

Separated quantum dynamics

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An approximation to the time-dependent Schrödinger equation for n distinguishable particles is proposed, for which the computational solution is an $O(n^2)$ problem. The Hamiltonian of the system is assumed to be a sum of single-particle operators and of pair-operators. The proposed modification of Hamiltonian dynamics is given by a set of n one-particle Schrödinger equations, in which the potential felt by each of the particles gets an additive contribution from each of the other particles. This contribution depends on the contributing particle only through the probability density associated with its one-particle wave function. These equations are similar to time-dependent Hartree-Fock equations, when the latter are formulated for wave functions instead of density operators. The difference reflects the fact that Hartree-Fock assumes identical particles, whereas the present work is about distinguishable particles. It is shown that the dynamical evolution of these one-particle wave functions changes neither the norm of these functions, nor the expectation value of the Hamiltonian with respect to the product of the one-particle wave functions. For the time step evolution operator of this modified dynamics, a simple definition is given in terms of the Hamiltonian evolution operators of the whole system and its subsystems. In a computational model of a three-particle system, the time-discrete trajectory starting from a product state was computed for the Schrödinger equation and its approximation. Very good agreement of the expectation values of particle positions was found over the whole course of the simulation. For the correlations between two or three particle positions, the agreement was found to decrease considerably with time.

1 Introduction

As is well known, non-relativistic quantum dynamics of many-particle systems, when taken literally, becomes rather intractable for large particle numbers. A direct computational approach requires exponentially growing computational resources with growing number of particles. On the other hand, the states which would require the highest rate

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of computational operations in an adaptive time evolution algorithm ¹ — linear combinations of complex many-particle states — seem to be reluctant to do this work in nature. They show a tendency to simplify themselves via decoherence — a phenomenon that cannot be understood as a consequence of quantum dynamics alone. If, by what mechanism ever, the execution of quantum dynamics would lack perfect precision (e.g. [10]), one would expect decoherence to be the consequence.

That the information content of the generic n -particle state grows exponentially with n , may be an artifact of the non-relativistic approximation. According to the view of non-relativistic physics, the physical situation prevailing at some space time point depends on the physical situation at arbitrarily many space-like separated points. This allows a non-relativistic n -particle wave function to express unthinkably complex physical situations, which neither are likely to result from state preparation in experiments, nor by dynamical evolution from experimentally accessible states.

In a theory which takes relativistic causality properly into account, an n -particle wave function is by no means a natural construct (e.g. [3] Introduction) since a state description is not complete unless it includes the interaction-mediating quanta. Eliminating the interaction quanta and replacing them by potential-like interaction operators works for two-particle bound states in Breit's equation (e.g. [3] Chapter IX). If one tries to define Breit-type Hamiltonians for n -particle systems, the physically indispensable requirement of macro-causality enforces a rather complicated structure, [4] and literature cited therein, of such *direct interaction theories*. This is one hint more that n -particle wave functions fail to be suitable state descriptors for interacting particles in a world that satisfies relativistic causality.

Despite these reservations, the present paper adopts non-relativistic many-particle quantum mechanics as a basis of argumentation. It develops a dynamical approximation in which interaction between subsystems is profoundly simplified compared to an exact quantum mechanical treatment, and therefore the states under consideration have a simple structure. So we escape the 'vastness of the Hilbert space' ² at a price, however, that may be too high for most applications related to quantum information processing: There are no entangled states in this approximation.

The rest of this section introduces the quantum system and its approximative version for which Section 3 develops a computational model. Further, it describes for the present system the results that will be formulated and proved in Section 2 for more general systems.

Let us consider an elementary quantum mechanical systems that is capable of describing an experiment: It is given by a bound particle acted on by an external field which the experimenter is able to control. This situation is described by the following time-dependent Schrödinger equation:

$$i \hbar \dot{\Psi}(x, t) = -\frac{\hbar^2}{2m} (\Delta \Psi)(x, t) + (V(x) + qg(x)) \Psi(x, t). \quad (1)$$

¹one which adjusts its space-time grid dynamically to computational needs

²[7], p. 2

where the potential V has a sufficiently deep minimum at some position $x = x_0$ to ensure the existence of bound states. In addition, V is assumed to be sufficiently localized that there is a neighborhood Ω of x_0 outside of which all bound state wave functions effectively vanish. Let us refer to Ω as the *biotope* of the bound particle in accordance with the common usage that functions ‘live’ on some subset of their domain (e.g. on their carrier). Let us assume that there are three experimental procedures: One that prepares the particle in the ground state ψ_0 determined by (1) for $q = 0$, the second one that applies field g over a known span of time, and the third one that measures the position of the particle at a chosen point in time t . Then equation (1) determines the statistical distribution of the particle position as a function of g , and of the time elapsed since the preparation of the ground state. It thus makes predictions concerning the statistics of experiments that can be done by the means just described. If one has more choices to prepare initial states and to make observations concerning particle states, there are more experiments for which equation (1) predicts the outcome, and which in this sense are *pertinent* to this equation, and to the physical system to which this equation refers.

Let us consider some concrete setup of an experiment pertinent to (1). Then it is a self-suggesting Gedankenexperiment, and, as Section 3 will show, also a feasible computer experiment, to build a copy of this setup such that the biotopes Ω_1 and Ω_2 associated with these two experiments are disjoint, but separated only by a fraction, e.g. one half, of their diameter. For real experiments it would be natural to implement these two setups as distinguishable substructures of a single experimental setup. This combined setup then is an experiment pertinent to some system and to some equation. If the two experiments don’t influence each other, despite the small separation, quantum theory suggests the following candidate for this equation:

$$\begin{aligned} i\hbar\dot{\Psi}(x_1, x_2, t) = & -\frac{\hbar^2}{2m_1}(\Delta_1\Psi)(x_1, x_2, t) + (V_1(x_1) + q_1g(x_1))\Psi(x_1, x_2, t) \\ & -\frac{\hbar^2}{2m_2}(\Delta_2\Psi)(x_1, x_2, t) + (V_2(x_2) + q_2g(x_2))\Psi(x_1, x_2, t) . \end{aligned} \quad (2)$$

Interaction between the two bound particles, can be represented by an interaction potential V_{12} :

$$\begin{aligned} i\hbar\dot{\Psi}(x_1, x_2, t) = & -\frac{\hbar^2}{2m_1}(\Delta_1\Psi)(x_1, x_2, t) + (V_1(x_1) + q_1g(x_1))\Psi(x_1, x_2, t) \\ & -\frac{\hbar^2}{2m_2}(\Delta_2\Psi)(x_1, x_2, t) + (V_2(x_2) + q_2g(x_2))\Psi(x_1, x_2, t) \\ & + V_{12}(x_1, x_2)\Psi(x_1, x_2, t) . \end{aligned} \quad (3)$$

A sufficiently general case for the present introductory discussion is

$$\begin{aligned} V_1(x_1) &= f_1(|x_1 - x_1^0|) \\ V_2(x_2) &= f_2(|x_2 - x_2^0|) \\ V_{12}(x_1, x_2) &= q_1q_2f(|x_1 - x_2|) \end{aligned} \quad (4)$$

with functions f_1, f_2, f of type $\mathbb{R}_+ \rightarrow \mathbb{R}$.

Here is a good place to discuss the particularities which arise if particles 1 and 2 belong to the same species, so that we are dealing with ‘identical particles’. In this case we have $q_1 = q_2$ and $m_1 = m_2$, and Pauli’s principle asks for symmetrical wave or anti-symmetrical wave functions. Since our particles were introduced as spin-less, only the first of these possibilities applies directly. It is, however, convenient to consider both cases in parallel.

