ON FERMIONIC MODELS OF A CLOSED ECOSYSTEM WITH APPLICATION TO BACTERIAL POPULATIONS

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ABSTRACT. This paper deals with the application of operatorial techniques of quantum physics to a theoretical model of closed ecosystems. The model is built by using fermionic operators whose evolution is ruled by a self–adjoint Hamiltonian operator. Adopting Heisenberg–like dynamics, we consider either linear or nonlinear models with the aim of describing the long–term survival of bacterial populations; the introduction of effective dissipative mechanisms is also considered. Moreover, a variant of linear models through the introduction of additional rules acting periodically on the system is proposed. Specifically, the evolution in a time interval is obtained by gluing the evolutions in a finite set of adjacent subintervals. In each subinterval the Hamiltonian is time independent, but the values of the parameters entering the Hamiltonian may be changed by the rules at the end of a subinterval on the basis of the actual state of the system. Within this context, a new approach is provided in order to obtain reliable results, without increasing the computational cost of the numerical integration of the differential equations involved.

1. Introduction

The description of the dynamics of classical complex systems may be profitably carried out with an operatorial approach, typical of quantum mechanics, even in the case of macroscopic systems (Bagarello 2012); in a series of recent papers, it has been shown how this method, based on raising and lowering operators, can be used to successfully analyze the dynamical aspects of stock markets (Bagarello 2006, 2007), love affairs (Bagarello 2011; Bagarello and Oliveri 2010), population migration phenomena (Bagarello and Oliveri 2013), escape strategies of crowds (Bagarello, Gargano, and Oliveri 2015), desertification processes (Bagarello, Cherubini, and Oliveri 2016).

In this paper, the operatorial approach is exploited to study the dynamics of a bacterial population constrained in a closed environment; the model here considered is derived from a general one developed in Bagarello and Oliveri (2014), and aims to describe some features of the long–term survival of bacterial populations.

Bacteria are highly–complex thermodynamic systems, requiring a source of energy for maintaining their structure and functions. Bacterial growth is influenced by nutrient availability and environmental conditions, such as pH, temperature, oxygen, presence of
toxic compounds, etc. When one or more environmental conditions become unfavourable, bacteria react in order to survive. Some genera, such as *Bacillus* and *Clostridium*, when under negative stimuli, produce endospores, *i.e.*, differentiated cells with no active metabolism, able to survive for an indefinite time in terms of “latent life”. When optimal conditions are restored, the endospores germinate, metabolism is activated, and new vegetative cells appear. On the contrary, there are non–sporulating genera which are able to trigger efficient resistance mechanisms. The survival of the latter genera attracted in the last 30 years the attention of many microbiologists with the aim of characterizing the molecular mechanisms underlying the bacterial stress response. In general, when under stress, several phenotypic variations are observed (reduction of cell size, morphological transitions from rod to spherical shape (Reeve, Amy, and Matin 1984), decrease in metabolic activity (Cabral 1995; Chapman, Fall, and Atkinson 1971; Kjelleberg *et al.* 1987), synthesis repression of constitutive proteins, synthesis activation of stress–induced proteins required for survival (Eberl *et al.* 1996; Givskov, Eberl, and Molin 1994; Van Overbeek *et al.* 1995)); parallely, increased resistance against external challenges (*e.g.*, $H_2O_2$, antibiotics, disinfecting solutions) and improved ability to persist in their habitat are displayed (Rockabrand *et al.* 1995; Van Overbeek *et al.* 1995).

Special attention has been devoted to *Pseudomonas aeruginosa*, an ubiquitous bacterium capable to use more than one hundred of chemical compounds as carbon and energy sources, and, due to its wide metabolic versatility, persist for prolonged periods of time without external sources of nutrients. Remarkably, it is the ethiological agent of several diseases, and represents an emergence in nosocomial infections, because of its high degree of resistance against several classes of antibiotics and persistence also in disinfecting solutions. For these features, it is important to develop models able to better comprehend, or at least describe, the observed long–term survival of such bacterial populations (Carnazza *et al.* 2008; Di Salvo and Oliveri 2016).

The closed ecosystem that will be considered in this paper is made by four compartments, representing the nutrients, the bacteria and two kinds of garbage, whose role will be detailed below.

The model is built by using some tools from quantum mechanics, like operator algebras and, in particular, the so–called number representation, which proved to be quite useful to set up a natural description of a system in rather different areas. In fact, there are situations (say, stock markets) where several quantities changing discontinuously are well described in terms of the integer eigenvalues of certain relevant self–adjoint operators, the observables of the system, and the dynamics ruled by an energy–like operator, the *Hamiltonian*. In such a framework, we associate to each compartment of our model an annihilation, a creation, and a number operator ($a_j$, $a_j^\dagger$, and $\hat{n}_j = a_j^\dagger a_j$, respectively).

