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Time-dependent density-functional theory for open spin chains

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The application of methods of time-dependent density-functional theory to systems of qubits provided the interesting possibility of simulating an assigned Hamiltonian evolution by means of an auxiliary Hamiltonian having different two-qubit interactions and hence a possibly simpler wave-function evolution. In this paper we extend these methods to some instances of Lindblad evolution of a spin chain.

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I. INTRODUCTION

The application of methods of time-dependent density-functional theory to systems of qubits has been proposed by Aspuru-Guzik and Tempel in Ref. [1]. In particular, these authors have given, for a family of Hamiltonian evolutions of qubit systems, a proof of the van Leeuwen (VL) theorem [2]. Our work is mostly based on their constructive proof of the VL theorem given in Sec. D of the Supplemental Material to Ref. [1].

We review their work on the Hamiltonian evolution of a spin chain in Sec. II: we explore the possibility offered by van Leeuwen's mapping from densities to potentials of simulating, by means of a spin chain having spatially homogeneous hopping parameters, the magnetization of an *engineered* spin chain [3]. Section III explores the possibility of extending these methods to some instances of dissipative evolution of a spin chain according to the Lindblad equation. We focus our attention on a class of models studied in all details by Žnidarič [4,5] and exemplified in Fig. 1.

The case in which only dephasing is present is of some interest on its own right: in Sec. III A we numerically explore the possibility (suggested in [6] for electronic systems) of simulating, in this case, the magnetization of an *open* quantum system with that of a driven *closed* system; then we discuss the complementary problem of compensating for the effects of dephasing on a spin chain. Section III B is devoted to the study of the dissipation current [7,8] present when we allow exchange of magnetization with the two reservoirs $\mathcal{B}_L$ and $\mathcal{B}_R$. In Sec. IV we discuss the difficulties, already evidenced in [9], that appear when the local kinetic energy is not everywhere nonzero, and present suggestions for further work.

II. THE MODELS: HAMILTONIAN EVOLUTION

We consider a chain of s spin-1/2 systems $\boldsymbol{\sigma}(1),\boldsymbol{\sigma}(2),\ldots,\boldsymbol{\sigma}(s)$, with $\boldsymbol{\sigma}(x)=(\sigma_1(x),\sigma_2(x),\sigma_3(x))$, evolving under the action of a Hamiltonian of the form

$$\begin{aligned} H(t) &= \sum_{x=1}^{s-1} J(x)[\sigma_1(x)\sigma_1(x+1)+\sigma_2(x)\sigma_2(x+1)] \\ &\quad + \sum_{x=1}^{s-1} K(x)\sigma_3(x)\sigma_3(x+1) + \sum_{x=1}^{s} h(x,t)\sigma_3(x) \\ &= H_0(J,K) + \sum_{x=1}^{s} h(x,t)\sigma_3(x). \end{aligned} \tag{1}$$

As our notations indicate, the two-qubit coupling constants $J(x)$ and $K(x)$ are supposed to be time independent, while the field $h(x,t)$ is allowed to depend on time.

The current operator field j is defined by

$$\begin{aligned} \mathrm{j}(0) = \mathrm{j}(s) &= 0, \\ \mathrm{j}(x) &= 2J(x)[\sigma_1(x)\sigma_1(x+1)-\sigma_2(x)\sigma_2(x+1)]. \end{aligned} \tag{2}$$

Its interest comes from the following commutator identity (from which the continuity equation easily follows):

$$-i[\sigma_3(x),H(t)]+[\mathrm{j}(x)-\mathrm{j}(x-1)]=0. \tag{3}$$

It is useful, in what follows, to consider also the identity

$$\mathrm{j}(x) = 4iJ(x)[\sigma_+(x)\sigma_-(x+1)-\sigma_-(x)\sigma_+(x+1)], \tag{4}$$

where $\sigma_\pm(x)=(\sigma_1(x)\pm i\sigma_2(x))/2$.

Using the above identities proof of the following further identity, of obvious relevance to the Heisenberg evolution of the current field, is immediate:

$$\begin{aligned} -i[\mathrm{j}(x),H(t)] = 8J(x)\{&J(x)[\sigma_3(x)-\sigma_3(x+1)] \\ &+ J(x-1)\sigma_3(x)\tau(x-1,x+1) \\ &- J(x+1)\sigma_3(x+1)\tau(x,x+2) \\ &+ K(x+1)\sigma_3(x+2)\tau(x,x+1) \\ &- K(x-1)\sigma_3(x-1)\tau(x,x+1) \\ &+ [h(x+1,t)-h(x,t)]\tau(x,x+1)\}. \end{aligned} \tag{5}$$

Here and in what follows we set

$$\tau(x,y)=\sigma_+(x)\sigma_-(y)+\sigma_-(x)\sigma_+(y).$$

Identities (3) and (5) have the obvious consequence that, if the state $|\psi(t)\rangle$ satisfies the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle \tag{6}$$

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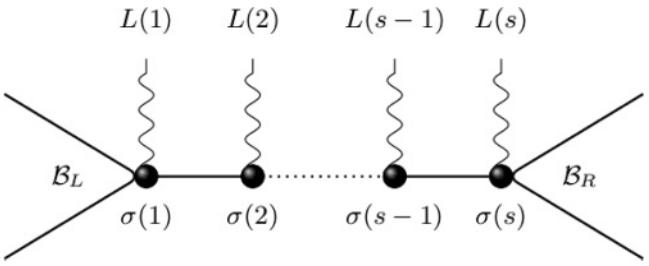

FIG. 1. The end points of a spin chain of length s interact with two reservoirs $\mathcal{B}_L$ and $\mathcal{B}_R$. Dephasing operators act independently on each site.