A physically correct ψ should thus be an eigenstate of the unitary, idempotent, and Hermitean operator U defined by

$$(U\psi)(x_1, x_2) := \psi(x_2, x_1). \quad (5)$$

Of course, the time-evolution has to conserve this property. This is, however, not the case with equations (3),(4). Fortunately, a slight modification corrects this:

$$\begin{aligned} V_1(x_1) &= f_1(|x_1 - x_1^0|) + f_2(|x_1 - x_2^0|) \\ V_2(x_2) &= f_1(|x_2 - x_1^0|) + f_2(|x_2 - x_2^0|). \end{aligned} \quad (6)$$

Then, there is a common function $f_c := f_1(|\bullet - x_1^0|) + f_2(|\bullet - x_2^0|)$ which allows writing $V_1(x_1) = f_c(x_1)$, $V_2(x_2) = f_c(x_2)$. This implies that the two binding potentials for the two particles enter as a single external field which influences the system as a whole, but is different from zero only on the disjoint sets Ω_1 and Ω_2 . With this definition of V_1 and V_2 the Hamiltonian belonging to (3) commutes with U , and thus also with the projectors $P_{\text{boson}} = (1 + U)/2$ and $P_{\text{fermion}} = (1 - U)/2$. Therefore, symmetrical wave functions remain symmetrical under time evolution, and anti-symmetrical wave functions behave correspondingly. Pauli’s principle is satisfied if it is satisfied for the initial state. Actually, more is true: The dynamical evolution of an initial product state $\psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2)$ determines the evolution of the initial bosonic state $P_{\text{boson}}\psi / \|P_{\text{boson}}\psi\|$, and of the initial fermionic state $P_{\text{fermion}}\psi / \|P_{\text{fermion}}\psi\|$, simply by applying the respective projectors to the state that evolved from ψ . If the particles respect their biotopes, the function ψ_1 vanishes outside Ω_1 and ψ_2 vanishes outside Ω_2 . Then ψ , as defined above, satisfies

$$\psi(x_1, x_2) \neq 0 \Rightarrow (x_1 \in \Omega_1 \vee x_2 \in \Omega_2) \quad (7)$$

which is a condition that makes sense also if ψ is not a product function. For strong binding potentials and weak interaction it is plausible that also in the course of dynamical evolution this condition will hold approximately. To enforce the strict conservation of (7) one may impose reflecting boundary conditions at the surface of the biotopes. Then the two definitions (4) and (6) of binding potentials strictly agree for all states that arise by time evolution from ψ . After having seen that in the present framework dynamics for identical particles can be obtained from the dynamics of distinguishable particles by simple means, the rest of the article will deal with the distinguishable case only, with exception of a remark on the central equation (9).

The situation discussed so far naturally extends to more particles: a third particle brings an equilibrium position x_3^0 and a binding potential f_3 wheres its interaction with

the other particles brings only a new coupling parameter q_3 which then describes interaction with the other particles via the same function f . The three particles then obey the following time-dependent Schrödinger equation:

$$\begin{aligned}
i\hbar\dot{\Psi}(x_1, x_2, x_3, t) = & \\
& \left(-\frac{\hbar^2}{2m_1}\Delta_1 + f_1(|x_1 - x_1^0|) + q_1 g(x_1) \right) \Psi(x_1, x_2, x_3, t) \\
& + \left(-\frac{\hbar^2}{2m_2}\Delta_2 + f_2(|x_2 - x_2^0|) + q_2 g(x_2) \right) \Psi(x_1, x_2, x_3, t) \\
& + \left(-\frac{\hbar^2}{2m_3}\Delta_3 + f_3(|x_3 - x_3^0|) + q_3 g(x_3) \right) \Psi(x_1, x_2, x_3, t) \\
& + (q_1 q_2 f(|x_1 - x_2|) + q_1 q_3 f(|x_1 - x_3|) + q_2 q_3 f(|x_2 - x_3|)) \Psi(x_1, x_2, x_3, t) \\
= & (H\Psi)(x_1, x_2, x_3, t).
\end{aligned} \tag{8}$$

In Section 2 we will include general pair interaction operators which then enable spin-dependent interaction. If experiments pertinent to the individual systems led us to ascribe the wave functions $\psi_1(x_1, t)$ ³, $\psi_2(x_2, t)$, $\psi_3(x_3, t)$ to the individual particles, the new combined system gets ascribed the wave function $\Psi(x_1, x_2, x_3, t) := \psi_1(x_1, t) \psi_2(x_2, t) \psi_3(x_3, t)$. When, however, this expression taken at some fixed time t_0 is taken as initial values for the differential equation (8), it will develop (unless all charges q_i are zero) into a state which has no longer a factorizing wave function and thus leaves us ignorant about the time evolution of the wave functions of the individual particles. Of course, if the influence from adjacent particles is to be taken into account, the concept of a single particle wave function is questionable. The usual procedure is to treat each particle as an open system, the state of which may be not pure. These impure single-particle states (density operators) can be obtained from an exact wave function of the whole system by 'tracing out' the neighboring particles. If the wave function of the whole system is a product function at time t_0 , the density operators of the individual particles start as pure states and evolve into less and less pure ones over the time.

Thus the concept of a wave function of an individual particle would only be a temporary one and even the slightest interaction between particles as taken into account in (8) would, in the course of time, invalidate the single particle theory (1). The present work tries to show that this is too pessimistic a view and that there is a natural and rather accurate way of describing the system state still by three one-particle wave functions $\psi_1(x_1, t)$, $\psi_2(x_2, t)$, $\psi_3(x_3, t)$ the time-dependence of which reflects also interaction of the particles via the potentials taken into account in (8). This time-dependence has to be

³ consider this an abbreviation of $x_1 \mapsto \psi_1(x_1, t)$ to correctly denote what is called *function* here; another consistent reading is to infer from the context that x_1 denotes not a *constant* ('arbitrary but fixed' such as t) but a *variable* (with a range implied by the context).

defined by what will be referred to as *separated dynamics*:

$$\begin{aligned}
i\hbar\dot{\Psi}_1(x_1,t) &= -\frac{\hbar^2}{2m_1}(\Delta\Psi_1)(x_1,t) + f_1(|x_1-x_1^0|)\Psi_1(x_1,t) \\
&\quad + q_1g(x_1)\Psi_1(x_1,t) \\
&\quad + q_1q_2\int dx_2|\Psi_2(x_2,t)|^2f(|x_2-x_1|)\Psi_1(x_1,t) \\
&\quad + q_1q_3\int dx_3|\Psi_3(x_3,t)|^2f(|x_3-x_1|)\Psi_1(x_1,t), \\
i\hbar\dot{\Psi}_2(x_2,t) &= -\frac{\hbar^2}{2m_2}(\Delta\Psi_2)(x_2,t) + f_2(|x_2-x_2^0|)\Psi_2(x_2,t) \\
&\quad + q_2g(x_2)\Psi_2(x_2,t) \\
&\quad + q_2q_3\int dx_3|\Psi_3(x_3,t)|^2f(|x_3-x_2|)\Psi_2(x_2,t) \\
&\quad + q_2q_1\int dx_1|\Psi_1(x_1,t)|^2f(|x_1-x_2|)\Psi_2(x_2,t), \\
i\hbar\dot{\Psi}_3(x_3,t) &= -\frac{\hbar^2}{2m_3}(\Delta\Psi_3)(x_3,t) + f_3(|x_3-x_3^0|)\Psi_3(x_3,t) \\
&\quad + q_3g(x_3)\Psi_3(x_3,t) \\
&\quad + q_3q_1\int dx_1|\Psi_1(x_1,t)|^2f(|x_1-x_3|)\Psi_3(x_3,t) \\
&\quad + q_3q_2\int dx_2|\Psi_2(x_2,t)|^2f(|x_2-x_3|)\Psi_3(x_3,t).
\end{aligned} \tag{9}$$

This is a set of three one-particle Schrödinger equations in which each particle feels a potential-like influence from all other particles. The basic feature of this influence is, that it is independent of the phase of the influencing wave function (only $|\Psi_2|$ and $|\Psi_3|$ appears in the equation for Ψ_1). More generally, the influence gives rise to expressions that are non-linear in the influencing wave functions and linear in the influenced wave function.

For identical particles which are not spatially separated, similar equations have been derived by Dirac [1] by transforming the time-independent Hartree-Fock equations into dynamical equations. These are, therefore, usually referred to as time-dependent Hartree-Fock equations (TDHF). Their derivation is usually based on a variation principle, e.g. [2]. A form of these equations, which can be most directly compared with (9) can be found as equation (32) in [5]. There the particles are assumed to be fermions with statistics taken into account. If the single fermion wave functions ('orbitals') are assumed to live in disjoint parts of space (a situation which is not considered in [5] and which is alien to the intent of that work), then equation [5],(32) coincides with (9) — up to a scaling factor in front of the potential, which there is introduced in view of letting the particle number tend to infinity. This, in turn, is alien to the intent of the present work.

Without change, the equations (9) also define the dynamics of identical particle if the initial state can be represented as a symmetrized or anti-symmetrized product state (a

‘Slater determinant’ in the latter case). Then we evolve the underlying product state according to (9) and obtain the evolved (anti-)symmetrized state by (anti-)symmetrizing the evolved product state. Describing the same process by using a more complicated equation (TDHF) that acts directly on the (anti-)symmetrical wave function is no improvement, at least not for a computational implementation of dynamics.