We shall use fermionic operators due to two main reasons. The first one is technical, since the Hilbert space of the model (involving a finite number of fermionic modes) will result finite–dimensional, and the operators $a_j$ are represented by $2^4 \times 2^4$ matrices. The second one is concerned with the biological interpretation of the model: for each compartment, we will have only two possible non–trivial situations. In the first one (the ground state) there is a very low density, while in the second one (the excited state), the density is very high. Hence, if we try to increase the density of the excited state, or if we try to decrease the density of the ground state, we simply annihilate that compartment. We can interpret this
fact just saying that there exist upper and lower bounds to the densities of the compartments which cannot be overcome for obvious reasons. Of course, this rather sharp division in just two levels may appear unsatisfactory.

All the fermionic operators involved in the model satisfy the Canonical Anti–commutation Rules (CAR)

$$\{a_j, a_k^\dagger\} := a_j a_k^\dagger + a_k^\dagger a_j = \delta_{j,k}, \quad \{a_j, a_k\} = \{a_j^\dagger, a_k^\dagger\} = 0, \quad j, k = 1, \ldots, 4;$$

(1)

furthermore, the states of the quantum system are vectors in the $2^4$–dimensional Hilbert space $\mathcal{H}$ constructed as the linear span of the vectors

$$\varphi_{n_1,n_2,n_3,n_4} := (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}(a_3^\dagger)^{n_3}(a_4^\dagger)^{n_4} \varphi_0,$$

where $n_j \in \{0, 1\}$ for all $j = 1, \ldots, 4$, and $\varphi_0$ is the vacuum of the theory, i.e., a vector that is annihilated by all the operators $a_j$.

The vectors $\varphi_{n_1,n_2,n_3,n_4}$ give an orthonormal set of eigenstates of the number operators, say

$$\hat{n}_j \varphi_{n_1,n_2,n_3,n_4} = n_j \varphi_{n_1,n_2,n_3,n_4}, \quad \text{for all} \ j = 1, \ldots, 4.$$

(2)

The dynamics is governed by a self–adjoint time independent Hamiltonian operator $H$ embedding the main effects deriving from the interactions among the compartments of the system, and has the property of determining the time evolution of any actor $X$ of the model, in the so–called Heisenberg representation, as in quantum mechanics:

$$X(t) = \exp(iHt)X \exp(-iHt),$$

(3)

or, equivalently, by the differential equation

$$\frac{dX(t)}{dt} = i \exp(iHt)[H,X] \exp(-iHt) = i[H,X(t)],$$

(4)

where $[A,B] := AB - BA$ is the commutator between $A$ and $B$.

Therefore, the description of the dynamics requires, in principle, the solution of $2^{10}$ differential equations (or, equivalently, the computation of the exponential of the Hamiltonian, which is a $2^4 \times 2^4$ matrix, and of its inverse); once defined a vector state $\varphi_{n_1,n_2,n_3,n_4}$ representing the initial configuration of the system, we compute the mean values

$$n_j(t) = \langle \varphi_{n_1,n_2,n_3,n_4}, \hat{n}_j(t) \varphi_{n_1,n_2,n_3,n_4} \rangle, \quad j = 1, \ldots, 4,$$

(5)

$\langle \cdot, \cdot \rangle$ being the scalar product in $\mathcal{H}$.

These average values are interpreted as the densities (Bagarello, Cherubini, and Oliveri 2016; Bagarello and Oliveri 2014) of the four compartments of the model.

Notice that the differential equations ruling the dynamics are nonlinear for non quadratic Hamiltonians, whereas, for quadratic Hamiltonians, the dynamic equations are linear, and it is possible to drastically reduce the computational complexity of the problem (Bagarello 2012). The methods for the numerical solution of the nonlinear equations encounter major obstacles due to the remarkable growth of the size of the problem as the number of the involved compartments increases, even in the case of models not too much complicated. Of course, this results in a strong limitation on the kind of systems that can be analyzed in practice by means of nonlinear models, and, in particular, makes the operatorial approach computationally unmanageable without large supercomputing resources, for instance in the
case of spatial models describing nonlinear interactions between compartments on a lattice (Di Salvo and Oliveri 2016).

The plan of the paper is the following. In Section 2, we consider both quadratic and non-quadratic Hamiltonians with the aim of describing a bacterial population in a batch culture as a closed ecosystem; moreover, a discussion concerning the matrix representation of the fermionic operators and how this reflects on the computational cost is done. The effects of some dissipative mechanisms, phenomenologically introduced, is also considered. In Section 3, we propose an alternative approach for the operatorial description of the dynamics of a closed ecosystem by considering the additional introduction of specific rules acting periodically on the system and combining their action with the usual quantum definition of the time evolution; these rules repeatedly modify some of the parameters entering the model so as to express the change of the rates of interactions which reasonably take place in the system during its evolution. We implement an innovative *reduced* strategy to efficiently deduce the stepwise time evolution of the observables of the system, which is crucial in the case of a large number of fermionic modes. Finally, Section 4 contains our conclusions.