(natural units are used throughout this paper), then its *mean magnetization* field

$$m_3(x,t) = \langle\psi(t)|\sigma_3(x)|\psi(t)\rangle$$

satisfies the continuity equation

$$\frac{dm_3(x,t)}{dt} + [j(x,t) - j(x-1,t)] = 0, \tag{7}$$

and its *mean current* field

$$j(x,t) = \langle\psi(t)|\,\mathrm{j}(x)|\psi(t)\rangle$$

satisfies the equation of motion

$$\frac{d}{dt}j(x,t) = -i\langle\psi(t)|[\mathrm{j}(x),H_0(J,K)]|\psi(t)\rangle + 8J(x) \times [h(x+1,t) - h(x,t)]\langle\psi(t)|\tau(x,x+1)|\psi(t)\rangle. \tag{8}$$

In Ref. [1] Tempel and Aspuru-Guzik take the following point of view: Suppose we are interested in attaining, in a neighborhood of $t = 0$, a preassigned magnetization field $\overline{m}_3(x,t)$; because of (7) and (2) this target will be reached if we are able to attain a current field $\overline{j}(x,t)$ given by

$$\overline{j}(x,t) = -\frac{d}{dt}\sum_{y\leqslant x}\overline{m}_3(x,t); \tag{9}$$

finding a Hamiltonian $H_0(J,K) + \sum_{x=1}^{s} h(x,t)\sigma_3(x)$ (where J and K are supposed to be assigned, and h is supposed to be unknown) that determines such a current field $\overline{j}(x,t)$ is, in turn, equivalent to solving the differential-algebraic problem

$$\frac{d}{dt}\overline{j}(x,t) = -i\langle\psi(t)|[\mathrm{j}(x),H_0(J,K)]|\psi(t)\rangle + 8J(x)[h(x+1,t) - h(x,t)]\langle\psi(t)|\tau(x,x+1)|\psi(t)\rangle, \tag{10}$$

$$i\frac{d}{dt}|\psi(t)\rangle = \left[H_0(J,K) + \sum_{x=1}^{s} h(x,t)\sigma_3(x)\right]|\psi(t)\rangle$$

in the unknown *force field* $h(x+1,t) - h(x,t)$ and in the unknown *wave function* $|\psi(t)\rangle$. Naturally, $|\psi(t)\rangle$ is required to have the correct initial magnetization $\overline{m}_3(x,0)$ and the correct initial current $\overline{j}(x,0)$. For this formulation of the van Leeuwen theorem [2] as a nonlinear Schrödinger equation in which the potential is itself a functional of the wave function, we refer the reader to Refs. [9] and [10].

In the applications, $H_0(J,K)$ typically describes the two-qubit interaction one is physically able to achieve. Suppose, however, that the task one has to undertake is the transfer of magnetization along the chain [11,12] realizable through a different two-qubit Hamiltonian $H_0(\overline{J},\overline{K})$. The question is whether a force field $h(x+1,t) - h(x,t)$ can compensate for the "wrong" choice of two-body couplings.

As an example, consider as a *target* system a spin chain evolving under the *engineered XY Hamiltonian*

$$\overline{H} = -\frac{1}{2}\sum_{x=1}^{s-1}\frac{\pi\sqrt{x(s-x)}}{s}\tau(x,x+1). \tag{11}$$

The Hamiltonian (11), first discussed in [13] and then renamed an *engineered XY chain* in [3], is quite interesting for the quantum-computing community: it induces a periodic behavior of the system with period $T = 2s$; in particular it realizes the *perfect transfer* of an excitation (spin up) initially located at the first site $x = 1$ to the final site $x = s$ in a time s [12].

Figure 2, to be compared with Fig. 3 of Ref. [1], summarizes some experience we have gained in the numerical integration of (10) for $s = 6$, starting from the initial condition

$$|\psi_0\rangle = \frac{1}{\sqrt{s}}\sum_{x=1}^{s}|x\rangle, \tag{12}$$

where we have indicated by

$$|x\rangle = |\sigma_3(x) = +1, \quad \sigma_3(y) = -1 \ \text{ for } y \neq x\rangle$$

the simultaneous eigenstate of the operators σ_3 in which only the spin at position x is "up." As Fig. 2 shows, without undertaking the difficult task of implementing the engineered couplings, varying as $\sqrt{x(s-x)}$, it is possible to obtain the same magnetization and current fields using spatially homogeneous two-body couplings and suitably chosen *control fields* $h^c(x,t)$, e.g., by letting, as we did, the initial condition $|\psi_0\rangle$ evolve under

$$H^c = -\frac{1}{2}\sum_{x=1}^{s-1}\tau(x,x+1) + \sum_{x=1}^{s}h^c(x,t)\sigma_3(x). \tag{13}$$

III. OPEN SPIN CHAINS

We discuss the possibility of extending the above discussion to the case in which the initial state of the system, described by a density matrix ρ_0, evolves according to a Lindblad equation of the form

$$\frac{d\rho(t)}{dt} = i[\rho(t),H(t)] + \mathcal{D}(\rho(t)), \tag{14}$$

where $H(t)$ is of the form (1). The dissipator $\mathcal{D}$ that we consider takes into account both the dephasing induced by the interaction of each spin with some external degrees of freedom (for example, phonons) and the coupling with unequal one-spin

