sum_{j=1}^{J}|c_j(t_0)|^2 \simeq 1$. Once these projections computed, in order to have the time evolution for any future time with very high precision we would only require a simple evaluation.

In fact, even in the case of a time dependent general potential, solving equations (11) is simple and does not scale exponentially with growing number of dimensions N, as would have a complexity $O(Jn_t)$ with n_t the number of time steps to compute. This would be true except if we consider that in order to compute the coupling integrals w^{jk}, we need to integrate at least over a whole n_x^N division grid (where n_x is the smallest number of divisions of an spatial axis). This has a complexity of $O(n_x^N)$, which is exponential in time for increasing number of dimensions N. But then, if we knew the eigenstates analytically, the integrals would not be required to be done numerically and the problem would really be linear in dimensions.

Clearly, the truly exponential problem in this algorithm would be the computation of the eigenstates of the full Hamiltonian. If we did not know them a priori, we would need to compute them, which requires at least an evaluation of the Hamiltonian, which is a sparse matrix of $O(n_x^N)$ rows and columns, with about $O(d^N)$ non-zero elements per column, where d is the average non-zero elements in the $N = 2$ case. Clearly, evaluating this would at least require $O(d^N)$ operations, which scale expoenntially with dimensions N.

A such, the whole many body problem has been injected into computing the eigenstates of the full hamiltonian, which if we do not know analytically, is exponentially growing with dimensions.

3 Expanding the Wavefunction in Transversal Section Eigenstates

If we now choose a certain spatial degree of freedom x_a with $a \in \{1, ..., N\}$ and rename it as x while we name the vector composed by the rest of degrees of freedom as $y := (y_1, ..., y_{N-1})$, then we can write the full hamiltonian to be:

$$\hat{H}(x, y, t) = \sum_{j=1}^{N-1} \hat{T}_{y_j} + U(x, y, t) + \hat{T}_x + V(x, t) = \hat{H}^x(y, t) + \hat{T}_x + V(x, t) \tag{21}$$

If we know the transversal section eigenstates (TSE) defined as the set of eigenstates $\{\Phi_x^j(y,t)\}_j$ of associated eigenvalues $\{\varepsilon_x(t)\}_j$ solution for each x of:

$$\hat{H}^x(y,t)\phi_k(y,t) = \varepsilon^j(t)\phi_k(y,t) \tag{22}$$

As we know that the hermiticity of the operator $\hat{H}^x(y,t)$ implies its eigenstates form a complete basis of the space y for all times, we could write any wavefunction as a linear combination of them for each x:

$$\Psi(x, y, t) = \sum_j \chi^j(x,t)\Phi_x^j(y,t) \tag{23}$$

with $\chi^j(x,t) := \int \Phi_x^{j\ \dagger}(y,t)\Psi(x,y,t)dy$ the projection coefficients.

If we introduce this shape into the TDSE, we can obtain the differential equations ruling the shape of the coefficients $\chi j(x,t)$ much like we did in the previous section (just that now the resulting equation system will no longer be an ordinary differential equation).

$$i\hbar\frac{\partial\Psi(x,y,t)}{\partial t} = \hat{H}\psi(x,y,t) \Rightarrow \sum_j i\hbar\frac{\partial(\chi^j(x,t)\Phi_x^j(y,t))}{\partial t} = \sum_j \Big(\hat{H}^x(y,t) + \hat{T}_x + V(x,t)\Big)(\chi^j(x,t)\Phi_x^j(y,t)) \tag{24}$$

$$\Rightarrow \sum_j i\hbar\left(\Phi_x^j(y,t)\frac{\partial\chi^j}{\partial t} + \chi^j\frac{\partial\Phi_x^j(y,t)}{\partial t}\right) = \sum_j \Big(\varepsilon_x^j(t) + \hat{T}_x + V(x,t)\Big)(\chi^j(x,t)\Phi_x^j(y,t))$$

Defining the constant $C_x := \frac{-\hbar^2}{2m_x}$ we can note that:

$$\hat{T}_x(\chi^j(x,t)\Phi_x^j(y,t)) = C_x\frac{\partial^2}{\partial x^2} = \tag{25}$$

$$= C_x\left(\Phi_x^j(y,t)\frac{\partial^2}{\partial x^2} + \chi^j(x,t)\frac{\partial^2}{\partial x^2} + 2\frac{\partial}{\partial x}\chi^j(x,t)\frac{\partial}{\partial x}\Phi_x^j(y,t)\right))$$

$$= \Phi_x^j(y,t)\ \hat{T}_x\chi^j(x,t) + \chi^j(x,t)\ \hat{T}_x\Phi_x^j(y,t) + 2C_x\ \frac{\partial}{\partial x}\chi^j(x,t)\ \frac{\partial}{\partial x}\Phi_x^j(y,t))$$

Then we can multiply equation (24) by $\Phi^{k\ \dagger}(y,t)$ and integrate both sides over all the domain for y to get applying the orthonormality condition $\int \Phi^{k\ \dagger}(y,t)\Phi^j(y,t)dy = \delta_{kj}$:

$$i\hbar\frac{\partial}{\partial t}\chi^k(x,t) = \Big(\varepsilon^k(x,t) + \hat{T}_x + V(x,t)\Big)\chi^k(x,t) + \sum_j \left\{W^{kj}(x,t) + S^{kj}(x,t) + F^{kj}(x,t)\frac{\partial}{\partial x}\right\}\chi^j(x,t) \tag{26}$$

where we have defined the coupling terms between the transversal section eigenstates:

$$W^{kj}(x,t) = -i\hbar\int \Phi^{k\ \dagger}(y,t)\frac{\partial\Phi_x^j(y,t)}{\partial t}dy \tag{27}$$

$$S^{kj}(x,t) = \int \Phi^{k\ \dagger}(y,t)\hat{T}_x[\Phi_x^j(y,t)]dy \tag{28}$$

$$F^{kj}(x,t) = \int \Phi^{k\ \dagger}(y,t) 2C_x \frac{\partial}{\partial x} \Phi_x^j(y,t) dy \tag{29}$$

Equation (26) is the system of linear and coupled partial differential equation system ruling the behaviour of the coefficients $\chi^k(x,t)$. This is a generalization of the equations found and used in Ref.[3].