2. The models of bacterial populations based on fermionic operators

The model presented in this paper is derived from the general scheme already introduced by Bagarello and Oliveri (2014); it aims to describe the experimentally observed long–term survival dynamics of specific bacterial populations in a closed environment. These are situations in which the living bacteria (like \textit{Pseudomonas aeruginosa}), as the nutrients disappear, besides reducing their metabolism, start to use as nutrients the components of dead cells. An operatorial linear model for the description of the colony morphology in stressed/aged bacterial populations of \textit{P. aeruginosa} on a square lattice has been already investigated by Di Salvo and Oliveri (2016).

The scheme of closed ecosystem into consideration from now on (see Fig. 1) is assumed to have 4 compartments, namely the nutrients, the bacteria and two garbages (the first one made up of the dead cells which are reusable as nutrients, and the second one with the waste material not yet reusable or requiring much more time to become recyclable). Some bacterial populations, when the nutrients disappear, use as a source of energy either dead
cells or the products of the metabolism; only a part of these chemical compounds is easily reusable; moreover, some of the products of metabolic activity contribute to degrade the environmental conditions, and, therefore, may act as a stress factor.

Both a linear and a nonlinear model are considered and briefly analyzed.

2.1. The linear dynamical model. The dynamics of the 4–compartment linear model of closed ecosystem is defined by means of the self–adjoint quadratic Hamiltonian operator

\[
\begin{align*}
H = H_0 + H_I, & \quad \text{with} \\
H_0 = \sum_{j=1}^{4} \omega_j a_j^\dagger a_j, & \\
H_I = \lambda \left( a_1 a_2^\dagger + a_2 a_1^\dagger \right) + \sum_{j=1}^{2} \left( v_j^{(1)} \left( a_j a_3^\dagger + a_3 a_j^\dagger \right) + v_j^{(2)} \left( a_4 a_j^\dagger + a_j a_4^\dagger \right) \right),
\end{align*}
\]

where the first mode is related to the nutrients, the second one to the bacteria, and the last two to the garbages. The real constants \( \omega_j \) appearing in the first standard part \( H_0 \) are related to the tendency of each degree of freedom to stay constant in time; the larger their values, the smaller the amplitudes of the oscillations of the related densities (Bagarello 2012); in some sense, they are a measure of the inertia of the various compartments. Moreover, the real parameters \( \lambda, v_j^{(1)} \) and \( v_j^{(2)} \) in \( H_I \) are concerned to the interactions among the bacteria, the nutrients, and the garbages. More in detail, the term \( \lambda a_1 a_2^\dagger \) describes an increasing of bacteria and a simultaneous decreasing of the density of nutrients, the terms involving the parameters \( v_j^{(1)} (v_j^{(2)}) \), respectively describe the analogous interactions between the nutrients (the bacteria, respectively) and the two garbages: the garbages are recycled and transformed into nutrients, and the bacteria, because of their metabolic activity, produce garbage. Of course, to make the Hamiltonian self–adjoint, we are also forced to add the adjoint contributions (see also Bagarello and Oliveri (2014)). Notice that, requiring that \( [H, \hat{n}_j] = [H_0, \hat{n}_j] = 0 \): even if the operators \( a_j \) and \( a_j^\dagger \) have a non trivial time dependence, the density of the \( j \)-th compartments of the system, described by the number operator \( \hat{n}_j \), stays constant in time. The dynamical equations of the system deduced in accordance with the Heisenberg scheme (4) read

\[
\begin{align*}
\dot{a}_1(t) &= i \left( -\omega_1 a_1(t) + \lambda a_2(t) + v_1^{(1)} a_3(t) + v_1^{(2)} a_4(t) \right), \\
\dot{a}_2(t) &= i \left( -\omega_2 a_2(t) + \lambda a_1(t) + v_2^{(1)} a_3(t) + v_2^{(2)} a_4(t) \right), \\
\dot{a}_3(t) &= i \left( -\omega_3 a_3(t) + v_1^{(1)} a_1(t) + v_2^{(1)} a_2(t) \right), \\
\dot{a}_4(t) &= i \left( -\omega_4 a_4(t) + v_1^{(2)} a_1(t) + v_2^{(2)} a_2(t) \right).
\end{align*}
\]

As widely discussed by Bagarello, Cherubini, and Oliveri (2016) and Bagarello and Oliveri (2014), the operatorial approach is suited to cover also dissipative systems, in order to deal with more realistic situations where one or more compartments can experience some stress; in this case, a simple and efficient strategy can be adopted (see Bagarello, Cherubini, and
Figure 2. Linear model: time evolution of the densities of the compartments both in the case of a purely conservative system (a), and in the case in which a dissipative effect is phenomenologically introduced (b).