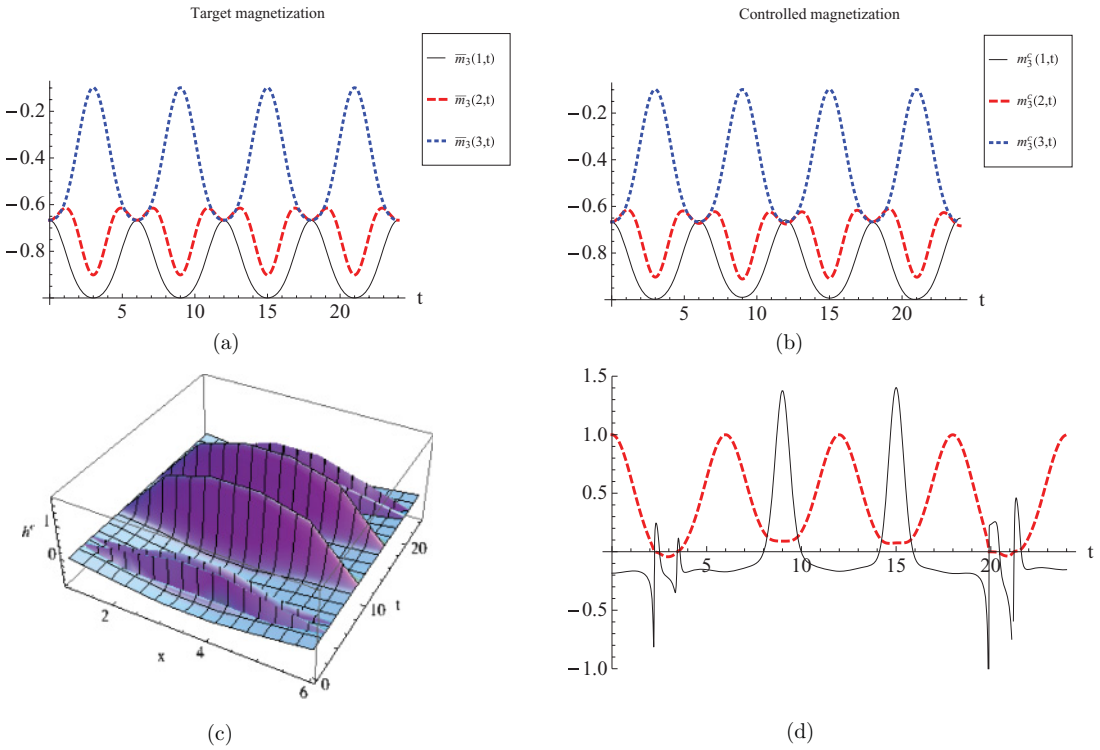

FIG. 2. (Color online) $s = 6$. (a) The magnetization field determined by the target Hamiltonian (11). (b) The magnetization field determined by the controlled Hamiltonian (13). (c) The control field $h^c(x,t)$, obtained by numerical integration of (10), as a function of x and t; interpolation in x is only for graphical convenience. (d) The control field $h^c(2,t)$ (solid line) and the the mean value of $\tau(1,2)$ in the controlled state (dashed line). In order to avoid singularities in $h^c(x,t)$ due to the zeros of this mean value, we have used Tikhonov regularization [16].

baths [14] $\mathcal{B}_L$ and $\mathcal{B}_R$ at both ends of the chain; it has the form

$$\mathcal{D}(\rho) = \mathcal{D}^{\text{deph}}(\rho) + \mathcal{D}^{\text{bath}}(\rho). \tag{15}$$

The dephasing superoperator is given, in Lindblad form [4,5], by

$$\mathcal{D}^{\text{deph}}(\rho) = \sum_{x=1}^{s} \{[L(x)\rho, L(x)^\dagger] + [L(x), \rho L(x)^\dagger]\}, \tag{16}$$

where the generator associated with each site x is

$$L(x) = \sqrt{\frac{\eta}{2}}\sigma_3(x).$$

$\mathcal{D}^{\text{bath}}$, instead, involves four generators:

$$\begin{aligned} L_1 &= \sqrt{\epsilon(1-\mu)}\sigma_+(1), \quad L_2 = \sqrt{\epsilon(1+\mu)}\sigma_-(1), \\ L_3 &= \sqrt{\epsilon(1+\mu)}\sigma_+(s), \quad L_4 = \sqrt{\epsilon(1-\mu)}\sigma_-(s), \end{aligned} \tag{17}$$

where the coupling parameter ϵ and the asymmetry parameter μ satisfy the conditions $\epsilon > 0$ and $-1 \leqslant \mu \leqslant 1$. The asymmetry parameter μ models a possible difference of the chemical potentials of $\mathcal{B}_L$ and $\mathcal{B}_R$. We refer the reader to the second section of [15] for a discussion of the range of validity of this approach and of the possible degree of control on the baths and on the bath-system interaction.

For the sake of clarity, we discuss the effect of the two sources of dissipation separately.

If there is no interaction with the baths ($\epsilon = 0$), for $1 \leqslant x \leqslant s$,

$$\text{Tr}[\sigma_3(x)\mathcal{D}(\rho)] = 0. \tag{18}$$

The continuity equation (3) retains, then, the form

$$\frac{dm_3(x,t)}{dt} + [j(x,t) - j(x-1,t)] = 0$$

where, now, $m_3(x,t) = \text{Tr}[\sigma_3(x)\rho(t)]$ and $j(x,t) = \text{Tr}[\text{j}(x)\rho(t)]$. Simple algebraic manipulations show that, for $1 \leqslant x < s$,

$$\text{Tr}[j(x)\mathcal{D}(\rho)] = -4\eta\text{Tr}[\text{j}(x)\rho]. \tag{19}$$

The evolution of the current field $j(x,t)$ is modified by the presence of dephasing, namely,

$$\frac{dj(x,t)}{dt} = -i\ \text{Tr}\{[\text{j}(x), H(t)]\rho(t)\} - 4\eta j(x,t). \tag{20}$$

The commutator on the right-hand side is given by (5).