3.1 Adiabatic (or constant) coupling potential with y for x and t

If we have that the potential energy term entangling the degrees of freedom x and y, which we called $U(x,y,t)$, is very slowly time dependent (or constant in time) and very slowly x dependent, then the eigenstates of the transversal sections to x fulfil $\frac{\partial}{\partial x}\Phi_x^j(y,t) \simeq 0$ and $\frac{\partial}{\partial t}\Phi_x^j(y,t) \simeq 0$. This would yield $W^{kj}(x,t), S^{kj}(x,t), F^{kj}(x,t) \simeq 0$, which would leave equations (26) uncoupled as:

$$i\hbar \frac{\partial}{\partial t}\chi^k(x,t) = \Big(\varepsilon^k(x,t) + \hat{T}_x + V(x,t)\Big)\chi^k(x,t) \tag{30}$$

Which is a single spatial dimension (1D) Schrödinger Equation (SE) for each of the eigenstates. This would mean that each coefficient $\chi(x,t)$ would preserve its norm $\int \chi(x,t)^{k\dagger}\chi^k(x,t)dx =: P^j(t)$ at all times due to the unitary time evolution of the Schrödinger Equation. This is exactly analogous to what happened when we expanded the wave-function in the energy eigenstates of the full hamiltonian.

We could now simply compute the initial coefficients $\chi^k(x,t_0)$ for a desired initial wavefunction by $\chi^k(x,t_0) = \int \chi(x,t)^{k\dagger}\psi(x,y,t_0)dy$ and then compute 1D SE-s for as many coefficients χ^k ad necessary to achieve a certain norm tolerance $\sum_{j=0}^{J} P^j(t) \simeq 1$ and then simply ensemble them to have the N dimensional full wavefunction as $\psi(x,y,t) = \sum_j \chi^j(x,t)\Phi^j(y,t)$.

In fact, in a sort of inception we could now compute the evolution of each of the coefficients χ^j of the transversal sections by computing the eigenstates $\phi^g(x,t)$ of their effective hamiltonian:

$$\hat{H}_{eff}(x,t) = \varepsilon^k(x,t) + \hat{T}_x + V(x,t) \Rightarrow \{\phi^g(x,t);\ \eta_g(t)\} \tag{31}$$

Then by the completeness of this basis in x there must exist some coefficients $c_{gj}(t)$ such that $\chi^j(x,t) = \sum_g c_{gj}(t)\phi^g(x,t)$. These coefficients will be uniquely defined by the equations we got in the first section:

$$\frac{\mathrm{d}}{\mathrm{d}t}c_{gj}(t) = -\frac{i}{\hbar}\eta^g(t)c_{gj}(t) + \sum_k M^{gk}(t)c_k(t) \tag{32}$$

with:

$$M^{gk}(t) := \int_{-\infty}^{\infty} \phi^{g\dagger}\frac{\partial \phi^k(x,t)}{\partial t}dx \tag{33}$$

If the part of the potential that was independent from y, $V(x,t)$, is also adiabatic in time, then as we proved earlier:

$$\chi^j(x,t) = c_{gj}(t_0)e^{\int_{t_0}^{t}\eta_g(t)dt}\phi^g(x,t) \tag{34}$$

Thus, by only knowing the projections $\chi^j(x,t_0) = \int \chi(x,t)^{j\dagger}\psi(x,y,t_0)dy$ and $c_{gj}(t_0) = \int \phi^g(x,t)^\dagger \chi^j(x,t)dx$, the solution of the full wavefunction would be uniquely defined at all future times.

3.2 Comments on General Potentials

In general in order to compute the coefficients of the expansion $\chi^j(x,t)$ we would first need to compute the coupling terms $W^{kj}(x,t), S^{kj}(x,t), F^{kj}(x,t)$. As we assume we know the eigenstates $\Phi_x^j(y,t)$, these can be trivially done even before we start to compute the time evolution for the coefficients $\chi^j(x,t)$. Then, we would need to solve the linear coupled system of partial differential equations for $\chi^j(x,t)$

given in equation (26). This system, truncated a t a certain maximum J could be stably evolved using a Crank Nicolson scheme which would only require to LU decompose a matrix of size SxS with $S = Jn_x$ with n_x the number of considered spatial divisions in x and J the number of terms in the expansion we considered to be relevant. At most this has a complexity of $O(Jn_xn_t)$ which is linear with the terms J and the divisions considered in time n_t and x n_x. So the question here would be, where has the many body problem gone? Well, on the one hand, the integrals $W^{kj}(x,t), S^{kj}(x,t), F^{kj}(x,t)$ are in the whole domain for all the spatial variables except for one $N-1$, so they each have a complexity of at least $O(n_y^{N-1})$ (where we assume n_y to be the smallest of the grids we consider for the non-x axes y). Clearly this is exponentially growing in time with the number of dimensions N. Still, if we knew analytically the eigenstates $\Phi_x^j(y,t)$ then the coupling terms would be resolved analytically and there would be no need for numerical integration. In fact, it would be enough that we got the eigenstates expressed as a combination of other analytical basis functions so that we could integrate symbolically and there would be no need for exponential complexity. So again, where is then the many body problem? Solved? No. The computation of the eigenstates Φ_x^j of the transversal hamiltonian $\hat{H}_x(y,t)$ requires at least one evaluation of the hamiltonian on a sequentialized vector $\Phi_x^j \in \mathbb{C}^{n_y^(N-1)}$, which will be the discretization of $\Phi_x^j(y,t)$. Thus the hamiltonian matrix will have a sparse number of rows and columns $O(n_y^{N-1})$, with a number of non-zero elements $O(d^{N-1})$ with d the average number of non-zero elements per row for the $N=2$ case. Therefore, the evaluation will at least have a complexity of $O(d^{N-1})$, which scales exponentially in time. Only if we knew the eigenstates a priori would this step be avoidable.