Oliveri (2016) and Bagarello and Oliveri (2014)) consisting in giving up the self–adjointness of $H$, allowing in this way complex–valued parameters; this is a standard procedure used in branches of quantum mechanics (like quantum optics), to describe simply (though not rigorously) decay processes (see Ben-Aryeh, Mann, and Yaakov (2004) and Cherbal et al. (2007) and references therein). We simply include this effect in the model by adding to some of the inertia parameters a small negative imaginary part. Figure 2(a) shows, as expected, the quasi–periodic oscillating behavior obtained in the conservative linear case; on the contrary,
when a small stress factor is introduced only for the second kind of garbage, the amplitude of the oscillations of the densities of all the compartments decays as time increases. Under the assumption that the ecosystem is unable to completely recycle all the produced garbage, as expected, after a sufficiently long time, a significant decay of the densities of all the levels in the model arises, as depicted in Figure 2(b). The simulations shown in Figure 2 are produced by selecting the following values of the parameters: $\omega_1 = 0.3$, $\omega_2 = 0.2$, $\omega_3 = 0.4$, $\omega_4 = 0.5$ ($\omega_4 = 0.5 - 0.05i$ in case of stress effects, respectively), $\lambda = 0.3$, $\nu_1^{(1)} = 0.25$, $\nu_1^{(2)} = 0.2$, $\nu_2^{(1)} = 0.15$, $\nu_2^{(2)} = 0.1$, and the following initial densities for the four compartments: $n_1 = 1$, $n_2 = 0.1$, $n_3 = 0$, and $n_4 = 0$.

As specified above, the fermionic operators $a_j$, $j = 1, \ldots, 4$, are represented by matrices of order 16; hence, the system (7) consists of 1024 differential equations to be solved with a suitable set of initial conditions, say:

$$a_1(0) = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},$$

$$a_2(0) = \begin{pmatrix}
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.\)
Once we know the entries of matrices $a_j(t)$ ($j = 1, \ldots, 4$) at time $t$, the local densities of the compartments are simply obtained by computing the sum of the squared absolute values of the elements in a row of matrices $a_j(t)$. The 16 rows produce the solutions for all the possible initial states, which are the combinations with repetition of 4 elements chosen in the set $\{0, 1\}$. Due to the linearity of the problem, actually we do not need to know the solutions for all possible initial data; it suffices to have the fundamental solutions corresponding to the initial data $(n_1 = \delta_{i1}, n_2 = \delta_{i2}, n_3 = \delta_{i3}, n_4 = \delta_{i4})$ ($i = 1, \ldots, 4$), where $\delta_{ij}$ is the Kronecker symbol, to get, through a linear combination, the solutions for all initial states. Also, we are not forced to use initial densities in the set $\{0, 1\}$, but we may choose the initial data for all compartments in the whole interval $[0, 1]$.

The linearity of equations (7) implies that we explicitly know their exact solution, and this allows us to drastically reduce the computational cost. In fact, the system of equations (7) may be written in compact form as

$$\dot{A}(t) = UA(t),$$

(8)
with
\[ A(t) = \begin{pmatrix} a_1(t) \\ a_2(t) \\ a_3(t) \\ a_4(t) \end{pmatrix}, \quad U = i \begin{pmatrix} -\omega_1 & \lambda & v_1^{(1)} & v_1^{(2)} \\ \lambda & -\omega_2 & v_2^{(1)} & v_2^{(2)} \\ v_1^{(1)} & v_2^{(1)} & -\omega_3 & 0 \\ v_1^{(2)} & v_2^{(2)} & 0 & -\omega_4 \end{pmatrix}. \tag{9} \]

By computing \( V(t) = \exp(Ut) \), the solution may be clearly expressed as
\[ A(t) = V(t)A(0). \tag{10} \]

If we call \( V_{jk}(t) \) the generic time–dependent matrix entry of \( V(t) \), and \( n_\ell \) the initial density of the \( \ell \)-th compartment of the system, from (5) we find that
\[ n_j(t) = \sum_{\ell=1}^{4} |V_{j\ell}(t)|^2 n_\ell. \tag{11} \]

The formula (11) allows to exactly obtain the local densities at time \( t \) of the various compartments of the model in a simple manner at the cost of computing the exponential of the \( 4 \times 4 \) matrix \( Ut \). This size reduction of the computational cost of the solution is not possible for nonlinear dynamic equations; in fact, in this case we do not have the exact solution and we are forced to numerically solve 1024 nonlinear differential equations, or, according to formula (3), compute at each time \( t \) the exponential of the matrix \( Ht \), which is a \( 2^4 \times 2^4 \) matrix, together with its inverse (conjugate).