The evolution in the presence of the interaction with the baths $\mathcal{B}_L$ and $\mathcal{B}_R$ ($\eta = 0$, $\epsilon > 0$), on the other side, determines a nontrivial modification of the continuity equation. For $1 \leqslant k \leqslant 4$, we set

$$\mathcal{D}L_k(\rho(t)) = [L_k\rho, L_k^\dagger] + [L_k, \rho L_k^\dagger]$$

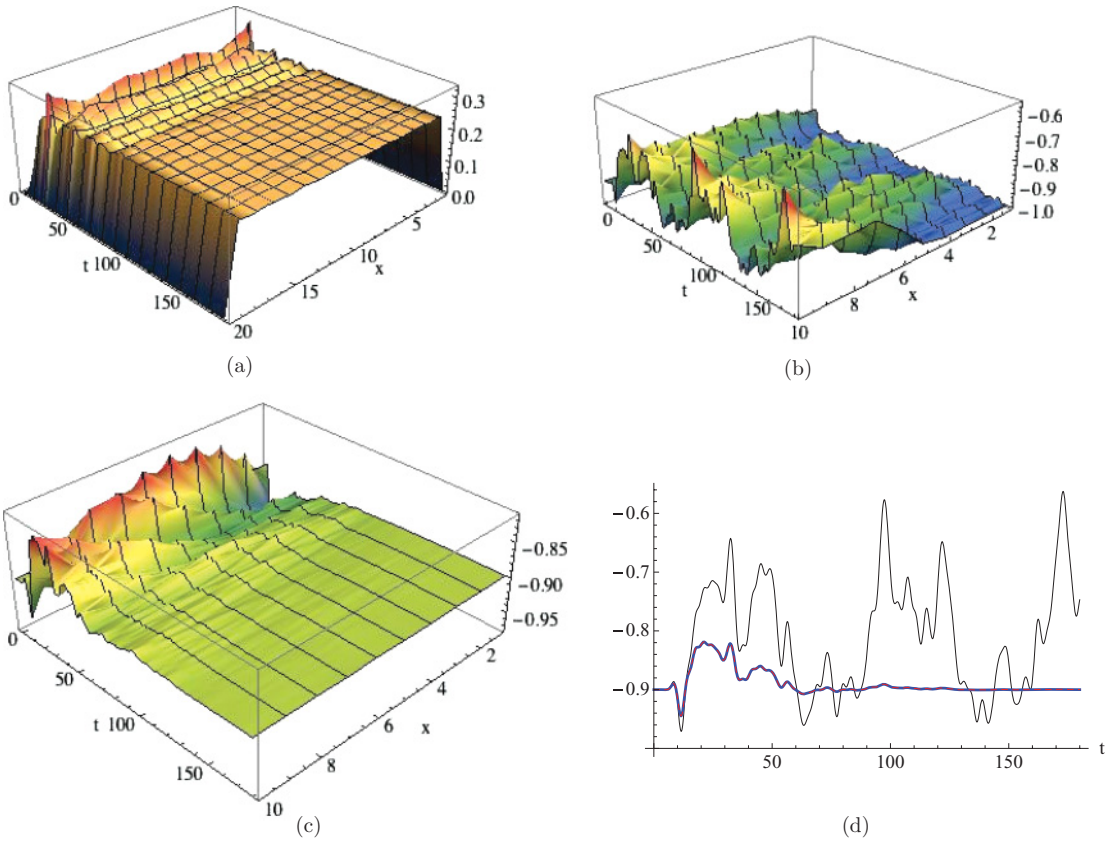

FIG. 3. (Color online) $s = 20$, $\eta = 0.01$, $\epsilon = 0$. (a) The Kohn-Sham potential $h^c(x,t)$. (b) The field $m_3(x,t)$ corresponding to purely unitary evolution of the initial condition ρ_0 under the Hamiltonian (25). (c) The magnetization field $m_3^c(x,t)$. (d) $m_3(10,t)$ (thin line) and $m_3^c(10,t)$ (thick line). The field $m_3^{\text{deph}}(x,t)$ is numerically indistinguishable from $m_3^c(x,t)$.

so that we have

$$\mathcal{D}^{\text{bath}}(\rho) = \sum_{k=1}^{4} \mathcal{D}L_k(\rho). \tag{21}$$

A little algebra shows now that the effect of the left bath $\mathcal{B}_L$ on the magnetization is

$$\begin{aligned}&\text{Tr}\{\sigma_3(x)[\mathcal{D}L_1(\rho) + \mathcal{D}L_2(\rho)]\}\\ &\quad = -\delta_{1,x} 4\epsilon\{\mu + \text{Tr}[\sigma_3(x)\rho]\},\end{aligned}$$

whereas the effect of the right bath $\mathcal{B}_R$ is

$$\begin{aligned}&\text{Tr}\{\sigma_3(x)[\mathcal{D}L_3(\rho) + \mathcal{D}L_4(\rho)]\}\\ &\quad = -\delta_{s,x} 4\epsilon\{-\mu + \text{Tr}[\sigma_3(x)\rho]\}.\end{aligned}$$

The continuity equation reads now

$$\begin{aligned}&\frac{dm_3(x,t)}{dt} + [j(x,t) - j(x-1,t)]\\ &\quad = -4\epsilon\{\delta_{1,x}[m_3(x,t) + \mu] + \delta_{s,x}[m_3(x,t) - \mu]\}.\end{aligned} \tag{22}$$

The right-hand side of (22) plays the role of a *dissipation current* [7].

As to the time evolution of the current field, it is

$$\begin{aligned}\frac{dj(x,t)}{dt} &= -i\text{Tr}\{[\text{j}(x), H(t)]\rho(t)\}\\ &\quad - 2\epsilon(\delta_{1,x} + \delta_{s-1,x}) j(x,t).\end{aligned} \tag{23}$$

Summarizing, the kinematical and dynamical equations in the presence of both dephasing and coupling with the baths ($\eta > 0$ and $\epsilon > 0$) are

$$\begin{aligned}&\frac{dm_3(x,t)}{dt} + [j(x,t) - j(x-1,t)]\\ &\quad = -4\epsilon\{\delta_{1,x}[m_3(x,t) + \mu] + \delta_{s,x}[m_3(x,t) - \mu]\}, \frac{dj(x,t)}{dt}\\ &\quad = -i\text{Tr}\{[\text{j}(x), H(t)]\rho(t)\} - [4\eta + (\delta_{1,x} + \delta_{s-1,x})2\epsilon] j(x,t).\end{aligned} \tag{24}$$

We conclude this section with a few numerical examples. In all the examples that follow, we take an initial condition of the form $\rho_0 = |\psi_0\rangle\langle\psi_0|$, with $|\psi_0\rangle$ given, for different values of s, by (12).