Equation (9) follows from a direct and simple algorithmic definition of the time evolution step: Assume that at time t we are given wave functions $\psi_1(x_1, t), \psi_2(x_2, t), \psi_3(x_3, t)$. We try to propagate the state to time $t + \Delta t$. For this purpose, we first consider the exact dynamics of all subsystems arising from elimination of just one of the particles. Let us consider the case that particle 2 is eliminated first: The initial wave function $\psi_{31}(x_3, x_1, t) := \psi_3(x_3, t) \psi_1(x_1, t)$ will propagate into $\psi_{31}(x_3, x_1, t + \Delta t)$. For ignoring particle 1 the same logic leads to $\psi_{23}(x_2, x_3, t + \Delta t)$, and for ignoring particle 3 to $\psi_{12}(x_1, x_2, t + \Delta t)$. The exact dynamics of the whole system propagates $\psi(x_1, x_2, x_3, t) := \psi_1(x_1, t) \psi_2(x_2, t) \psi_3(x_3, t)$ into $\psi(x_1, x_2, x_3, t + \Delta t)$. Here, and also for the subsystems considered before, the initially factorizing state will lose the factorizing property through propagation (it will become *entangled*). However, the subsystem states constructed so far, allow us to extract single-particle states by a self-suggesting and symmetrical tracing out process which here applies to wave functions instead of density operators:

$$\begin{aligned}\psi_1(x_1, t + \Delta t) &:= \int dx_2 \int dx_3 \overline{\psi_{23}(x_2, x_3, t + \Delta t)} \psi(x_1, x_2, x_3, t + \Delta t) \\ \psi_2(x_2, t + \Delta t) &:= \int dx_3 \int dx_1 \overline{\psi_{31}(x_3, x_1, t + \Delta t)} \psi(x_1, x_2, x_3, t + \Delta t) \\ \psi_3(x_3, t + \Delta t) &:= \int dx_1 \int dx_2 \overline{\psi_{12}(x_1, x_2, t + \Delta t)} \psi(x_1, x_2, x_3, t + \Delta t) .\end{aligned}\tag{10}$$

This process can also be seen as applying two-particle destruction operators⁴ to the propagated three-particle state. It will be shown in the next section that scheme (10) yields the equations (9) in the limit of decreasing Δt . Since (10) makes use of the full quantum mechanical time evolution operator, it does not provide a simplification in comparison to the exact quantum mechanical time evolution operator. Unlike the scheme (10), the separated dynamics equations never encounter a full state of the interacting system (a function of three variables), only functions of two spatial variables appear. This does not change if new particles are added. Let n be the number of particles then the computational effort needed for a time step behaves as $O(n^2)$ and, if only a fixed number of neighbors is considered as interacting with a particle, this behavior reduces to the more favorable $O(n)$.

Since the dynamical law (9) thus is seen to result from the exact law by a simple and natural modification, one may expect that the main properties of the exact law translate into properties of the modified law: It will be shown in the next section that we still have

⁴ the well known creation and destruction operators in Fock space result from creation and destruction operators defined on the whole tensor algebra. These enjoy a simpler definition, but less canonical algebraic properties. I expect that using Fock states and Fock-space operators here leads to the TDHF evolution step in an analog manner.

conservation of the norm:

$$\int dx_1 |\psi_1(x_1, t)|^2, \quad \int dx_2 |\psi_2(x_2, t)|^2, \quad \int dx_3 |\psi_3(x_3, t)|^2 \quad (11)$$

are constant as functions of t . We also have *conservation of energy* in the form that the expectation value

$$\langle \psi_1(t) \otimes \psi_2(t) \otimes \psi_3(t) | H(\psi_1(t) \otimes \psi_2(t) \otimes \psi_3(t)) \rangle \quad (12)$$

is constant as functions of t . Here H is the Hamiltonian defined in (8).

2 Quantum systems made of interacting subsystems

We consider n distinguishable quantum systems S_j ($n < \infty$). For each $j \in J := \{1, \dots, n\}$ let \mathcal{H}_j be the *state space* (\equiv Hilbert space of pure states) of S_j . For the present purpose it is convenient to represent \mathcal{H}_j as a space of complex-valued functions on a measure space of configurations: $\mathcal{H}_j = L^2(X_j, \mathbb{C}, d\mu_j)$. A point $x \in X_j$ can typically be specified by giving values of position components and spin components of particles which make up S_j . Thus S_j needs not to be a one-particle system as assumed in the introduction. Actually, it is not assumed to be a particle system at all.

As far as the connection of the mathematical construct to the real world is concerned, there is no difference between the situation that X_j is a differential manifold endowed with a regular Borel measure, and the situation that it is a finite set endowed with some weighted counting measure. In the following section we will be concerned explicitly with the finite case. More generally, all theoretical constructs which are relevant to physics, can be expressed (in some cases with a loss of elegance) in the *Grothendieck universe of hereditarily finite sets*. Interestingly, this universe, with all common set theoretic operations, can be coded as a single class in any object oriented programming language. My C++ implementation is, together with full explanation of all functions, much shorter than the present article.

For each subset $\alpha \subseteq J$ there is a well defined Cartesian product space $X_\alpha = \prod_{j \in \alpha} X_j$, a product measure $\mu_\alpha = \prod_{j \in \alpha} \mu_j$, and a state space $\mathcal{H}_\alpha = L^2(X_\alpha, \mathbb{C}, d\mu_\alpha)$ of a system S_α that consists of the subsystems S_j , $j \in \alpha$. Obviously we may identify \mathcal{H}_j with $\mathcal{H}_{\{j\}}$ and S_j with $S_{\{j\}}$. Consider a *partition* of α , i. e. a list $\alpha_1, \dots, \alpha_p$ of pairwise disjoint subsets of α which satisfy $\alpha = \bigcup_{k=1}^p \alpha_k$. Then there is a natural p -linear mapping of the Cartesian product $\prod_{k=1}^p \mathcal{H}_{\alpha_k}$ into the Hilbert space \mathcal{H}_α defined by $(\psi_k)_{k=1}^p \mapsto \psi$, where $\psi((x_i)_{i \in \alpha}) = \psi_1((x_i)_{i \in \alpha_1}) \dots \psi_p((x_i)_{i \in \alpha_p})$. As is common practice, we write $\psi_1 \otimes \dots \otimes \psi_p$ for this ψ and let the context determine the set and the partition to which this *tensor product* refers. Notice that according to the present usage the same space \mathcal{H}_α is co-domain of various tensor products, so that here the role of a tensor product is not to create a Hilbert space out of given tensorial factors but to analyze a given Hilbert space in terms of simpler ones, by allowing a product decomposition (representation as a tensor product) for some of its elements. Therefore, it is adequate to refer to the mapping introduced before as a (*tensor*) *decomposition* of \mathcal{H}_α into the factors \mathcal{H}_{α_k} and of ψ into the

factors ψ_k . Let A be a bounded linear operator on one of the factors, say \mathcal{H}_{α_i} , then there is a natural way to ‘extend’ the operator from one factor to the whole of \mathcal{H}_α by letting it act as the identity on all the other factors:

$$A(\psi_1 \otimes \dots \otimes \psi_{i-1} \otimes \psi_i \otimes \psi_{i+1} \otimes \dots \otimes \psi_p) := \psi_1 \otimes \dots \otimes \psi_{i-1} \otimes A\psi_i \otimes \psi_{i+1} \otimes \dots \otimes \psi_p. \quad (13)$$

By linearity and continuity this extends to the definition of a bounded operator on \mathcal{H}_α . If the context tells on which Hilbert space an operator is acting, there is no danger in using the same name for operators acting on different spaces, just as the two operators A in (13). Notice that for each β satisfying $\alpha_i \subseteq \beta \subseteq J$ there may be many partitions of β which have α_i among their components⁵. So the procedure (13) defines many concrete ways to extent A to a linear operator on \mathcal{H}_β . In the present framework of dealing with function spaces it is easy to show that all these different concrete procedures give rise to the same result — which is indispensable for the formalism to make sense. This would be less obvious for tensor products defined by the more abstract methods of multi-linear algebra. Such abstract frameworks are less convenient for the proofs to be presented, and they give no direct guidance for defining computational models of the mathematical structure under consideration.

It may be instructive to explicitly write down the term, which gives the action of $A : L^2(X_\alpha, \mathbb{C}, d\mu_\alpha) \rightarrow L^2(X_\alpha, \mathbb{C}, d\mu_\alpha)$ after ‘extension’ to an operator $L^2(X_\beta, \mathbb{C}, d\mu_\beta) \rightarrow L^2(X_\beta, \mathbb{C}, d\mu_\beta)$ for the general situation $\alpha \subseteq \beta \subseteq J$. By definition, A maps functions $\psi : X_\alpha \rightarrow \mathbb{C}$ into functions of type $X_\alpha \rightarrow \mathbb{C}$. The result $A\psi$ is therefore also of type $X_\alpha \rightarrow \mathbb{C}$ so that an expression $f(\psi, (x_i)_{i \in \alpha})$ for the values $(A\psi)((x_i)_{i \in \alpha})$ of this function is the algorithmic content of A . By the same token, the ‘extension’ of A to $L^2(X_\beta, \mathbb{C}, d\mu_\beta)$ corresponds to an expression $g(\phi, (y_i)_{i \in \beta})$ for $\phi : X_\beta \rightarrow \mathbb{C}$. This expression can be directly given in terms of f as $g(\phi, (y_i)_{i \in \beta}) := f((x_i)_{i \in \alpha} \mapsto \phi(x \vee y), (y_i)_{i \in \alpha})$ ⁶, where for families $x := (x_i)_{i \in \alpha}$ and $y := (y_i)_{i \in \beta}$ the family $x \vee y := (x \vee y)_{i \in \beta}$ is defined as $(x \vee y)_i := (i \in \alpha ? x_i : y_i)$, where a notation for conditional terms is employed which is common in programming languages. Notice that $(x_i)_{i \in \alpha} \mapsto \phi(x \vee y)$ is a function of the type which expression f needs as its first argument. We will need a further operation of multi-linear algebra which has a direct representation in function spaces: Let $\phi_\alpha \in L^2(X_\alpha, \mathbb{C}, d\mu_\alpha)$, $\psi_\beta \in L^2(X_\beta, \mathbb{C}, d\mu_\beta)$, $\alpha \subseteq \beta$ then there is a well-defined state $\chi_\gamma \in L^2(X_\gamma, \mathbb{C}, d\mu_\gamma)$, $\gamma := \beta \setminus \alpha$ given by $\chi_\gamma := \langle \phi_\alpha | \psi_\beta \rangle$ where $\langle \phi_\alpha | \psi_\beta \rangle((x_i)_{i \in \gamma}) := \int \prod_{i \in \alpha} d\mu_i(x_i) \overline{\phi_\alpha((x_i)_{i \in \alpha})} \psi_\beta((x_i)_{i \in \beta})$. This generalization of the scalar product corresponds to the operation of contraction in tensor calculus.