From (10), it is trivial to observe that
\[ A(t_1 + t_2) = V(t_1 + t_2)A(0) = \exp(U(t_1 + t_2))A(0) = \exp(U_{t_2})\exp(U_{t_1})A(0) = \exp(U_{t_2})A(t_1); \tag{12} \]
on the contrary, by considering (11), if we compute
\[ \tilde{n}_j = n_j(t_1 + t_2) = \sum_{\ell=1}^{4} |V_{j\ell}(t_1 + t_2)|^2 n_\ell, \]
\[ n_j^* = n_j(t_1) = \sum_{\ell=1}^{4} |V_{j\ell}(t_1)|^2 n_\ell, \tag{13} \]
\[ n_j^{**} = \sum_{\ell=1}^{4} |V_{j\ell}(t_2)|^2 n_\ell, \]

it is
\[ \tilde{n}_j \neq n_j^{**}. \tag{14} \]

In other words, formula (11), starting from the initial values \( n_j \ (j = 1, \ldots, 4) \), computing \( n_j(t_1) \)'s, and using these values as new initial data for computing the value after time \( t_2 \) has elapsed, does not provide the same result as the one given by computing \( n_j(t_1 + t_2) \) starting from the initial data \( n_j \ (j = 1, \ldots, 4) \). This is a serious problem if we divide in subintervals the time interval in which we follow the dynamics, and use the final values of the \( n_j \)'s in a subinterval as the initial data for the evolution in the next subinterval. In such cases, we need to compute the evolution of the entries of the operators, and therefore do a much more lengthy computation.
2.2. The nonlinear dynamical model. We may consider nonlinear effects in the model by including in the Hamiltonian contributions of order greater than two. In particular, we introduce in the interaction part $H_I$ of the Hamiltonian cubic terms, say

$$
H = H_0 + H_I, \quad \text{with}
$$

$$
\begin{align*}
H_0 &= \sum_{j=1}^{4} \omega_j a_j^\dagger a_j, \\
H_I &= \lambda \left( a_2 a_3^\dagger a_4^\dagger + a_4 a_3 a_2^\dagger \right) + \mu \left( a_1 a_2^\dagger + a_2 a_1^\dagger \right) \\
&\quad + \sum_{k=3}^{4} v^{(k)} \left( a_1 a_k^\dagger + a_k a_1^\dagger \right);
\end{align*}
$$

(15)

the real parameters $\omega_j$ ($j = 1, \ldots, 4$), $\lambda$, $\mu$, $v^{(k)}$ ($k = 3, 4$) are to be interpreted once again as being related to the inertia and the strength of the interactions among the compartments (Bagarello and Oliveri 2014). The differential equations derived from (15) now take the following more complicated form:

$$
\begin{align*}
\dot{a}_1 &= i \left( -\omega_1 a_1 + \mu a_2 + 2\lambda a_2 a_1 a_3^\dagger a_4^\dagger + 2\lambda a_4 a_3 a_2^\dagger a_1 + v^{(3)} a_3 + v^{(4)} a_4 \right), \\
\dot{a}_2 &= i \left( -\omega_2 a_2 + \mu a_1 + \lambda a_4 a_3 (2a_3^\dagger a_2^\dagger - \mathbb{I}) \right), \\
\dot{a}_3 &= i \left( -\omega_3 a_3 + \lambda a_2 a_4^\dagger (2a_3^\dagger a_2^\dagger - \mathbb{I}) + v^{(3)} a_1 \right), \\
\dot{a}_4 &= i \left( -\omega_4 a_4 + \lambda a_2 a_3^\dagger (2a_4^\dagger a_2^\dagger - \mathbb{I}) + v^{(4)} a_1 \right).
\end{align*}
$$

(16)

The solutions of the nonlinear system (16) can be found numerically, once the parameters involved in the Hamiltonian have been fixed. Similarly to what already discussed for the linear model, also in the nonlinear case the effect of some stress factor acting on the system can be taken into account by considering some of the inertia coefficients having a small negative imaginary part. The evolutions drawn in Figure 3, obtained using the following values of the parameters: $\omega_1 = 0.3$, $\omega_2 = 0.2$, $\omega_3 = 0.4$, $\omega_4 = 0.5$ ($\omega_4 = 0.5 - 0.05i$ in case of stress effects, respectively), $\lambda = 0.1$, $\mu = 0.25$, $v_3 = 0.15$, $v_4 = 0.15$, and the initial densities for the four compartments ($n_1 = 1, n_2 = n_3 = n_4 = 0$), show once again irregular oscillatory behaviors for the nonlinear conservative model compared to the decay of the system due to the lack of recycling of part of the garbage produced by the ecosystem in the non–conservative case.