A. Pure dephasing

In the case of pure dephasing, the observable

$$N_3 = \sum_{x=1}^{s} \frac{1 + \sigma_3(x)}{2},$$

namely, the number of *particles* (spins up), is a constant of motion. It has been shown in Ref. [6] that it is possible to reproduce the current and density of an electronic system subject to a number-conserving dissipation by letting the

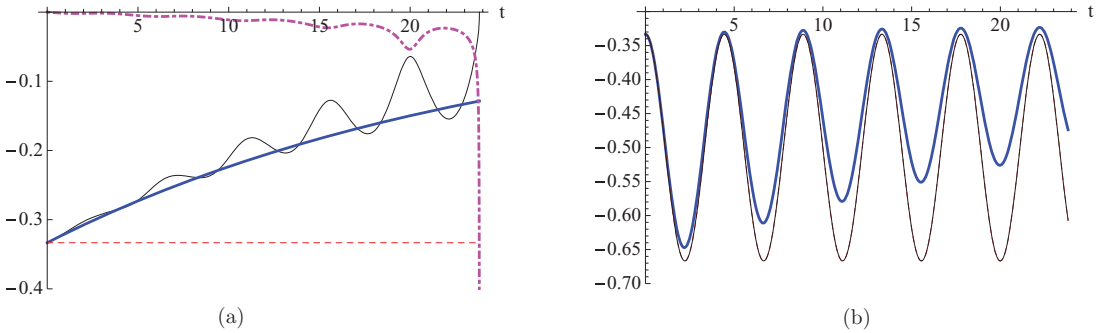

FIG. 4. (Color online) $s = 3$, $\eta = 0.01$, $\epsilon = 0$. (a) The control field $h^c(2,t)$ is represented (rescaled by a factor 0.1 for graphical convenience) as a function of time as a dot-dashed thick line. Expectations of the local kinetic energy $T(1)$, under three different evolutions, are represented as functions of time: the dashed line corresponds to the pure Hamiltonian; the solid thick line to Hamiltonian + dephasing; the solid thin line to Hamiltonian+dephasing+control field. (b) The expectations of $\sigma_3(1)$ for the same three systems. Same graphical conventions as in (a); the dashed line is not visible since the magnetizations of the target and controlled systems are, as long as both exist, numerically indistinguishable.

same quantum system evolve unitarily under a time-dependent Hamiltonian with suitably chosen control field $h^c(x,t)$. We wish to show that the same considerations apply to open spin chains as well.

Suppose that the interactions in the chain are described by the XY Hamiltonian

$$H_0 = -\frac{1}{2}\sum_{x=1}^{s-1}[\sigma_+(x)\sigma_-(x+1) + \sigma_+(x+1)\sigma_-(x)], \quad (25)$$

which can be obtained from the Hamiltonian family described by (1) by setting $J(x) = -1/4$, $K(x) = h(x,t) = 0$. The evolution of the chain under the sole effect of dephasing from the initial state ρ_0 is determined by the Lindblad equation (14) with $\mathcal{D} = \mathcal{D}^{\text{deph}}$ defined as in (16). We indicate by $j^{\text{deph}}(x,t)$ and $m_3^{\text{deph}}(x,t)$ the ensuing current and magnetization fields.

We wish to determine an external field $h^c(x,t)$ such that the evolution $\rho^c(t)$ of the initial state ρ_0 under the Hamiltonian

$$H^c(t) = H_0 + \sum_{x=1}^{s} h^c(x,t)\sigma_3(x) \quad (26)$$

determines the same magnetization and current fields as in the dissipating system, that is,

$$\begin{aligned} m_3^c(x,t) &= \text{Tr}[\sigma_3(x)\rho^c(t)] = m_3^{\text{deph}}(x,t), \\ j^c(x,t) &= \text{Tr}[\text{j}(x)\rho^c(t)] = j^{\text{deph}}(x,t). \end{aligned} \quad (27)$$

It is sufficient to solve, for the state $\rho^c(t)$, the Liouville problem

$$\rho^c(0) = \rho_0, \quad \frac{d\rho^c(t)}{dt} = i[\rho^c(t), H^c(t)], \quad (28)$$

where the unknown field $h^c(x,t)$ is itself a functional of ρ^c through the algebraic equation

$$\begin{aligned} \frac{dj^{\text{deph}}(x,t)}{dt} &= -i\text{Tr}\{[\text{j}(x), H_0]\rho^c(t)\} + 8J(x)[h^c(x+1,t) \\ &\quad - h^c(x,t)]\text{Tr}[\tau(x,x+1)\rho^c(t)]. \end{aligned} \quad (29)$$

In the numerical example that we discuss below, $dj^{\text{deph}}(x,t)/dt$ is known, having been determined by numerical integration of the Lindblad equation for pure dephasing under the initial condition $|\psi_0\rangle\langle\psi_0|$ with $s = 20$ and $\eta = 0.01$.

Figure 3 shows that, for this example, the differential-algebraic problem posed by (28) and (29) does have a solution that very well attains the current of the dissipating system ($j^c = j^{\text{deph}}$) and, because of the continuity equation (3), also the magnetization ($m_3^c = m_3^{\text{deph}}$). The Kohn-Sham potential [6] shown in Fig. 3(a) is able to reduce the amplitude of the oscillations visible, for Hamiltonian evolution under H_0, in Fig. 3(b); this leads to the magnetization profile of Fig. 3(c), in which the controlled magnetization is reported: it is numerically indistinguishable from the target magnetization (not reported). Because of the left-right symmetry of our problem we have found it sufficient to let x go only from 1 to $s/2$.