For subsystem S_j , there is a Hamiltonian h_j , a self-adjoint linear operator on \mathcal{H}_j , and for each two-element set $\rho = \{i, j\} \subseteq J$ there is a self-adjoint operator v_ρ in \mathcal{H}_ρ which describes the interaction between S_i and S_j . In the sequel ρ is always to be understood as denoting a subset of J which has just two elements, i. e. $|\rho| = 2$. This is a good place to state explicitly the name-based declarations used so far tacitly: $i, j, k, l \in J$, $\alpha, \beta, \gamma \subseteq J$, $\psi_\alpha \in \mathcal{H}_\alpha$.

⁵lists have components

⁶defining nameless functions in this manner is referred to as λ -abstraction

The state space of the whole system S is \mathcal{H}_J and the Hamiltonian of the whole system is

$$H = \sum_{j \in J} H_j + \sum_{\rho \subseteq J} V_\rho =: T + V, \quad (14)$$

where $H_j := h_j \otimes \mathbf{1}$ with respect to the tensor decomposition of \mathcal{H} determined by the partition $J = \{j\} \cup (J \setminus \{j\})$, and $V_\rho := v_\rho \otimes \mathbf{1}$ with respect to the tensor decomposition of \mathcal{H} determined by the partition $J = \rho \cup (J \setminus \rho)$. Let for each $j \in J$ be $\psi_j \in J$ a normalized state (i.e. $\|\psi_j\| = 1$). Then we define $\psi := \psi_1 \otimes \dots \otimes \psi_n$ and the propagated state $\psi^{\Delta t} := \exp(-i\Delta t H) \psi$ ⁷. To reproduce the definition of separated dynamics, as given in Section 1, in the present general setting, we have to consider the systems originating from S by elimination of a single subsystem. Let $S.j$ denote such a system, where S_j is the eliminated subsystem. The state space of $S.j$ is $\mathcal{H}_{J.j}$, where $J.j := J \setminus \{j\}$ and the Hamiltonian of the system is

$$H.j = \sum_{i \in J.j} H_i + \sum_{\rho \subseteq J.j} V_\rho. \quad (15)$$

That (15) employs the same names of operators as (14) although the respective state spaces are different is to be understood in the light of the foregoing discussion.

In $S.j$ we consider the state $\psi.j := \otimes_{i \in J.j} \psi_j \in \mathcal{H}_{J.j}$ and the propagated state $(\psi.j)^{\Delta t} := \exp(-i\Delta t H.j) \psi.j$. This allows us to propose an evolved state $(\psi_j)_{\Delta t}$ of the single system S_j by

$$(\psi_j)_{\Delta t} := \langle (\psi.j)^{\Delta t} | \psi^{\Delta t} \rangle. \quad (16)$$

This definition can easily be generalized to defining evolved states of system pairs, triplets, or higher aggregates by replacing $S.j$ by systems in which pairs, triplets, or higher aggregates of subsystems were eliminated. Particular to our present case of single systems elimination is the simplicity of the dynamical scheme resulting from it: Using definition (16) for all $j \in J$ we may form the state $\psi_{\Delta t} := (\psi_1)_{\Delta t} \otimes \dots \otimes (\psi_n)_{\Delta t}$ which is said to result from the initial state $\psi := \psi_1 \otimes \dots \otimes \psi_n$ by *separated dynamics*.

We have now to show that separated dynamics is actually given by much simpler equations than the exact quantum dynamics which in the present definition is still involved.

From (16) we see

$$(\psi_j)_{\Delta t} = \langle \psi.j | \exp(-i\Delta t (H - H.j)) \psi \rangle \quad (17)$$

so that the time derivative under separated dynamics is given by

$$i\dot{\psi}_j = \langle \psi.j | (H - H.j) \psi \rangle = \langle \psi.j | (H_j + \sum_{j \in \rho \subseteq J} V_\rho) \psi \rangle = h_j \psi_j + \sum_{j \in \rho \subseteq J} \langle \psi.j | V_\rho \psi \rangle \quad (18)$$

and after eliminating from ψ the many factors that get integrated out without change due to the pair operator nature of the interaction

$$i\dot{\psi}_j = h_j \psi_j + \sum_{k=1, k \neq j}^n \langle \psi_k | v_{\{k,j\}} (\psi_k \otimes \psi_j) \rangle. \quad (19)$$

⁷this section puts $\hbar = 1$

This reduces to (9) in the case that $n = 3$ and that v_ρ are multiplication operators in \mathcal{H}_ρ , and that the h_j are Hamiltonians of particles as considered there. It is the general definition of separated dynamics for the case that interaction is mediated by pair-interaction operators. Notice that the most complex states appearing in (19) are two particle states. This reduces the computational complexity of the quantum dynamical initial value problem profoundly.

2.1 Norm conservation

Let us repeat that part of (18) which will be used in this and the next subsection

$$i\dot{\Psi}_j = h_j\Psi_j + \sum_{j \in \rho \subseteq J} \langle \Psi \cdot j | V_\rho \Psi \rangle. \quad (20)$$

We study the time dependence of the norm of an arbitrarily selected Ψ_j :

$$\begin{aligned} \frac{d}{dt} \langle \Psi_j | \Psi_j \rangle &= \langle \dot{\Psi}_j | \Psi_j \rangle + \langle \Psi_j | \dot{\Psi}_j \rangle = 2\Re \langle \Psi_j | \dot{\Psi}_j \rangle \\ &= 2\Re(-i) \left(\langle \Psi_j | h_j \Psi_j \rangle + \sum_{j \in \rho \subseteq J} \langle \Psi_j | \langle \Psi \cdot j | V_\rho \Psi \rangle \right) \\ &= 2\Im \left(\langle \Psi_j | h_j \Psi_j \rangle + \sum_{j \in \rho \subseteq J} \langle \Psi | V_\rho \Psi \rangle \right) = 0 \end{aligned} \quad (21)$$

since expectation values of Hermitean operators are real.

2.2 Energy conservation

Also here computing the imaginary part of terms will play the decisive role. The argument is rather complex. Without the opportunity to monitor all these terms in a computational model it would have been much harder to identify the terms the cancellation of which entails the result. We get two terms of quite different behavior:

$$\frac{d}{dt} \langle \Psi | H \Psi \rangle = \frac{d}{dt} \langle \Psi | T \Psi \rangle + \frac{d}{dt} \langle \Psi | V \Psi \rangle =: \dot{Y} + \dot{Z} \quad (22)$$

and analyze \dot{Y} and \dot{Z} in turn. From

$$\dot{Y} = \frac{d}{dt} \sum_{j=1}^n \langle \Psi_j | h_j \Psi_j \rangle = \sum_{j=1}^n 2\Im \langle h_j \Psi_j | i \dot{\Psi}_j \rangle \quad (23)$$

we pick a generic term for further analysis

$$\begin{aligned} \langle h_j \Psi_j | i \dot{\Psi}_j \rangle &= \langle h_j \Psi_j | h_j \Psi_j \rangle + \sum_{j \in \rho \subseteq J} \langle h_j \Psi_j | \langle \Psi \cdot j | V_\rho \Psi \rangle \rangle \\ &= \|h_j \Psi_j\|^2 + \sum_{j \in \rho \subseteq J} \langle H_j \Psi | V_\rho \Psi \rangle. \end{aligned} \quad (24)$$

Thus

$$\Im \langle h_j \psi_j | i \dot{\psi}_j \rangle = \Im \sum_{j \in \rho \subseteq J} \langle H_j \psi | V_\rho \psi \rangle \quad (25)$$

and

$$\frac{1}{2} \dot{Y} = \Im \sum_{j=1}^n \sum_{j \in \rho \subseteq J} \langle H_j \psi | V_\rho \psi \rangle = \Im \sum_{j=1}^n \langle H_j \psi | V \psi \rangle = \Im \langle T \psi | V \psi \rangle. \quad (26)$$