In a nutshell, only if these eigenstates are known analytically will this method scale linearly in dimensions N.[1] But this was already true for the even simpler case of Section 1. There, if we knew the eigenstates of the full hamiltonian, then the time evolution of the full wave-function was reduced into a yet simpler system of equations. In fact, with the hamiltonian being time adiabatic there was already no need to compute overlap integrals, unlike here, where overlap integrals are required while the transversal hamiltonian has non-adiabatic dependence on time or x. So it does not seem like we have gained so much. Just that before we needed at least $O(d^N)$ operations to get the eigenstates of the full hamiltonian and now we just need $O(d^{N-1})$. Instead, we now require a harder equation for the time evolution of the coefficients where a partial differential equation system (with a complexity around $O(Jn_xn_t)$) must be solved instead of an ordinary differential equation system (with a complexity of $O(Jn_t)$). Of course, overall the complexity has been reduced in one N, yet it is exponential $O(d^N)$.

The natural question would then be: can we find an scheme where we can choose conveniently how many of the exponential complexity N is migrated from the Schrödinger Equation to an eigenstate problem? Clearly, it is pure fantasy to believe there is an scheme where we just have a linear complexity in the SE (the coefficients) and in the eigenvalue problem. Perhaps trying to iteratively solve higher and higher dimensional coefficient problems like we did here in the last step, but solving 1D coefficient problems in each iteration could achieve so. It is not entirely clear. Still, what we have done in the first section is to migrate all the n_x^N from the Schrödinger Equation to the eigenstate problem. Then here we have migrated one of those n_x from the eigenvalue problem to the Schrödinger Equation, leaving a joint complexity $O(n_y^{N-1}) + O(n_x) = O(n_y^{N-1})$. It seems possible that we will be able to migrate any number of n_y from the Schrödinger Equation to the eigenvalue problem and viceversa. If this was so, we could minimize the overall complexity if we set half of the multiplicative n_y in one side and the other half in the other side. This would leave a complexity $O(n_y^{N/2}) + O(n_x^{N/2}) = O(n_x^{N/2})$ which is still exponential, but it is the square-root of the exponential increase that the full Schrödinger Equation supposes! And this is precisely what we can achieve with the approach of the next section.

[1] If we only knew them numerically, then the problem would still be exponential due to the coupling integrals.

4 Expanding the Wavefunction in Custom Section Eigenstates

We will now divide the spatial degrees of freedom as follows: we will have some main degrees of freedom $x = (x_1, .., x_m)$ in each of which we will slice the whole set of degrees of freedom $(x_1, ..., x_N)$. Then we will have the set of non-main degrees of freedom $y = (x_{m+1}, ...x_N)$ for which we will need to know the eigenstates. As such, we will have a general decomposition of the Hamiltonian:

$$\hat{H}(x,y,t) = \sum_{j=1}^{N} \hat{T}_{x_j} + G(x,y,t) = \sum_{j=m}^{N} \hat{T}_{x_j} + U(x,y,t) + \sum_{j=1}^{m} \hat{T}_{x_j} + V(x,t) = \hat{H}_x(y,t) + \sum_{j=1}^{m} \hat{T}_{x_j} + V(x,t) \tag{35}$$

We then define the set of eigenstates $\{\Phi_x^j(y,t)\}_j$ with eigenvalues $\{\varepsilon_x(t)\}_j$ to be the solution to:

$$\hat{H}_x(y,t)\Phi_x^j(y,t) = \varepsilon_x^j(t)\Phi_x^j(y,t) \tag{36}$$

As we know that the hermiticity of the operator $\hat{H}_x(y,t)$ implies its eigenstates form a complete basis of the space y for all times, we could write any wavefunction as a linear combination of them for each x:

$$\Psi(x,y,t) = \sum_j \Lambda^j(x,t)\Phi_x^j(y,t) \tag{37}$$

with $\Lambda^j(x,t) := \int {\Phi_x^j}^\dagger(y,t)\Psi(x,y,t)dy$ the projection coefficients.

If we introduce this shape into the TDSE, we can obtain the differential equations ruling the shape of the coefficients $\Lambda j(x,t)$ much like we did in the previous section (just that now the resulting equation system will no longer be a 1D coupled system of Schrödinger like equations).

$$i\hbar\frac{\partial\Psi(x,y,t)}{\partial t} = \hat{H}\psi(x,y,t) \Rightarrow \sum_j i\hbar\frac{\partial(\Lambda^j(x,t)\Phi_x^j(y,t))}{\partial t} = \sum_j \left(\hat{H}_x(y,t) + \sum_{s=1}^{m}\hat{T}_{x_s} + V(x,t)\right)(\Lambda^j(x,t)\Phi_x^j(y,t)) \tag{38}$$

$$\Rightarrow \sum_j i\hbar\left(\Phi_x^j(y,t)\frac{\partial\Lambda^j}{\partial t} + \Lambda^j\frac{\partial\Phi_x^j(y,t)}{\partial t}\right) = \sum_j \left(\varepsilon_x^j(t) + \sum_{s=1}^{m}\hat{T}_{x_s} + V(x,t)\right)(\Lambda^j(x,t)\Phi_x^j(y,t))$$