As a further example, we pose the following, complementary, problem: we are given an open quantum system affected only by dephasing ($\epsilon = 0, \eta > 0$) and evolving under a master equation of the form (14). Is it possible to determine an external control field h^c that compensates for the effects of dissipation, at least as far as the magnetization m_3 and the current j fields are concerned?

For the sake of definiteness, we consider a spin chain with XY interaction H_0, as in (25). The system is affected by noise: the dissipator $\mathcal{D}^{\text{deph}}$ [see Eq. (16)] intervenes in the evolution of the system as in (14). We are looking for a choice of a control field h^c such that the current and magnetization fields evolve in time as if the dissipator were not acting at all; namely, the target is

$$\begin{aligned} \overline{m}_3(t,x) &= \text{Tr}[\sigma_3(x)\overline{\rho}(t)], \\ \overline{j}(x,t) &= \text{Tr}[\text{j}(x)\overline{\rho}(t)], \end{aligned}$$

where $\overline{\rho}(t)$ is the solution of

$$\frac{d\overline{\rho}}{dt} = i[H, \overline{\rho}(t)]$$

with the initial condition $\overline{\rho}(0) = \rho_0$.

Figure 4 refers to a system of $s = 3$ spins. It shows that our control scheme works only *locally*; in fact, as soon as one of the local kinetic energy terms $T(x) = 2J(x)\tau(x,x+1)$ hits the value zero, the corresponding control field h^c develops a singularity, as shown in Fig. 4(a). It is not surprising that the control problem posed above admits only a solution that

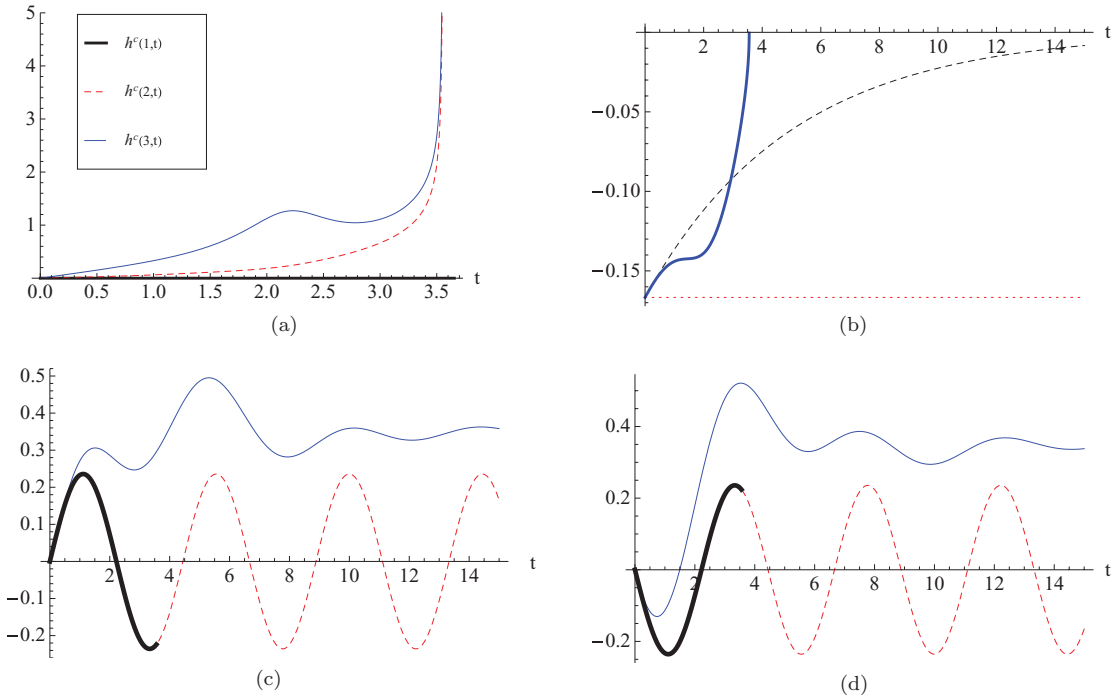

FIG. 5. (Color online) $s = 3$, $\epsilon = 0.1$, $\mu = -1$, $\eta = 0$. (a) The field $h^c(x,t)$. (b) $\mathrm{Tr}[T(1)\overline{\rho}(t)]$ (dotted line); $\mathrm{Tr}[T(1)\rho^{\mathrm{actual}}(t)]$ (dashed line); $\mathrm{Tr}[T(1)\rho^c(t)]$ (solid thick line). (c) $\bar{j}(1,t)$ (dashed line); $j^c(1,t)$ (solid thick line); $j^{\mathrm{actual}}(1,t)$ (solid thin line). (d) $\bar{j}(2,t)$ (dashed line); $j^c(2,t)$ (solid thick line); $j^{\mathrm{actual}}(2,t)$ (solid thin line). The current field $j^c(x,t)$ is, as long as it exists, numerically indistinguishable from the target field $\overline{j}(x,t)$.

is local in time. This aspect of the problem has already been discussed in [9] and [16].

B. Dissipation current

In order to discuss the role of Eq. (22), we analyze here, for the sake of definiteness, the same problem posed at the end of the previous section (is there an external field that "compensates" for dissipation?) in the presence of interaction with the baths $\mathcal{B}_L$ and $\mathcal{B}_R$. The novel feature that appears in the case $\epsilon > 0$ is the fact that the number operator N_3 ceases to be a constant of motion: "charges" in the form of spins up can be pumped into or drained from the chain by the baths. It is well known that conventional time-dependent density-functional theory (TDDFT), as discussed in Ref. [6], does not hold when the total particle number is not conserved. Here we focus our attention on the modifications needed when one considers a variant of the context of Ref. [1] in which the total magnetization is not conserved. One must carefully distinguish between magnetization and current. In the discussion that follows, we set

$$H^c(t) = H_0 + \sum_{x=1}^{s} h^c(x,t)\sigma_3(x),$$

with H_0 given by Eq. (25), and consider the dissipator (21)

$$\mathcal{D}^{\mathrm{bath}}(\rho) = \sum_{k=1}^{4} \mathcal{D}L_k(\rho);$$

for the definition of the current operator $\mathrm{j}(x)$ we refer to Eq. (2) and, as usual, we take in our numerical example $\rho_0 = |\psi_0\rangle\langle\psi_0|$ with $|\psi_0\rangle$ as in (12).