The term \dot{Z} is more complicated since it contains the time derivative of the product state ψ :

$$\frac{1}{2} \dot{Z} = \frac{1}{2} \frac{d}{dt} \langle \psi | V \psi \rangle = \Im \langle V \psi | i \dot{\psi} \rangle, \quad (27)$$

$$\begin{aligned} i \dot{\psi} &= i \dot{\psi}_1 \otimes \psi_2 \otimes \dots \otimes \psi_n + \dots + \psi_1 \otimes \dots \otimes \psi_{n-1} \otimes i \dot{\psi}_n \\ &= h_1 \psi_1 \otimes \psi_2 \otimes \dots \otimes \psi_n + \dots + \psi_1 \otimes \dots \otimes \psi_{n-1} \otimes h_n \psi_n \\ &\quad + \sum_{l \in \rho} \langle \psi.l | V_\rho \psi \rangle \otimes \psi_2 \otimes \dots \otimes \psi_n + \dots + \psi_1 \otimes \dots \otimes \psi_{n-1} \otimes \sum_{n \in \rho} \langle \psi.n | V_\rho \psi \rangle \\ &= T \psi + \sum_{l \in \rho} \langle \psi.l | V_\rho \psi \rangle \otimes \psi_2 \otimes \dots \otimes \psi_n + \dots + \psi_1 \otimes \dots \otimes \psi_{n-1} \otimes \sum_{n \in \rho} \langle \psi.n | V_\rho \psi \rangle. \end{aligned} \quad (28)$$

Thus

$$\frac{1}{2} \dot{Z} = \Im \langle V \psi | i \dot{\psi} \rangle = \Im \langle V \psi | T \psi \rangle + \Im \sum_{j=1}^n \langle V \psi | (\psi_1 \otimes \dots \otimes \psi_n) \Big|_{\psi_j \rightarrow \langle \psi.j | V \psi \rangle} \rangle. \quad (29)$$

In the last line there is a term substitution symbol where an arrow connects the symbol to be replaced with the symbol to be used for replacement. By the last line of (28) one would expect not the whole potential V appearing in the substitution but only the two terms V_ρ satisfying $j \in \rho$. However, the sets ρ which do not satisfy this condition give real contributions, which vanish since we only take the imaginary part of the whole term. To see this, we note that for $j \notin \rho$ we have $\langle \psi.j | V_\rho \psi \rangle = \langle \psi | V_\rho \psi \rangle \psi_j$ which is ψ_j times a real number. What we have found is

$$\frac{d}{dt} \langle \psi | H \psi \rangle = \dot{Y} + \dot{Z} = 2 \Im \sum_{j=1}^n \langle V \psi | (\psi_1 \otimes \dots \otimes \psi_n) \Big|_{\psi_j \rightarrow \langle \psi.j | V \psi \rangle} \rangle \quad (30)$$

so that energy conservation is equivalent to the property of the term

$$X := \sum_{j=1}^n \langle V \psi | (\psi_1 \otimes \dots \otimes \psi_n) \Big|_{\psi_j \rightarrow \langle \psi.j | V \psi \rangle} \rangle \quad (31)$$

to be real-valued. For the following calculations it is convenient to write this as $X \sim 0$, where $z \sim z'$ means $\Im z = \Im z'$. To show this, we study the terms of which X is a sum:

$$A(\rho) := V_\rho \psi, \quad B(i, j) := \psi_1 \otimes \dots \otimes \psi_n \Big|_{\psi_i \rightarrow \langle \psi.i | V_{\{i,j\}} \psi \rangle}, \quad C(\rho, i, j) := \langle A(\rho) | B(i, j) \rangle. \quad (32)$$

It is convenient to extend this definitions by allowing instead of ρ (which satisfies $|\rho| = 2$ by definition) also one-element sets: $A(\{i\}) = 0 \cdot \psi$ and therefore also $B(i, i) = 0 \cdot \psi$. These terms will be shown to satisfy

$$C(\rho, i, j) \sim 0 \text{ if } i \notin \rho \quad (33)$$

$$C(\{i, k\}, i, j) + C(\{i, j\}, i, k) \sim 0. \quad (34)$$

This then implies

$$\begin{aligned} X &= \sum_{i=1}^n \sum_{j=1}^n \sum_{\rho \subseteq J} C(\rho, i, j) \sim \sum_{i=1}^n \left(\sum_{j=1}^n \sum_{k=1}^n C(\{i, k\}, i, j) \right) \\ &= \sum_{i=1}^n \left(\sum_{j=1}^n \sum_{k=1}^n \frac{1}{2} (C(\{i, k\}, i, j) + C(\{i, j\}, i, k)) \right) \sim 0 \end{aligned} \quad (35)$$

which is the main conclusion. So it remains to show (33) and (34): We consider (33) first: Since $i \notin \rho$ there is a partition $J = \rho \cup \{i\} \cup \alpha$ so that for the tensor decomposition of \mathcal{H}_J with respect to this partition we have $A(\rho) = (v_\rho \Psi_\rho) \otimes \Psi_i \otimes \Psi_\alpha$ and $B(i, j) = \Psi_\rho \otimes \tilde{\Psi}_{ij} \otimes \Psi_\alpha$ where $\tilde{\Psi}_{ij} := \langle \Psi_j | v_{\{i, j\}} \Psi_i \otimes \Psi_j \rangle$. Then $\langle A(\rho) | B(i, j) \rangle = \langle v_\rho \Psi_\rho | \Psi_\rho \rangle \cdot \langle \Psi_i | \tilde{\Psi}_{ij} \rangle \cdot \langle \Psi_\alpha | \Psi_\alpha \rangle$. The factor in the middle can be processed further $\langle \Psi_i | \langle \Psi_j | v_{\{i, j\}} \Psi_i \otimes \Psi_j \rangle \rangle = \langle \Psi_i \otimes \Psi_j | v_{\{i, j\}} \Psi_i \otimes \Psi_j \rangle \in \mathbb{R}$. So all factors in $C(\rho, i, j)$ are seen to be real, thus $C(\rho, i, j) \sim 0$. Now we consider (34) and thus $C(\{i, k\}, i, j)$. The partition $J = \{i, k\} \cup \alpha$ induces a tensor decomposition $\mathcal{H}_J = \mathcal{H}_{\{i, k\}} \otimes \mathcal{H}_\alpha$ and a representation $C(\{i, k\}, i, j) = \langle v_{\{i, k\}} \Psi_{\{i, k\}} | \tilde{\Psi}_{ij} \otimes \Psi_k \rangle = \langle v_{\{i, k\}} \Psi_i \otimes \Psi_k | \langle \Psi_j | v_{\{i, j\}} \Psi_i \otimes \Psi_j \rangle \otimes \Psi_k \rangle = \langle (v_{\{i, k\}} \Psi_i \otimes \Psi_k) \otimes \Psi_j | (v_{\{i, j\}} \Psi_i \otimes \Psi_j) \otimes \Psi_k \rangle$. From this formula we see that the exchange $j \leftrightarrow k$ just exchanges the two factors of the scalar product, and thus changes $C(\{i, k\}, i, j)$ into its complex conjugate. Thus $C(\{i, k\}, i, j) = \overline{C(\{i, j\}, i, k)}$ and thus $C(\{i, k\}, i, j) + C(\{i, j\}, i, k) \sim 0$, which completes the proof.

It is interesting that according to [2] the ‘customary Hartree-Fock Hamiltonian has an expectation value given by the sum of the kinetic energy and twice the potential energies’ and that it is only by a modification of this Hamiltonian proposed by these authors the conserved quantity becomes the expectation value of $T + V$. Therefore they suggest the name ‘constant- $\langle H \rangle$ ’ Hamiltonian for their modification. In the light of this observation, one may state as a merit of the present approach that it left no choice to end up with a ‘wrong conserved quantity’.

3 A computational comparison of exact, separated, and classical dynamics

The model to be presented in this section is a special case of the one discussed in the Introduction. However, instead of ranging over physical 3-space, as was suggested there, the variables x_1, x_2, x_3 range here over linear lattices.

Each of the linear lattices is obtained from an interval I in \mathbb{R} by partitioning it in d congruent subintervals and taking the centers of the subintervals as lattice points. The

Laplacian on such a finite lattice is defined by

$$(\Delta\Psi)_i := \frac{\Psi_{i-1} - 2\Psi_i + \Psi_{i+1}}{h^2}, \quad (36)$$

where $h := |I|/d$ is the lattice spacing and $\Psi_i := 0$ for $i \notin \{1, \dots, d\}$. This corresponds to reflecting boundary conditions, whereas in [11] periodic boundary conditions were employed.