Defining the constant $C_j := \frac{-\hbar^2}{2m_{x_j}}$ we can note that:

$$\hat{T}_{x_j}(\Lambda^j(x,t)\Phi_x^j(y,t)) = C_j\frac{\partial^2}{\partial x_j^2} = \tag{39}$$

$$= C_j\left(\Phi_x^j(y,t)\frac{\partial^2}{\partial x_j^2} + \Lambda^j(x,t)\frac{\partial^2}{\partial x_j^2} + 2\frac{\partial}{\partial x_j}\Lambda^j(x,t)\frac{\partial}{\partial x_j}\Phi_x^j(y,t)\right))$$

$$= \Phi_x^j(y,t)\ \hat{T}_{x_j}\Lambda^j(x,t) + \Lambda^j(x,t)\ \hat{T}_{x_j}\Phi_x^j(y,t) + 2C_j\ \frac{\partial}{\partial x_j}\chi^j(x,t)\ \frac{\partial}{\partial x_j}\Phi_x^j(y,t))$$

Then we can multiply equation (38) by ${\Phi^k}^\dagger(y,t)$ and integrate both sides over all the domain for y to get applying the orthonormality condition $\int {\Phi^k}^\dagger(y,t)\Phi^j(y,t)dy = \delta_{kj}$:

$$i\hbar\frac{\partial}{\partial t}\Lambda^k(x,t) = \left(\varepsilon^k(x,t) + \sum_{s=1}^{m}\hat{T}_{x_s} + V(x,t)\right)\Lambda^k(x,t) + \sum_j\left\{W^{kj}(x,t) + \sum_{s=1}^{m}S_s^{kj}(x,t) + F_s^{kj}(x,t)\frac{\partial}{\partial x_s}\right\}\Lambda^j(x,t) \tag{40}$$

where we have defined the coupling terms between the transversal section eigenstates:

$$W^{kj}(x,t) = -i\hbar\int {\Phi^k}^\dagger(y,t)\frac{\partial\Phi_x^j(y,t)}{\partial t}dy \tag{41}$$

$$S_s^{kj}(x,t) = \int {\Phi^k}^\dagger(y,t)\hat{T}_{x_s}[\Phi_x^j(y,t)]dy \tag{42}$$

$$F_s^{kj}(x,t) = \int {\Phi^k}^\dagger(y,t)2C_s\frac{\partial}{\partial x_s}\Phi_x^j(y,t)dy \tag{43}$$

4.1 Adiabatic (or constant) coupling potential with y for x and time

If we have that the potential energy term entangling the degrees of freedom x and y, which we called $U(x,y,t)$, is very slowly time dependent (or constant in time) and very slowly x dependent, then the eigenstates of the transversal sections to x fulfil $\frac{\partial}{\partial x_s}\Phi_x^j(y,t) \simeq 0$ and $\frac{\partial}{\partial t}\Phi_x^j(y,t) \simeq 0$. This would yield $W^{kj}(x,t), S_s^{kj}(x,t), F_s^{kj}(x,t) \simeq 0$, which would leave equations (48) uncoupled as:

$$i\hbar\frac{\partial}{\partial t}\Lambda^k(x,t) = \left(\varepsilon^k(x,t) + \sum_{s=1}^{m}\hat{T}_{x_s} + V(x,t)\right)\Lambda^k(x,t) \tag{44}$$

Which is an m spatial dimension (mD) Schrödinger Equation for each of the eigenstates. This would mean that each coefficient $\Lambda^j(x,t)$ would preserve its norm $\int \chi(x,t)^{j\dagger}\chi^j(x,t)dx =: P^j(t)$ at all times due to the unitary time evolution of the Schrödinger Equation. This is exactly analogous to what happened when we expanded the wave-function in the time stationary energy eigenstates of the full hamiltonian.

We could now simply compute the initial coefficients $\Lambda^k(x,t_0)$ for a desired initial wavefunction by $\Lambda^k(x,t_0) = \int \Phi(x,t)^{k\dagger}\psi(x,y,t_0)dy$ and then compute mD SE-s for as many coefficients Λ^k, say J as necessary to achieve a certain norm tolerance $\sum_{j=0}^{J} P^j(t) \simeq 1$ and then simply ensemble them to have the N dimensional full wavefunction as $\psi(x,y,t) = \sum_j \Lambda^j(x,t)\Phi^j(y,t)$.

The fun point now is that we could now solve each of the mD SE-s (52) using precisely the same method described in this section! We could now choose a new subset $z = (x_1, ..., x_r)$ as main degrees of freedom and $w = (x_{r+1}, ..., x_m)$ as the transverse degrees, for which we will now compute the eigenstates using the decomposition of the effective Hamiltonian for the m degrees of freedom:

$$\hat{H}_{eff}(x,t) = \varepsilon^k(x,t) + \sum_{s=1}^{m}\hat{T}_{x_s} + V(x,t) = \sum_{s=r+1}^{m}\hat{T}_{x_s} + \tilde{U}(z,w,t) + \sum_{s=1}^{r}\hat{T}_{x_s} + V(\tilde{z},t)$$

And proceeding as explained.

4.2 Comments on General Potentials

For a general potential, the set of coupled linear partial differential equations (48) can be solved if we first compute the coupling integrals $W^{kj}(x,t), S_s^{kj}(x,t), F_s^{kj}(x,t)$ which have a complexity $O(n_y^{N-m})$[2]. Then the equations may be solved using a Cranck Nicolson scheme by LU decomposing sparse matrices of $O(Jn_x^m)$ rows and columns n_t times, where J is the number of coefficients in the expansion we consider to be important. Then the time evolution of the system, once we know the coupling terms and the eigenstates would require $O(Jn_t n_x^m)$.

If we did not know the eigenstates, we would need to compute them, which requires at least $O(Jd^{N-m})$ operations as we said in the previous section (with d the average number of non-zero elements per column in the Hamiltonian for the $m = N-1$ case).