Figure 5 answers, in the particular case $s = 3$, the following question: is there a field $h^c(x,t)$ such that, under the action of a Hamiltonian of the form $H^c(t)$, and of the dissipator $\mathcal{D}^{\mathrm{bath}}(\rho)$, the initial condition $\rho(0)$ evolves into a state $\rho^c(t)$ for which the expectation value $\mathrm{Tr}[\rho^c(t)j(x)]$ coincides, for $1 \leqslant x \leqslant s-1$ and at least in a neighborhood of $t = 0$, with

$$\overline{j}(x,t) \stackrel{\mathrm{def}}{=} \langle\psi_0|\exp(+itH_0)\mathrm{j}(x)\exp(-itH_0)|\psi_0\rangle?$$

The behavior of the control field $h^c(x,t)$ satisfying the condition

$$\mathrm{Tr}[\rho^c(t)\mathrm{j}(x)] = \overline{j}(x,t) \tag{30}$$

posed above shows [see Fig. 5(a)] that the existence of the solution is again local, because of the vanishing [Fig. 5(b)] of the expected local kinetic energy $T(1)$ in the controlled evolution. Figures 5(c) and 5(d) show that, as long as it is defined, the field $h^c(x,t)$ does enforce the target current: this is hardly surprising since it has been found by imposing precisely this condition.

In order to compare, in the figures, the controlled evolution with the Lindblad evolution without control, we define $\rho^{\mathrm{actual}}(t)$ as the evolution of the initial condition ρ_0 determined solely by the Hamiltonian H_0 and the dissipator $\mathcal{D}^{\mathrm{bath}}$. Setting

$$\overline{m}_3(x,t) \stackrel{\mathrm{def}}{=} \langle\psi_0|\exp(+itH_0)\sigma_3(x)\exp(-itH_0)|\psi_0\rangle,$$

Fig. 6 answers, in the same situation as above, the following different question: for which values of x does the state

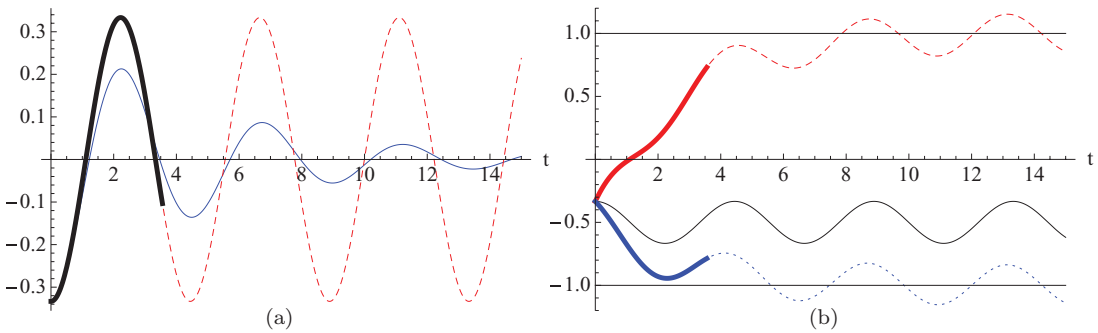

FIG. 6. (Color online) $s = 3$, $\epsilon = 0.1$, $\mu = -1$, $\eta = 0$. (a) $\mathrm{Tr}[\sigma_3(2)\rho^{\mathrm{actual}}(t)]$ (solid thin line); $\overline{m}_3(2,t)$ (dashed line); $m_3^c(2,t)$ (solid thick line). The magnetization $m^c(2,t)$ is, as long as it exists, numerically indistinguishable from the target magnetization $\overline{m}_3(x,t)$. (b) $a(t)$ and $b(t)$ as functions of time (dashed and dotted thin lines, respectively); the corresponding fields $m_3^c(1,t)$ and $m_3^c(3,t)$ determined by numerical (local) solution of the VL problem are represented as thick lines; solid thin line: the target magnetization $\overline{m}_3(1,t) = \overline{m}_3(3,t)$. For the extremal sites of the chain, the controlled system does not attain, even locally, the target magnetization.

$\rho^c(t)$ determined by imposing the condition (30) satisfy the additional condition

$$\mathrm{Tr}[\rho^c(t)\sigma_3(x)] = \overline{m}_3(x,t)? \tag{31}$$

In order to answer this question, we must use Eq. (22). For $1 < x < s$ we have

$$\begin{aligned}\frac{dm_3^c(x,t)}{dt} &= -[j^c(x,t) - j^c(x-1,t)] \\ &= -[\overline{j}(x,t) - \overline{j}(x-1,t)] = \frac{d\overline{m}_3(x,t)}{dt}\end{aligned}$$

and

$$m_3^c(x,0) = \overline{m}_3(x,0).$$

Therefore, the controlled magnetization $m_3^c(x,t)$ at sites $2,3,\ldots,s-1$ is, as long as it exists, identical to the target one [Fig. 6(a)].