The introduction of terms of order greater than two in $H$ thus entails the lack of an exact solution of (4) so that no less than 1024 nonlinear differential equations need to be solved in order to deduce the evolution of the system and, according to quantum theory, the initial densities of the compartments are flattened to the integer values 0 (completely empty) or 1 (completely filled). Numerically solve such a system of nonlinear differential equations obviously becomes a huge task as the number of compartments of the system grows, requiring very high computational costs. Moreover, the size of the problem almost immediately exceeds the limit of manageability with ordinary computing resources in the event that the operatorial approach is intended to be generalized to the case of a nonlinear spatial model.
3. Rule induced dynamics

An alternative to the use of a nonlinear model is to start from a quadratic Hamiltonian (hence, from a linear set of differential equations), and enrich the description of the dynamics by introducing some rules repeatedly acting on the parameters involved in the Hamiltonian to account for a sort of dependence of the parameters on the current state of the system; thus, we have an extended version of quantum dynamics. We notice that extended versions of quantum dynamics of a system $\mathcal{S}$ determined by a self–adjoint Hamiltonian $H$, by the initial conditions, and by a certain rule $\rho$ acting periodically on $\mathcal{S}$, though slightly different from the approach here considered, have been recently proposed for analyzing the quantum game of life (Bagarello et al. 2016).

Let us consider a self–adjoint quadratic Hamiltonian operator $H^{(1)}$ like (6), and let $X$ be one of the number operators. Consider the evolution

$$X(t) = \exp(iH^{(1)}t)X\exp(-iH^{(1)}t),$$

and compute the mean value

$$x(t) = \langle \phi_{n_1,n_2,n_3,n_4}, X(t)\phi_{n_1,n_2,n_3,n_4} \rangle$$

in a time interval of length $\tau > 0$. Then, let us use the values of the various $x(\tau)$ in order to modify some of the parameters involved in $H^{(1)}$: as a result, we are led to a new Hamiltonian operator $H^{(2)}$, having the same functional form as $H^{(1)}$ but (in general) with a different set of the values of the involved parameters. Starting from the current state reached by the system at time $\tau$ under the action of the Hamiltonian $H^{(1)}$, we consider the evolution of the system again in a time interval of length $\tau$ with the new Hamiltonian $H^{(2)}$, and so on. Therefore, the global evolution will be governed by a sequence of similar Hamiltonian operators, and the parameters entering the model are stepwise (in time) constant.

This kind of rule–induced dynamics clearly may produce discontinuities in the first order derivatives of the operators, which in turn determine discontinuities in the first order
derivatives of the average values, but prevents the occurrence of jumps in the evolutions of the latter.

Since in each time interval we use as initial datum the new state reached by the system, we can not use the compact representation (8) of the model. In fact, in the case in which no rule is applied, the evolution provided by equation (11) in a time interval $[0, n\tau]$ ($n$ positive integer) can not be reproduced by gluing the $n$ evolutions in a time interval of length $\tau$. However, equation (3) provides that, by transitionally breaking down the process of evolution of the fermionic operators $a_j$ ($j = 1, \ldots, 4$), we can evidently reach the state of the system at a specific time by allowing this state to evolve over a certain number of time units. Hence, we can not use for our purposes the minimal approach as expressed in (11); instead, we need to follow the evolution of the components of the operators $a_j$ ($j = 1, \ldots, 4$), according to the standard representation of fermions. This means that we have to solve in our case 1024 differential equations in each time interval. Such a computational effort can be drastically reduced by defining and implementing a new method, as explained in next subsection.

3.1. A reduced approach. We introduce here a new approach leading to a drastic reduction of the computational complexity of the implementation of models based on fermionic operators and ruled by quadratic Hamiltonians. Let us consider the usual canonical basis for the 4-dimensional vector space:

$$ (e_i)_{i \in I} = \left( (\delta_{i,j})_{j \in I} \right)_{i \in I} $$

(17)

with $I = \{1, \ldots, 4\}$. The squared Euclidean norm of the $k$–th vector of this basis gives the initial condition $n_i = \delta_k$. Of course, all the possible initial conditions may be expressed as a linear combination of these basic initial conditions. Recall once again that each operator $a_j, j = 1, \ldots, 4$, is represented in the standard mode by a $2^4 \times 2^4$ matrix. Now we construct a new family composed of 4 operators $b_j$, represented by $4 \times 4$ matrices, whose entries are given in such a way that each of them contains a single row whose Euclidean norm is equal to 1 (and zero elsewhere) and those non-zero rows are mismatched. A possible choice is given by:

$$ b_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad b_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad b_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad b_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. $$