This means that even without knowing the eigenstates a priori, we could achieve the solution of the full TDSE for a fixed n_t in a time $O(n_y^{N-m}) + O(n_x^m) = O(n_x^{max(m,N-m)})$ (where we consider $n_x = n_y$). This is minimized clearly if we chose $m = N/2$. In that case, as we argued in the conclusions of the previous section, we would square root the computation time for the TDSE from $O(n_x^N)$ to $O(n_x^{N/2}$, which is already a good thing, even if the many body problem is not surpassed[3]!

[2] n_y is the smallest number of spatial divisions we consider for the spatial axes in y. n_x is the same for x, while n_t is the number of time steps we consider.

[3] In fact, we can not expect to get rid of the exponential complexity if we do not make any approximation to the approach, so perhaps it is as good as we could get for an exact solution!

4.3 The Spectrum of possibilities of the algorithm

It is at this point clear that the present algorithm is a generalization of the examples given in the first two sections. In particular, if we choose $m = 0$, we recover the expansion of the wavefunction in the eigenstates of the full hamiltonian, if $m = 1$, we get the expansion of the full wavefunction in the transversal eigenstates and if $m = N$ we recover the full Schrödinger Equation. In the last case we have $O(n_x^N)$ on the equation system side while in the first we have $O(n_x^N)$ on the eigenstate obtention side. For intermediate m, we transfer workload from computing the system of differential equations to computing the eigenstate problem. The balance is optimal when we set $m = N/2$, where the complexity is square-rooted.

Therefore, this algorithm might be specially useful to reduce the complexity of the time evolution if we know the eigenstates of the sections analytically for any of the $m < N$, as this would immediately erase the eigenstate and overlap integral numerical obtention from the scheme and we would be left with the resolution of the coupled Schrödinger like equation system of $O(n_x^m)$.

Now, in the eyes of the "inception" like approach we suggested two subsections ago, it is a natural question whether we can iteratively apply the algorithm for the simplest case in order to solve it everything with rather a series of 1D Schrödinger like Equations and one 1D eigenvalue problem or a series of 1D eigenvalue problems and a 1D Schrödinger like Equation. If yes, any of those two approaches would have a linear complexity in N. Of course it is not possible to do it for the general non-adiabatic case. But it turns out it is indeed possible for the adiabatic case! Let us try the $m = N - 1$ case!

5 Expanding the Wavefunction in 1D Eigenstates

If we apply the generalized algorithm (48) for the case in which $x = (x_1, ..., x_{N-1})$ and $y = x_N$, we will have that :

$$\hat{H}(x,y,t) = \sum_{j=1}^{N} \hat{T}_{x_j} + G(x,y,t) = \hat{T}_{x_N} + U(x,y,t) + \sum_{j=1}^{N-1} \hat{T}_{x_j} + V(x,t) = \hat{H}_x(y,t) + \sum_{j=1}^{N-1} \hat{T}_{x_j} + V(x,t) \quad (45)$$

We then define the set of eigenstates $\{\Phi_x^j(y,t)\}_j$ with eigenvalues $\{\varepsilon_x(t)\}_j$ to be the solution to:

$$\hat{H}_x(y,t)\Phi_x^j(y,t) = \varepsilon_x^j(t)\Phi_x^j(y,t) \quad (46)$$

As we know that the hermiticity of the operator $\hat{H}_x(y,t)$ implies its eigenstates form a complete basis of the space y for all times, we could write any wavefunction as a linear combination of them for each x:

$$\Psi(x,y,t) = \sum_j \Lambda^j(x,t)\Phi_x^j(y,t) \quad (47)$$

with $\Lambda^j(x,t) := \int {\Phi_x^j}^\dagger(y,t)\Psi(x,y,t)dy$ the projection coefficients.

This would leave the equation for the coefficients (48) as:

$$i\hbar\frac{\partial}{\partial t}\Lambda^k(x,t) = \left(\varepsilon^k(x,t) + \sum_{s=1}^{N-1}\hat{T}_{x_s} + V(x,t)\right)\Lambda^k(x,t) + \sum_j \left\{W^{kj}(x,t) + \sum_{s=1}^{N-1} S_s^{kj}(x,t) + F_s^{kj}(x,t)\frac{\partial}{\partial x_s}\right\}\Lambda^j(x,t) \quad (48)$$

where we have defined the coupling terms between the transversal section eigenstates:

$$W^{kj}(x,t) = -i\hbar\int {\Phi^k}^\dagger(y,t)\frac{\partial\Phi_x^j(y,t)}{\partial t}dy \quad (49)$$

$$S_s^{kj}(x,t) = \int \Phi^{k\ \dagger}(y,t)\hat{T}_{x_s}[\Phi_x^j(y,t)]dy \tag{50}$$

$$F_s^{kj}(x,t) = \int \Phi^{k\ \dagger}(y,t)2C_s\frac{\partial}{\partial x_s}\Phi_x^j(y,t)dy \tag{51}$$

5.1 Adiabatic (or constant) coupling potential with y for x and t

If we have that the potential energy term entangling the degrees of freedom x with y, which we called $U(x,y,t)$, is very slowly time dependent (or constant in time) and very slowly x dependent, then the eigenstates of the transversal sections to x fulfil $\frac{\partial}{\partial x_s}\Phi_x^j(y,t) \simeq 0$ and $\frac{\partial}{\partial t}\Phi_x^j(y,t) \simeq 0$. This would yield $W^{kj}(x,t), S_s^{kj}(x,t), F_s^{kj}(x,t) \simeq 0$, which would leave equations (48) uncoupled as:

$$i\hbar\frac{\partial}{\partial t}\Lambda^k(x,t) = \left(\varepsilon^k(x,t) + \sum_{s=1}^{N-1}\hat{T}_{x_s} + V(x,t)\right)\Lambda^k(x,t) \tag{52}$$