As to the sites coupled to the reservoirs, because, again, of Eq. (22), the following differential equation holds for $m_3^c(1,t)$:

$$\begin{aligned}\frac{dm_3^c(1,t)}{dt} &= -j^c(1,t) - 4\epsilon\mu - 4\epsilon m_3^c(1,t) \\ &= -\overline{j}(1,t) - 4\epsilon\mu - 4\epsilon m_3^c(1,t) \\ &= \frac{d\overline{m}_3(1,t)}{dt} - 4\epsilon\mu - 4\epsilon m_3^c(1,t).\end{aligned}$$

Under the initial condition $m_3^c(1,0) = \overline{m}_3(1,0)$, this implies that

$$\begin{aligned}m_3^c(1,t) = \overline{m}_3(1,t) &- \mu(1 - e^{-4\epsilon t}) \\ &- 4\epsilon e^{-4\epsilon t}\int_0^t \overline{m}_3(1,\tau)e^{4\epsilon t}d\tau.\end{aligned} \tag{32}$$

Similarly, at site s, we have

$$\begin{aligned}m_3^c(s,0) &= \overline{m}_3(s,0), \\ \frac{dm_3^c(s,t)}{dt} &= \frac{d\overline{m}_3(s,t)}{dt} + 4\epsilon\mu - 4\epsilon m_3^c(s,t),\end{aligned}$$

and, therefore,

$$\begin{aligned}m_3^c(s,t) = \overline{m}_3(s,t) &+ \mu(1 - e^{-4\epsilon t}) \\ &- 4\epsilon e^{-4\epsilon t}\int_0^t \overline{m}_3(s,\tau)e^{4\epsilon t}d\tau.\end{aligned} \tag{33}$$

Therefore, the controlled magnetizations at sites 1 and s are, as long as they exist, different from the target ones [see the initial part of Fig. 6(b)].

By explicit computation it is easy to see that, in the simple example $s = 3$ at hand, the target magnetizations are given by

$$\overline{m}_3(2,t) = -\frac{1}{6}\cos(\sqrt{2}t)$$

and

$$\overline{m}_3(1,t) = \overline{m}_3(3,t) = -\frac{1}{2} + \frac{1}{6}\cos(\sqrt{2}t).$$

With the above explicit expressions for $\overline{m}_3$ and $m_3^c(3,t)$, the right-hand sides of Eqs. (32) and (33) can immediately be computed, namely,

$$\begin{aligned}a(t) &= \overline{m}_3(1,t) - \mu(1 - e^{-4\epsilon t}) - 4\epsilon e^{-4\epsilon t}\int_0^t \overline{m}_3(1,\tau)e^{4\epsilon t}d\tau, \\ b(t) &= \overline{m}_3(s,t) + \mu(1 - e^{-4\epsilon t}) - 4\epsilon e^{-4\epsilon t}\int_0^t \overline{m}_3(s,\tau)e^{4\epsilon t}d\tau.\end{aligned}$$

These are the two quantities represented by the thin dashed and dotted lines in Fig. 6(b), extending well beyond the interval $0 \leqslant t \leqslant 3.55$ of existence of the solution of the VL problem.

The fact that there is a value of t beyond which $a(t)$ and $b(t)$ can go out of the interval $[-1,1]$ of physically acceptable values of magnetization convinces us of the fact that the determination of a control field compensating for the dissipation induced by the interaction with the baths $\mathcal{B}_L$ and $\mathcal{B}_R$ admits a solution that is *at most local* in t. The local character of the solution is therefore determined neither by the choice of the initial condition, nor by the Hamiltonian and dissipator, nor by the numerical algorithm for solution of the differential algebraic problem.

IV. CONCLUSIONS AND OUTLOOK

We have probed the interesting idea, advanced in Ref. [1], of quantum computing, by means of spin-1/2 arrays, without use of the wave function. In our exposition we have stressed the dynamic control perspective advanced in [1]: the components of the wave function or, in our generalization to the case of open quantum systems, of the density matrix, are *latent* dynamical variables, that in their evolution (parametrized by $J,K,\epsilon,\mu,\eta,|\psi_0\rangle$) determine the response, in terms of output magnetization and/or current, to the time-dependent input variables $h^c(x,t)$.

In our choice of numerical examples, we have concentrated on themes motivated by our previous experience with Feynman's model of a quantum computer [13,17,18]. For instance, the numerical example of Fig. 2 can be rephrased in the following way: can one use the freedom of reparametrizing the system $(J,K,\ldots,|\psi_0\rangle \to J',K',\ldots,|\psi_0'\rangle)$, without altering the input-output response, in such a way as to simulate, on a transitionally invariant structure, the delicate tailoring of hopping parameters required for perfect transfer of the cursor along the program line? The example of Fig. 4 can be similarly reformulated as follows: can one compensate by external fields for, in the words of Feynman [17], imperfections and free energy losses in the motion of the clocking cursor?

In answering the above questions, the success of TDDFT has been only partial because the solutions exist only locally in time: the point is that in Eqs. (10) and (29) the unknown gradient $h^c(x+1,t)-h^c(x,t)$ appears with the local mean kinetic energy as a coefficient. This difficulty would turn out to be particularly severe if one tried to simulate a sharp initial condition in the Hamiltonian context of Fig. 2: the local mean kinetic energy terms are in this case initially zero. In the context of Fig. 4 (dephasing), vanishing of the expected values of the operators $\tau(x,y)$ is unavoidable, because they are precisely the nondiagonal matrix elements of the density matrix that dephasing is supposed to damp.

The example of Figs. 5 and 6 (interaction with baths) shows that it is indeed possible to compensate for dissipation even when the number of particles is no longer a constant of motion, at least for the spins that are not coupled with the baths. It is not surprising that the magnetizations of the extremal sites are not attainable by means of the control field: the field h^c does commute with the number operator and therefore is not able to absorb injected charges or to create new ones.

Further efforts are needed, we think, in the choice and/or in the smoothing of the initial condition and in the introduction of "convergence factors" [1] that extend the existence interval of the solution with small errors in the overall propagation. As a final remark, we observe that a numerical analysis of the size-dependence of problems associated with the vanishing of kinetic energy [19] would greatly benefit from application of numerical methods, such as wave-function Monte Carlo simulations, more efficient than the brute-force numerical integration we have adopted.

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