It should be noted that the operators $b_j$ ($j = 1, \ldots, 4$) can not actually be considered as fermionic operators since, as they are defined, they no longer satisfy the CAR. In any case, let us assume that the evolution equations for the reduced operators $b_j(t)$ are formally the...
same as those for $a_j$, i.e., those given in (7), say

$$\begin{align*}
\dot{b}_1(t) &= i \left( -\omega_1 b_1(t) + \lambda b_2(t) + v_1^{(1)} b_3(t) + v_1^{(2)} b_4(t) \right), \\
\dot{b}_2(t) &= i \left( -\omega_2 b_2(t) + \lambda b_1(t) + v_2^{(1)} b_3(t) + v_2^{(2)} b_4(t) \right), \\
\dot{b}_3(t) &= i \left( -\omega_3 b_3(t) + v_1^{(1)} b_1(t) + v_1^{(2)} b_2(t) \right), \\
\dot{b}_4(t) &= i \left( -\omega_4 b_4(t) + v_1^{(2)} b_1(t) + v_2^{(2)} b_2(t) \right).
\end{align*}$$

(18)

Once computing the solution $b_j(t)$ of (18), the formula

$$\sum_{k=1}^{4} |(b_j(t))_{ik}|^2, \quad j = 1, \ldots, 4$$

(19)

provides the solutions corresponding to the initial conditions $\mathbf{e}_i$, which are the same as those provided by the standard approach, as shown in Figure 4.

As soon as these fundamental solutions are known, all the other possible evolutions of every initial state are simply recoverable through trivial linear combinations of them, i.e., the expression

$$\tilde{n}_j(t) = \sum_{i=1}^{4} \alpha_i \sum_{k=1}^{4} |(b_j(t))_{ik}|^2, \quad j = 1, \ldots, 4$$

(20)

gives the solution corresponding to the initial condition $(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$. Therefore, instead of solving the 1024 differential equations for the entries of the fermionic operators $a_j(t)$ ($j = 1, \ldots, 4$), we need to solve only 64 equations for the operators $b_j(t)$. We remark that this size reduction, which surely is not convenient in the case of standard linear models (where we integrate only 4 equations), results really useful (essential for a large number of operators) for the implementation of an efficient stepwise method.

### 3.2. Numerical results

A first comment is concerned with the numerical comparison between the solutions obtained with the classical approach and the ones computed using our reduced method.

As it is evident in Figure 4, as well as from the data reported in Table 1, the global evolution of the densities $n_i$ and $\tilde{n}_j$, corresponding to the fundamental solutions $a_i$ (computed using the classical model) and $b_j$ (computed using the reduced method) starting from the initial conditions $\mathbf{e}_i$, $i = 1, \ldots, 4$, are the same, assessing the numerical equivalence between

<table>
<thead>
<tr>
<th>I.C.</th>
<th>$|n_1 - \tilde{n}<em>1|</em>{\infty}$</th>
<th>$|n_2 - \tilde{n}<em>2|</em>{\infty}$</th>
<th>$|n_3 - \tilde{n}<em>3|</em>{\infty}$</th>
<th>$|n_4 - \tilde{n}<em>4|</em>{\infty}$</th>
</tr>
</thead>
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<td>$\mathbf{e}_1$</td>
<td>$1.8763468 \times 10^{-7}$</td>
<td>$3.7085755 \times 10^{-8}$</td>
<td>$7.1483147 \times 10^{-8}$</td>
<td>$1.0132139 \times 10^{-7}$</td>
</tr>
<tr>
<td>$\mathbf{e}_2$</td>
<td>$3.7085734 \times 10^{-8}$</td>
<td>$1.1176913 \times 10^{-8}$</td>
<td>$1.0100925 \times 10^{-8}$</td>
<td>$1.1962275 \times 10^{-8}$</td>
</tr>
<tr>
<td>$\mathbf{e}_3$</td>
<td>$7.1483147 \times 10^{-8}$</td>
<td>$1.0100928 \times 10^{-8}$</td>
<td>$9.7523852 \times 10^{-8}$</td>
<td>$4.3765407 \times 10^{-8}$</td>
</tr>
<tr>
<td>$\mathbf{e}_4$</td>
<td>$1.0132139 \times 10^{-7}$</td>
<td>$1.962279 \times 10^{-8}$</td>
<td>$4.3765407 \times 10^{-8}$</td>
<td>$1.5132622 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

Table 1. Linear model: norm of the difference between the solutions obtained with the reduced representation of the operators and the ones computed with the standard approach starting from initial conditions belonging to the canonical basis $\mathbf{e}_1 = (1,0,0,0)$, $\mathbf{e}_2 = (0,1,0,0)$, $\mathbf{e}_3 = (0,0,1,0)$, and $\mathbf{e}_4 = (0,0,0,1)$. 
Figure 4. Linear model: time evolution of the densities of the compartments corresponding to the initial conditions belonging to the canonical basis \([1,0,0,0], [0,1,0,0], [0,0,1,0], [0,0,0,1]\) computed using the classical representation of the operators (on the left) and their reduced one (on the right).
the two approaches; in fact, the absolute difference does not exceed the value of $10^{-7}$ over long periods of time.