Which is an $N-1$ spatial dimension (N-1)D Schrödinger Equation for each of the eigenstates. As they are uncoupled Schrödinger Equations, each of them could now be solved in parallel using the same approach, now defining $x^{(2)} = (x_1, ..., x_{N-2})$ and $y^{(2)} = x_{N-1}$. We could obtain the transversal sections for the hamiltonian including the potential that couples $x^{(2)}$ to $y^{(2)}$:

$$\varepsilon^k(x,t)+\sum_{s=1}^{N-1}\hat{T}_{x_s}+V(x,t) = U^{(2)}(x^{(2)},y^{(2)},t)+\hat{T}_{x_{N-1}}+\sum_{s=1}^{N-1}\hat{T}_{x_s}+V^{(2)}(x^{(2)},t) = \hat{H}_{x^{(2)}}+\sum_{s=1}^{N-1}\hat{T}_{x_s}+V^{(2)}(x^{(2)},t) \tag{53}$$

Then defining the 1D eigenstate problem to get the set $\{\Phi_{x^2}^{j2}(y^{(2)},t)\}_j$ with eigenvalues $\{\varepsilon_{x^2}^{j2}(t)\}_j$:

$$\hat{H}_{x^{(2)}}\Phi_{x^2}^{j2}(y^{(2)},t) = \varepsilon_{x^2}^{j2}(t)\Phi_{x^2}^{j2}(y^{(2)},t) \tag{54}$$

We would have that there exist some coefficients $\Lambda^{j2}(x^{(2)},t)$ such that:

$$\Lambda(x^{(2)},y^{(2)},t) = \sum_j \Lambda^{j2}(x^{(2)},t)\Phi_{x^2}^{j2}(y^{(2)},t) \tag{55}$$

which would follow the dynamical equation:

$$i\hbar\frac{\partial}{\partial t}\Lambda^{k2}(x^{(2)},t) = \left(\varepsilon^{j2}(x^{(2)},t) + \sum_{s=1}^{N-2}\hat{T}_{x_s} + V^{(2)}(x^{(2)},t)\right)\Lambda^{k2}(x^{(2)},t)+\sum_j\left\{W^{kj2}(x^{(2)},t) + \sum_{s=1}^{N-1}S_s^{kj2}(x^{(2)},t) + F_s^{kj} \right. \tag{56}$$

Which again if we had that the coupling potential $U^{(2)}(x^{(2)},y^{(2)},t)$ was adiabatic in $x^{(2)}$ and t, $W^{kj2}(x^{(2)},t), S_s^{kj2}(x^{(2)},t), F_s^{kj2}(x^{(2)},t) \simeq 0$ would mean that the coefficients would obey a Schrödinger Equation:

$$i\hbar\frac{\partial}{\partial t}\Lambda^{k2}(x^{(2)},t) = \left(\varepsilon^{j2}(x^{(2)},t) + \sum_{s=1}^{N-2}\hat{T}_{x_s} + V^{(2)}(x^{(2)},t)\right)\Lambda^{k2}(x^{(2)},t) \tag{57}$$

Where we could repeat the process of "marginalising" one spatial variable iteratively N times, until we would arrive to a 1D Schrödinger equation set for the coefficients $\Lambda^{kN}(x^{(N)},t)$. With them and each set of 1D parametrized eigenstate we would then be able to rebuild the whole Schrödinger Equation.

The fun point of such a procedure would be that computing the eigenstates of 1D Hamiltonians has a complexity $O(Jd)$ so doing the process for each of the N stages of inception would require $O(NJd)$ operations, together with the overlap integrals to get the initial coefficients, which would now be 1D integrals of complexity $O(n_y)$ and the resolution of the last J 1d Schrödinger like equations (where we could compute the coupling terms without neglecting them), that would take $O(Jn_x)$ operations: overall the complexity would be $O(NJn_x)$, which scales linearly with dimensions! Well, that is not

completely honest... It will be true as long as parametrically computing the eigenstates can be done in one step. That is, if in order to compute the eigenstates of the section for $(x_1, x_2, ...x_m)$ requires computing the eigenstates for each possible value of $(x_1, ..., x_m)$ in a given grid of size n_x^m, then computing the eigenstates at the first inception step would require $O(Jdn_x^{N-1})$ operations, which still scales exponentially in space! But we were pretty close this time!

In fact, if it really was as simple to compute the section eigenstates with a parametric dependence, at least as simple as (or lienarly more complex than) computing them for a single section, then we could achieve a linear algorithm inspired by this inception as shown in the following section. The good point about the one shown in the following section is that we will not require to approximate the adiabaticity and still we will convert the Schrödinger Equation into a set of 1D eigenstate problems and 1D Schrödinger Equations or ordinary differential equations.

6 Expanding the Wavefunction in 1D Section Eigenstates 2.0

Following the idea seeded in the previous section of only needing to solve 1D eigenstate problems, we could try the following: given we can iteratively isolate the interaction Hamiltonians of one degree of freedom with the rest:

$$\hat{H}(x_1, ..., x_N) = \sum_{j=1}^{N} \hat{T}_{x_j} + V^{(0)}(x_1, ..., x_N, t) = \tag{58}$$

$$= \hat{T}_{x_N} + U^{(1)}(x_1, ..., x_N, t) + \sum_{j=1}^{N-1} \hat{T}_{x_j} + V^{(1)}(x_1, ..., x_{N-1}, t) =$$

$$= \hat{H}_{x_1,...,x_{N-1}}(x_N, t) + \sum_{j=1}^{N-1} \hat{T}_{x_j} + V^{(1)}(x_1, ..., x_{N-1}, t) =$$

$$= \hat{H}_{x_1,...,x_{N-1}}(x_N, t) + \hat{T}_{x_{N-1}} + U^{(2)}(x_1, ..., x_{N-1}, t) + \sum_{j=1}^{N-2} \hat{T}_{x_j} + V^{(2)}(x_1, ..., x_{N-2}, t) =$$