For the sake of simplicity, this article deals with a single computation (computer run), and for all system parameters the values chosen for this particular computer run will be given now. All these values refer to an arbitrary system of physical units in which the numerical value of \hbar is 1. For the three particles the intervals are $[0, 1]$, $[1.1, 2.1]$, $[2.2, 3.2]$ respectively, and $d = 16$ for all of them. Further $m_1 = m_2 = m_3 = 4$, $q_1 = q_2 = q_3 = 1$, $x_1^0 = 0.51$, $x_2^0 = 1.59$, $x_3^0 = 2.7$. The spacing between these equilibrium positions are not precisely equal in order not to create very special numerical conditions. The functions f_i are of the form $f_i(r) = \lambda_i r^p$, with $\lambda_1 = 947.482$, $\lambda_2 = 884.317$, $\lambda_3 = 941.165$, $p = 4$. The interaction potential f is given as $f(r) = \alpha r^q$ with $\alpha = 5$, $q = 1.5$. It is given as increasing with distance in order to avoid that only next neighbors interact considerably. If one sets $q = 1$ ('quark potential'), the classical forces are independent of the distance. In this case all our test quantities come out as practically identical for separated and for exact dynamics. The external field is set as homogeneous: $g(x) = \beta x$ with $\beta = 5$. By these 23 numbers the Hamiltonian in (8) and also all coefficients in equation (9) are defined.

The initial state is the ground-state of the non-interacting system, i.e. the system for which the q_i are set to zero. Then we have three one-particle Hamiltonians, each of which determines a $d \times d$ -matrix for which the eigenstates are easily determined by numerical methods as pointed out for instance in [11]. It is very instructive to employ also excited states and linear combinations of those, but this is not reported here.

As discussed in detail in [11], a finite configuration space ('biotope') does not change the quantum mechanical interpretation. The points of the biotope carry complex numbers — quantum amplitudes — and not small quantum systems like qubits as considered in quantum cellular automata (QCA), see e.g. [9], [13]. Therefore, a finite biotope system would belong to orthodox Hilbert space quantum mechanics, if it would work with complex numbers rather than with finite bit approximations of those. Of course, for a computational model the time evolution is in finite propagation steps. They have the form of the update rule of an automaton, since for each point of the biotope, the old amplitude value gets replaced by a new one, which is determined by all the old ones. The update rule has to be implemented by arithmetical operations. Since these have to be executable in finite time, it is essential that numbers are finitely coded. Our update rule thus maps a finite set of states into itself, so that we have a finite state automaton. Actually, by considering all the finitely many biotope points as neighbors of each other, the present model is a classical cellular automaton — not a quantum one.

Some 'lack of perfect precision' in executing quantum dynamics, which was mentioned in the introduction as a possible origin of decoherence, is inherent in any computational implementation with finite precision numbers. Due to the enormous amount of precision that these numbers, nevertheless, provide, 'decoherence by roundoff-errors'

is hard to observe in actual computations. If, however, the accuracy of quantum amplitudes is spoiled intentionally by adding random noise to their phases it is hard not to see decoherence.

The computational version of the exact quantum dynamics is implemented as in [11] by the *direct midpoint method*. Since separated dynamics is not determined by a Hamiltonian but by non-linear integro-differential equations one needs a different numerical method in this case. Here I use the *modified leap-frog integrator* which is defined in [12] as an intermediate method on an evolutionary path leading from the normal leap-frog method to the direct midpoint method. For the convenience of the reader, the definition of these methods will be repeated here: Their common basic concept is to employ the ‘quantum velocity’ $\phi := \dot{\psi}$ as an additional state descriptor in a simulation. Propagating a state thus means to compute $\psi(t + \Delta t), \phi(t + \Delta t)$ from given $\psi(t), \phi(t)$. At the beginning of a simulation we only know $\psi(t_0)$ and have to find the velocity from the ‘equation of motion’ which may be written in the form $\phi(t_0) = D(t_0)\psi(t_0)$. Here, D is the operational expression that allows us to compute $\phi(t_0)$ for given t_0 and $\psi(t_0)$. Equations (9) and (20) define expression D in the case of separated dynamics. In the case of exact dynamics we have $D = -i\hbar H$, which is assumed not depend on t .

For exact dynamics, the time propagation step according to the direct midpoint method is

$$\psi += \frac{\Delta t}{2} \phi, \quad \phi += \Delta t D^2 \psi, \quad \psi += \frac{\Delta t}{2} \phi, \quad t += \Delta t \quad (37)$$

where a self-explanatory programming-style notation is employed. For time-dependent Hamiltonians, which naturally arise in interaction picture computations, and also if the external field is allowed to depend on time, a minor modification is necessary that is given in equation (16) of [12]. One also may use in this case the next method (38) as it stands.

For separated dynamics, D necessarily depends on t (since it includes the influencing states, which change with time) and the propagation step according to the modified leap-frog method is ⁸

$$t += \frac{\Delta t}{2}, \quad \psi += \frac{\Delta t}{2} \phi, \quad \phi_m := D(t) \psi, \quad \phi = 2\phi_m - \phi, \quad \psi += \frac{\Delta t}{2} \phi, \quad t += \frac{\Delta t}{2}. \quad (38)$$

Both methods are explicit, second order accurate, and asynchronous, i.e. they allow changing Δt after each step. This is important for using these methods as building blocks for adaptive methods. Since the propagation step (37) applies D twice, whereas (38) applies its D only once, it is natural to define the Δt -step of separated dynamics as the succession of two $\Delta t/2$ -steps (38). This gives the two stepping methods very similar stability properties. Therefore a common time step $\Delta t = 3.3104374 \cdot 10^{-4}$ was used for both methods. This value was computed by the program as one tenth of the stability limit $\Delta t_{crit} = 2\hbar / \|H\|$, see [11]. Computing the operator norm $\|H\|$ is alike computing about 100 propagation steps, which is negligible in a computation that does 10000 propagation steps as we do here.

⁸ That $D(t)$ in equation (1) of [12] was introduced as a linear operator is an unnecessary restriction that was suggested by the context there.

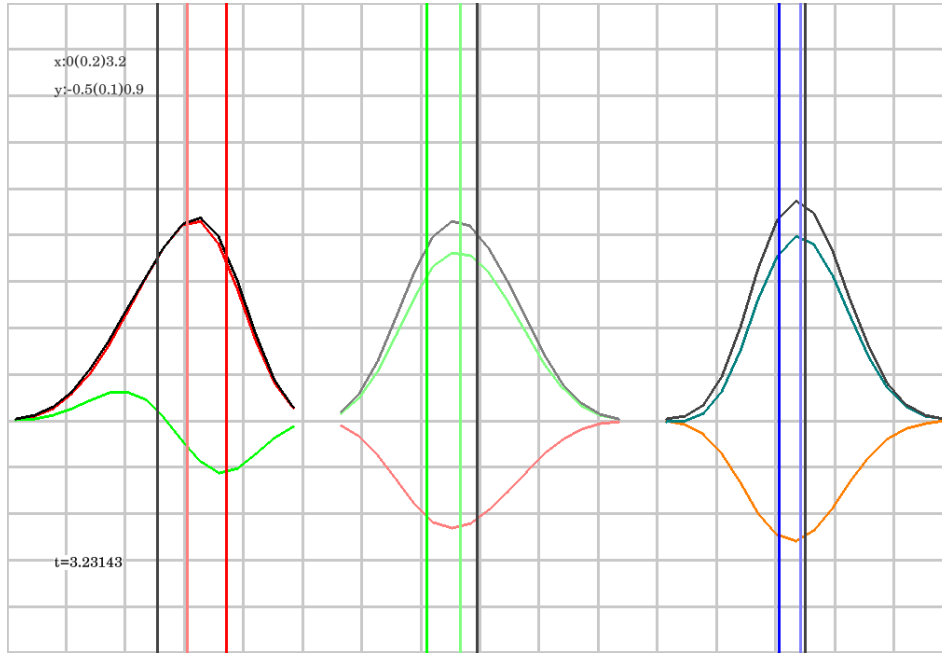


Figure 1: Wave functions of three particles in separated dynamics

A screen-shot of the final state of the separated dynamics part of the simulation is reproduced in Figure 1. Here, vertical black lines mark the equilibrium positions, pale colored vertical lines mark the quantum expectation value of particle position, and the vivid color vertical lines mark the positions of the classical particles. The classical particles are initially at rest at the equilibrium positions and their motion is followed by the classical mechanics version of the direct midpoint method [6] and with the same time step which was used for the two quantum methods. The wave functions themselves are represented as a red curve for the real part, a green curve for the imaginary part, and a black curve for the absolute value. It is obvious from this representation that each particle lives in its own biotope, and that it would not be necessary to distinguish the partial curves by color nuances as done in the figure. A different representation of the same state is given in Figure 2 as a quantum mechanical three-particle state which determines a $16 \times 16 \times 16$ array of complex numbers. These can be conveniently visualized as a 4×4 array of 16×16 color images. In the same format also the exact dynamics final state is shown in this figure. Notice that the difference is mostly in the overall color (total phase) of the images, not in the detail. This rule holds over the the whole run, where there are periods in which there is more detail. I made a gif-animation of 200 such image pairs created for each 50th simulation step. Unfortunately it is 16 MB in size and will not be attached to this article, but I'll send it on request.

The numerical methods of the simulation run are not capable of conserving norm and energy exactly. Rather they give rise to tiny oscillatory variations of these quantities and the energy may get a small oscillatory imaginary part. These quantities are shown

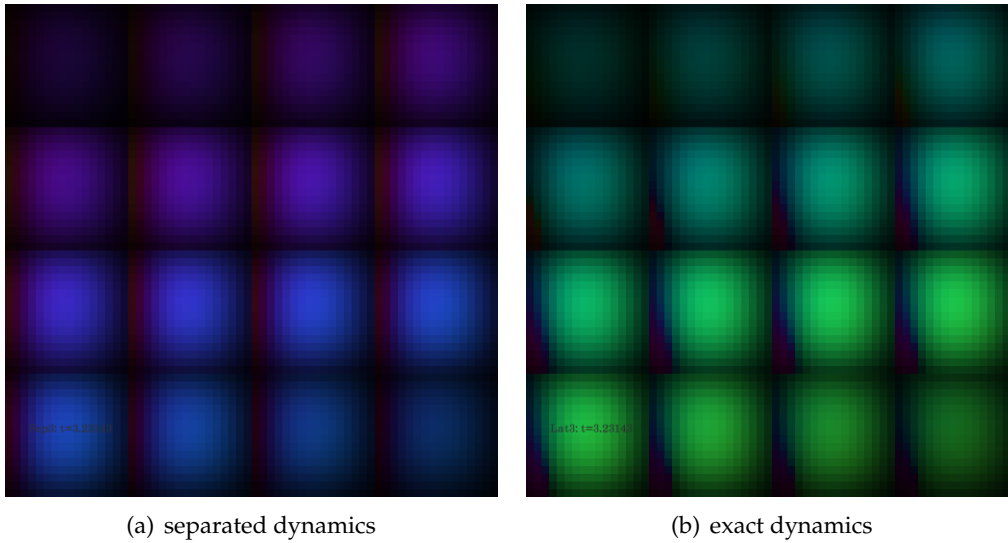


Figure 2: Areal state representations

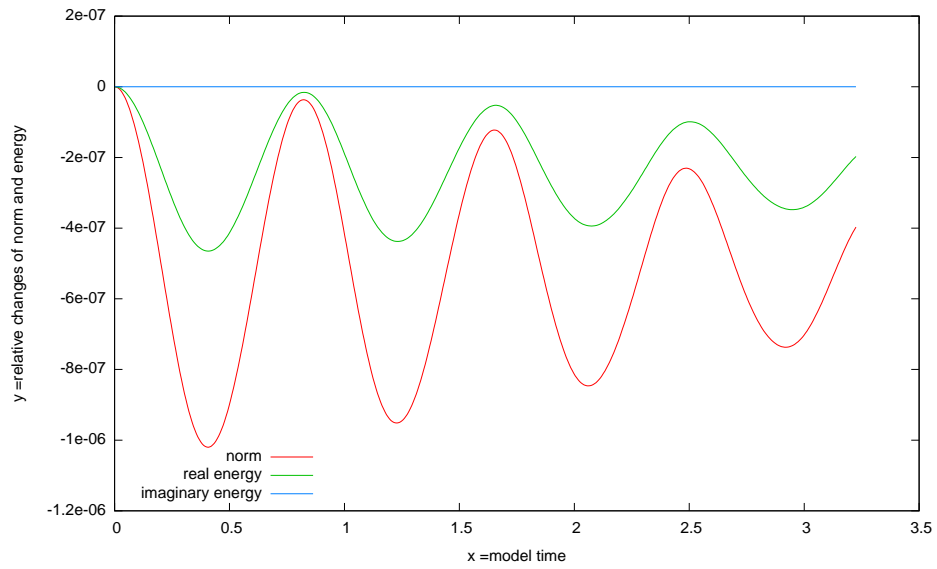


Figure 3: Deviations from norm conservation and energy conservation for separated dynamics

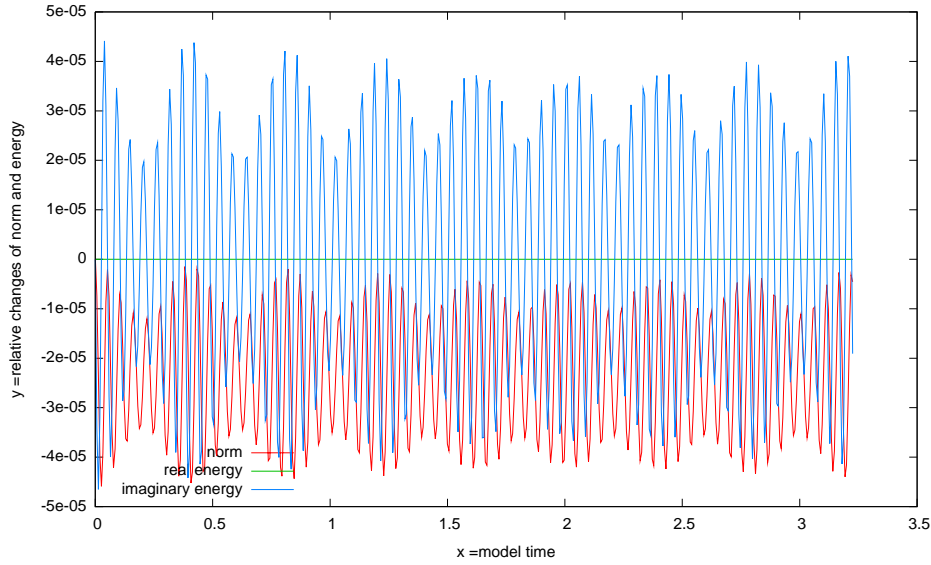


Figure 4: Deviations from norm conservation and energy conservation for exact dynamics

in Figure 3 and Figure 4 as relative changes with respect to the initial state. For exact dynamics these variations are completely understood, [11], [12], but for the numerical method used to treat separated dynamics a comparable analysis has not yet been done. As the figure shows, these deviations are much smoother and smaller for separated dynamics. If, however, the time step of separated dynamics would be defined as a single step of the modified leap-frog integrator (instead of a combination of two such steps) these curves would be zig-zag with two steps period, so that the diagram would be much more busy than the one of exact dynamics.

Finally we study quantities which are observable in principle and which can be computed both in exact dynamics and in separated dynamics. This is the computer version of the Gedankenexperiment considered in the introduction. A natural choice for the observable quantities are expectation values and correlations of the particle positions relative to their equilibrium positions. Precisely, we consider the seven quantities $s_1(t), s_2(t), s_3(t), s_{12}(t), s_{23}(t), s_{31}(t), s_{123}(t)$ for which the following definition of $s_{12}(t)$ gives the pattern:

$$s_{12}(t) := \int dx_1 dx_2 dx_3 \overline{\psi(x_1, x_2, x_3, t)} (x_1 - x_1^0) (x_2 - x_2^0) \psi(x_1, x_2, x_3, t). \quad (39)$$

For separated dynamics, due to $\psi(x_1, x_2, x_3, t) = \psi_1(x_1, t) \psi_2(x_2, t) \psi_3(x_3, t)$, this simplifies to a product

$$s_{12}(t) = \int dx_1 \overline{\psi_1(x_1, t)} (x_1 - x_1^0) \psi_1(x_1, t) \cdot \int dx_2 \overline{\psi_2(x_2, t)} (x_2 - x_2^0) \psi_2(x_2, t). \quad (40)$$

In Figure 5 we see the sum $s_1(t) + s_2(t) + s_3(t)$ of these shifts. The figure shows that the two quantum curves cannot be discerned at the given graphical resolution. It also

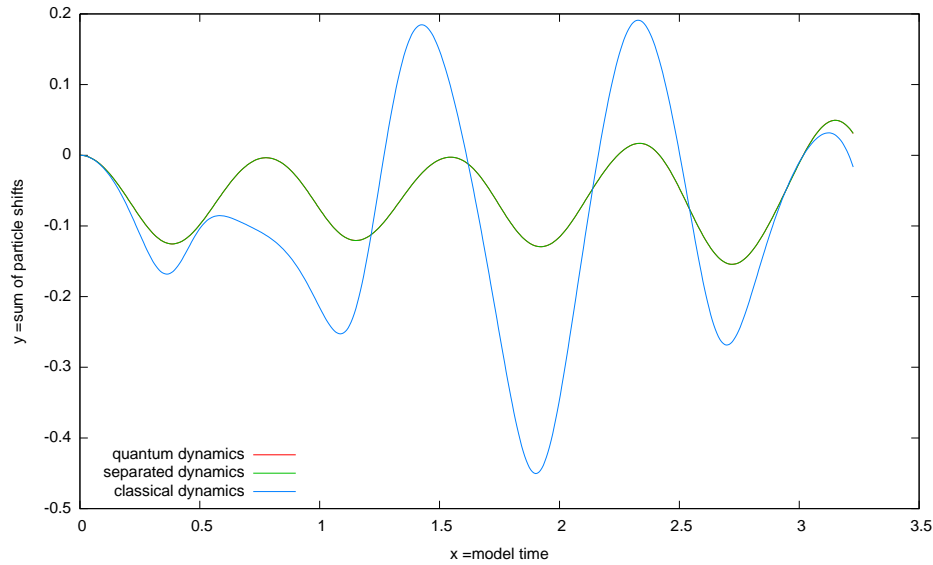


Figure 5: Total particle shift for separated, exact, and classical dynamics

shows that the quantum curve deviates considerably from the curve obtained from the classical particles, which were introduced earlier. Therefore, our selection of test quantities did avoid the fallacy of dealing with situations for which quantum results are predetermined by Ehrenfest's theorem. We also see that quantum dynamics and classical dynamics agree rather well for the very early phase of the motion. This shows that the initial state of the classical particles, as defined earlier, fits the quantum mechanical initial state.