$$= \hat{H}_{x_1,...,x_{N-1}}(x_N, t) + \hat{H}_{x_1,...,x_{N-2}}(x_{N-1}, t) + \sum_{j=1}^{N-1} \hat{T}_{x_j} + V^{(1)}(x_1, ..., x_{N-1}, t) =$$

$$\cdots$$

$$= \hat{H}_{x_1,...,x_{N-1}}(x_N, t) + \cdots + \hat{H}_{x_1,x_2}(x_3, t) + \hat{T}_{x_2} + U^{(N-2)}(x_1, x_2, t) + \hat{T}_{x_1} + V^{(N-2)}(x_1, t) =$$

$$\hat{H}_{x_1,...,x_{N-1}}(x_N, t) + \cdots + \hat{H}_{x_1}(x_2, t) + \hat{T}_{x_1} + V^{(N-2)}(x_1, t)$$

We arrive at the decomposition of the full hamiltonian:

$$\hat{H}(x_1, ..., x_N) = \hat{H}_{x_1,...,x_{N-1}}(x_N, t) + \cdots + \hat{H}_{x_1}(x_2, t) + \hat{H}(x_1, t) \tag{59}$$

Where we see that $\hat{H}_{x_1,...,x_m}(x_{m+1})$ is the coupling hamiltonian between the degree of freedom x_{m+1} and the first m.

Then, we could find the parametric 1D eigenstates for each $m \in \{1, ...N-1\}$ $\{\Phi^j_{x_1,...x_m}(x_{m+1}, t)\}_j$ with eigenvalues $\{\varepsilon^j_{x_1,...x_m}(t)\}_j$ to be the solutions of:

$$\hat{H}_{x_1,...,x_m}(x_{m+1}, t)\Phi^j_{x_1,...x_m}(x_{m+1}, t) = \varepsilon^j_{x_1,...x_m}(t)\Phi^j_{x_1,...x_m}(x_{m+1}, t) \tag{60}$$

6.1 Variant 1

We could then expand the wavefuntion in those eigenstates iteratively to get:

$$\psi(x_1,...,x_N,t) = \sum_{j_N,...,j_2} \chi^{j_N,...,j_2}(x_1,t)\Phi^{j_2}_{x_1}(x_2,t)\Phi^{j_3}_{x_1,x_2}(x_3,t)\Phi^{j_4}_{x_1,x_2,x_3}(x_4,t)\cdots\Phi^{j_N}_{x_1,...,x_{N-1}}(x_N,t) \quad (61)$$

Introducing this ansatz into the TDSE, we can get the time evolution of the coefficients $\chi^{j_N,...,j_2}(x_1,t)$:

$$i\hbar\frac{\partial}{\partial t}\psi(x_1,...,x_N,t) = \hat{H}(x_1,...,x_N,t)\psi(x_1,...,x_N,t) \quad (62)$$

$$i\hbar\sum_{j_N,...,j_2}\Phi^{j_2}_{x_1}(x_2)\cdots\Phi^{j_N}_{x_1,...,x_{N-1}}(x_N)\frac{\partial}{\partial t}\chi^{j_N,...,j_2}(x_1,t)+\chi^{j_N,...,j_2}(x_1,t)\frac{\partial}{\partial t}\Big(\Phi^{j_2}_{x_1}(x_2)\cdots\Phi^{j_N}_{x_1,...,x_{N-1}}(x_N)\Big) =$$

$$= \Big(\hat{H}_{x_1,...,x_{N-1}}(x_N,t)+\cdots+\hat{H}_{x_1}(x_2,t)+\hat{H}(x_1,t)\Big)\sum_{j_N,...,j_2}\chi^{j_N,...,j_2}(x_1,t)\Phi^{j_2}_{x_1}(x_2)\cdots\Phi^{j_N}_{x_1,...,x_{N-1}}(x_N) =$$

$$= \sum_{j_N,...,j_2}\Big(\chi^{j_N,...,j_2}(x_1,t)\Phi^{j_2}_{x_1}(x_2)\cdots\Phi^{j_{N-1}}_{x_1,...,x_{N-2}}(x_{N-1})\hat{H}_{x_1,...,x_{N-1}}(x_N,t)\Phi^{j_N}_{x_1,...,x_{N-1}}(x_N)+\cdots$$

$$+\chi^{j_N,...,j_2}(x_1,t)\hat{H}(x_1,t)\Phi^{j_2}_{x_1}(x_2)\cdots\Phi^{j_{N-1}}_{x_1,...,x_{N-2}}(x_{N-1})+\hat{H}(x_1,t)\Phi^{j_2}_{x_1}(x_2)\cdots\Phi^{j_{N-1}}_{x_1,...,x_{N-2}}(x_{N-1})\chi^{j_N,...,j_2}(x_1,t)\Big)$$

6.2 Variant 2

6.3 Generalization

7 What if we used any other (known) Orthonormal Basis for the Sections

We have clearly seen that there were three bottlenecks with which we could play and swing from side to side were: the obtention of more or less complicated eigenstate problems, the resolution of more or less complicated systems of partial differential equations and the computations of more or less complicated integrals of variations of the eigenstates. We found a method to transfer all the complexity we wanted into the eigenstate problem from the differential equations. Then the obvious idea here is, how can we avoid needing to compute the eigenstates, where all the exponential problem may be placed? Would we have enough with using a general orthonormal basis of functions? If yes, then we could have solved the millenia problem. The answer most likely will be not, else it would have already been found. Still, lets see what we can get.

7.1 If we knew an orthonormal basis for N

This is the analogous case of using the full hamiltonian eigenstates. Representing by $x = (x_1, ..., x_N)$, if we knew a set of orthonormal functions $\{f^j(x,t)\}_j$ spanning the whole Hilbert space of the system, then by the completeness of the basis we know that there should exist some coefficients $c_j(t) \in \mathbb{C}$ such that any arbitrary wavefunction should be expansible as a linear combination at any time (note that the basis functions need not be time dependent, but for the sake of generality we will consider so):

$$\psi(x,y,t) = \sum_j c_j(t) f^j(x,t) \tag{63}$$

Introducing it into the TDSE, we would obtain the dynamical equations for the coefficients $c_j(t)$:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \Rightarrow i\hbar \sum_k \frac{\partial (c_k(t) f^k(x,t))}{\partial t} = \sum_k \left(\sum_{j=1}^{N} \hat{T}_{x_j} + U(x,t) \right) (c_k(t) f^k(x,t)) \tag{64}$$

Using the orthonormality condition $\int f^{j\dagger}(x,t) f^k(x,t) dx = \delta_{j,k}$ and wrapping stuff up:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} c_j(t) = \sum_k \Big(W^{j,k}(t) + S_s^{j,k}(t) + D^{j,k}(t) \Big) c_k(t) \tag{65}$$

with:

$$W^{j,k}(t) := \int f^{j\dagger}(x,t) \frac{\partial f^k(x,t)}{\partial t} dx \tag{66}$$

$$S_s^{j,k}(t) := \int f^{j\dagger}(x,t) T_{x_j}[f^k(x,t)] dx \tag{67}$$

$$D^{j,k}(t) := \int f^{j\dagger}(x,t) U(x,t) f^k(x,t) dx \tag{68}$$

Where as we already knew the basis functions, presumably in their analytic shape, we would be left with a computation of the coupling integrals (which could perhaps be evaluated symbolically) and the resolution of the linear coupled ordinary differential equation for the coefficients $c_j(t)$.

If we only knew the basis functions numerically then the integrals would have a complexity $O(n_x^N)$ which scales exponentially. However, if we were able to have the coupling terms computed symbolically, then we would only need to simulate the system for the coefficients. This has a complexity of about $O(Jn_t)$, meaning the problem would be at most linearly scaling with dimensions! Now all the complexity has been transferred into computing integrals instead of eigenstates. In fact, because the coupling terms $S_s^{j,k}, W^{j,k}(t)$ are system independent they could be pre-computed for any N dimensional system. Only the term $D^{j,k}(t)$ which does depend on the particular system would need to be computed!

On the bad side, using generic orthonormal functions we would have lost the ability to approximate the coupling terms due to the adiabaticity of the potential.

7.2 If we knew an orthonormal basis for $N-m$

We will build here the analogue of the generalized method (48). Using the notation $x=(x_1,..,x_m)$ and $y=(x_{m+1},...,x_N)$, we will assume we know an arbitrary orthonormal set of functions $\{f^j(y,t)\}_j$ spanning the space y. Once again, they need not depend on time, but for generality we will consider so (the difference will be that the coupling terms will simplify. For the completeness of the basis for the subspace, we could find coefficients $\Lambda^j(x,t)$ such that:

$$\psi(x,y,t)=\sum_j \Lambda^j(x,t)f^j(y,t) \tag{69}$$

Note that unlike the transversal section eigenstates, these do not depend on x! (SHOULD THEY?)

Then introducing this ansatz into the full TDSE, we can get the dynamic equations for the coefficients $\Lambda^j(x,t)$, by using again the orthonormality condition $\int f^{k\dagger}(y,t)f^k(y,t)dy=1$ we can get:

$$i\hbar\frac{\partial}{\partial t}\Lambda^j(x,t)=\sum_{s=1}^{m}\hat{T}_m\Lambda^j(x,t)+\sum_k\left(W^{jk}(t)+\sum_{r=m}^{N}S_r^{jk}(t)+D^{jk}(x,t)\right)\Lambda^k(x,t) \tag{70}$$

with:

$$W^{jk}(t):=\int f^{j\dagger}(y,t)\frac{\partial f^k(y,t)}{\partial t}dy \tag{71}$$

$$S_r^{jk}(t):=\int f^{j\dagger}(y,t)\hat{T}_{x_s}[f^k(y,t)]dy \tag{72}$$

$$W^{jk}(x,t):=\int f^{j\dagger}(y,t)U(x,y,t)f^k(y,t)dy \tag{73}$$

Again, we achieve a similar equation, where the only task we would need would be to compute the coupling integrals and then evolving the coupled linear system of equations for the coefficients $\Lambda^j(x,t)$. The integrals would require a time $O(n_y^{N-m})$, while the coupled system would require $O(Jn_x^m)$, resulting in a complexity $O(n_x^{max(m,N-m)})$. The fun point is that if we knew analytically the orthonormal functions, we might be able to compute the integrals symbolically, which would allow us to safe the numerical integration and the complexity would be left $O(n_x^m)$, where if we fix m, the problem will at most be linearly increasing in complexity with dimensions N!

Once again though, we will have lost the possibility to study the adiabaticity and approximate the coupling terms in consequence.

7.3 If we only knew an orthonormal basis for each of the dimensions independently

Finally, in the spirit of the previous developments, if we knew an orthonormal set of functions spanning each of the spatial axes $\{f_r^j(x_r,t)\}_j$

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https://github.com/Oiangu9/The_Quantum_Many_Body_Problem_-Bachellors_Thesis-/blob/master/TheQuantumManyBodyProblem__BachelorsThesis_XabierOyangurenAsua.pdf

[5] Albareda G, Kelly A, Rubio A. *Nonadiabatic quantum dynamics without potential energy surfaces.* Phys Rev Materials. 2019; 3: 023803.

[6] All the animations employed for the analysis of Section 3.2 can be found in the following link: https://drive.google.com/drive/folders/1vnNDZrIYDlAhd-kVmmnVJgXmcdE2gxAV?usp=sharing