Due to the rapidly growing discrepancy of classical motion and quantum motion it makes no sense to include the classical particles in the presentation of the correlations. Thus Figure 6, 7 deal only with the two quantum motions. Again, within the graphical resolution one gets nearly identical curves when showing the two cases in one diagram. Therefore I use one diagram for the curves of exact dynamics, and a second one for the differences. Since the relative size of correlations depends on the unit of length, the curves of exact dynamics were scaled with a positive factor such that the maximum of their absolute value gets the value 1. Of course, in forming the difference between 'exact and separated curves', the same scaling factor is used for both. Notice that the difference is smallest for the s_i , larger for the s_{ik} , and largest for s_{123} .

At least particle shifts behave according to separated dynamics rather accurately as in exact dynamics, and quite different from classical dynamics. It may be interesting to compare this approach to method comparison with analytical approaches to the similar problem for the time-dependent Hartree-Fock approximation [8].

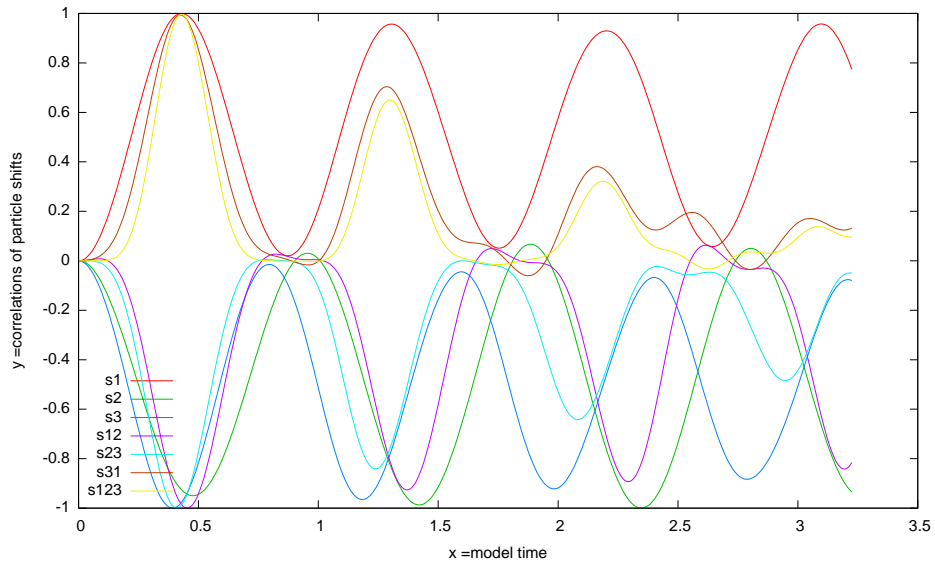


Figure 6: Correlations of particle shifts according to exact dynamics

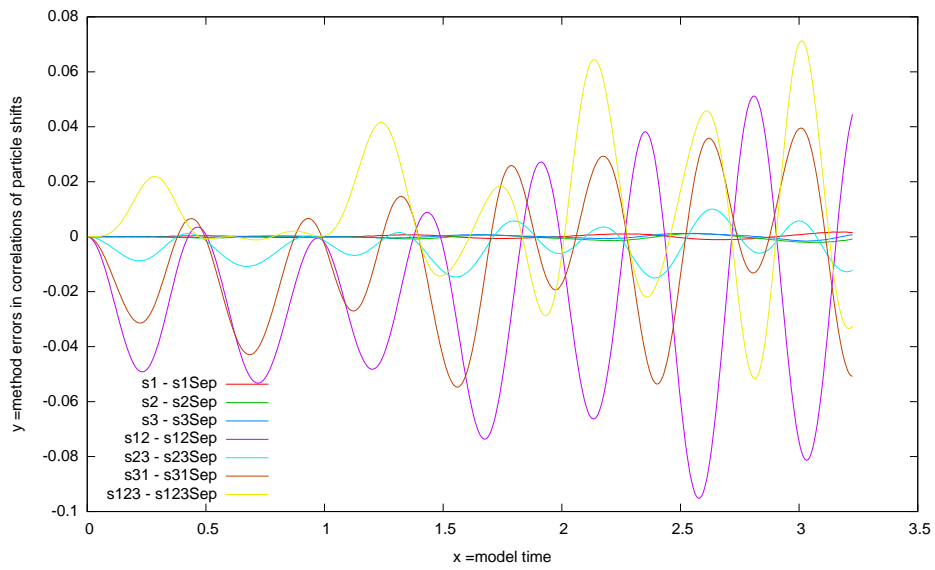


Figure 7: Difference of correlations: exact minus separated

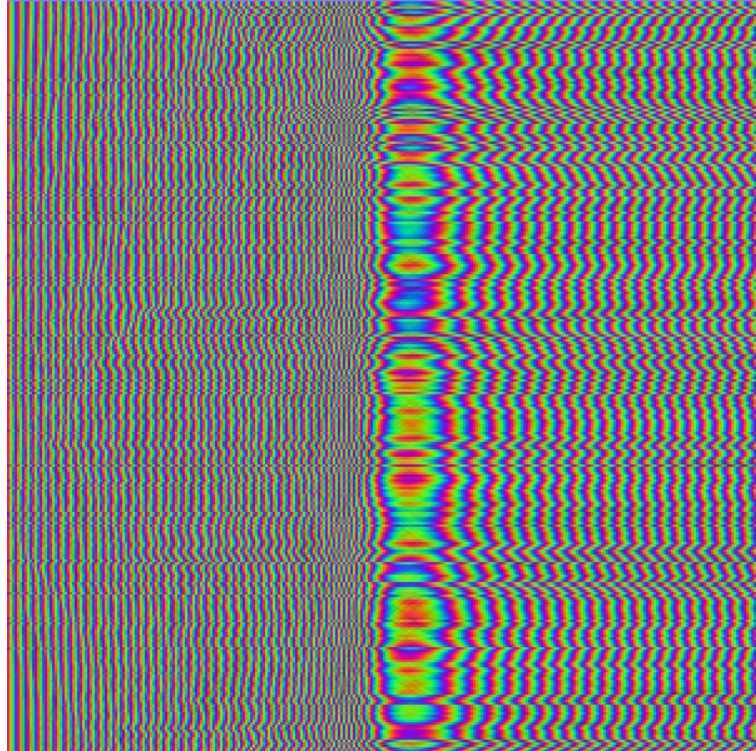


Figure 8: Chain of 300 spins evolving over 30 000 steps in separated dynamics

4 Outlook

The computational model in this article dealt only with three particles since it aims at comparing separated dynamics with exact quantum dynamics and the latter demands prohibitively heavy computational resources for large particle numbers. For the present run of 10000 time steps of 3 particles each living on a 16 point linear lattice the computation time was about three minutes on an off-the-shelf 2.08 GHz desktop computer. When applying the separated dynamics method to a Heisenberg spin chain with nearest neighbor interaction, I can run 600 particles (for more graphical representation becomes difficult) for 10 times more steps in the same time. So far, I did not extract physically relevant information from these experimental runs. The phenomena that express themselves in the graphical representation of the dynamics invite investigation. An example of 300 spins initially a fixed orientation which is modified by a stochastic spin flip of probability 0.25 is shown in Figure 8. In this figure time grows from left to right and in vertical direction one goes along the spin chain. The colors code the location of the spin on the Bloch sphere. After the obvious transition phase in the middle of the run, the expectation value of σ_3 that fluctuated a lot before becomes practically constant. The run is 30000 steps and took 56 seconds. This is not intended to be complete information. Rather, it is intended as an invitation to spin chain experts

to test separated dynamics within their problem field.

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