Once checked the effectiveness of the reduced model, this kind of representation may be used to test the effect on the description of the long-term survival of bacterial populations produced by the application of specific rules modifying the original linear model according to the state reached by the system after several time steps.

In practice, we consider the Heisenberg dynamics of the closed ecosystem for a time interval of length $\tau$ before applying the rule $\rho$; then, we assume the state reached by the system as the starting point for the next iteration of the time evolution, now governed by the new time-independent Hamiltonian operator deduced after the rule acting on the parameters has worked. At the end of this new iteration, $\rho$ is applied again, a new set of values for the parameters deduced, and a new integration performed. The stepwise dynamics we deduce in this way is driven by the particular functional form of the Hamiltonian $H$, the initial values for the parameters and the initial status of the system, and, of course, the rule $\rho$. In particular, two different rules, $\rho_1$ and $\rho_2$, have been devised taking into account the dynamical mechanisms implied by the variation of the scarcely recyclable garbage (21) and the nutrients (22), respectively; also, different values of $\tau$ have been tested. Our purpose is to reproduce the qualitative behavior of viability data (see Figure 5) of bacterial batch cultures where no nutrients at all were added after bacterial inoculum (Carnazza et al. 2008).
defined as follows:

\[
\begin{align*}
\text{if } n_4(k\tau) - n_4((k-1)\tau) > 0 \\
\quad & \begin{cases} 
\rho_1(\lambda) = \lambda(1 - 0.4) \\
\rho_1(v_1^{(2)}) = v_1^{(2)}(1 - 0.4) \\
\rho_1(v_2^{(2)}) = v_2^{(2)}(1 - 0.4)
\end{cases} \\
\text{else} \\
\quad & \begin{cases} 
\rho_1(\lambda) = \lambda(1 + 0.4) \\
\rho_1(v_1^{(2)}) = v_1^{(2)}(1 + 0.4) \\
\rho_1(v_2^{(2)}) = v_2^{(2)}(1 + 0.4)
\end{cases}
\end{align*}
\]

\(k = 1, 2, \ldots\) being the number of times the procedure is repeated. In a very simple way, \(\rho_1\) checks if the density of the scarcely recyclable garbage has increased compared to that of the previous step, and then modifies the values of the involved interaction parameters. The numerical simulations shown in Figure 6 have been produced by choosing the initial values for the parameters \(\omega_1 = 0.3, \omega_2 = 0.2, \omega_3 = 0.4, \omega_4 = 0.5, \lambda = 0.3, v_1^{(1)} = 0.25, v_1^{(2)} = 0.2, v_2^{(1)} = 0.15, v_2^{(2)} = 0.1\), the initial densities for the compartments \(n_1 = 1, n_2 = 0.1, n_3 = 0, n_4 = 0.1\), and by imposing the rule \(\rho_1\) after a time interval of length \(\tau = 2, \tau = 5\) or \(\tau = 10\), respectively. Due to the facts that the density of the scarcely recyclable waste material has reasonably damped oscillations and that, since it turns into nutrients rather hardly, this garbage has a low influence on the transformation of the system, we can observe that for values of length \(\tau\) of the interval of quantum evolution below 10, \(\rho_1\) seems not to be a fitting rule for the description of the long–term survival of the bacteria, whereas for \(\tau = 10\) the results are quite satisfactory.

Let us now consider another rule \(\rho_2\) based on the control of the variation of the density of the nutrients at each step and acting both on the values of the inertia and of the involved
interaction parameters according to the law

\[
\begin{align*}
\text{if} & \quad n_1(k\tau) - n_1((k-1)\tau) > 0 \\
\rho_2(\omega_1) &= \omega_1(1 - 0.4) \\
\rho_2(\omega_2) &= \omega_2(1 - 0.4) \\
\rho_2(\omega_3) &= \omega_3(1 + 0.2) \\
\rho_2(\omega_4) &= \omega_4(1 + 0.2) \\
\rho_2(\lambda) &= \lambda(1 + 0.4) \\
\rho_2(v_1^{(1)}) &= v_1^{(1)}(1 - 0.4) \\
\rho_2(v_2^{(1)}) &= v_2^{(1)}(1 - 0.4) \\
\end{align*}
\]

\text{else}

\[
\begin{align*}
\rho_2(\omega_1) &= \omega_1(1 + 0.4) \\
\rho_2(\omega_2) &= \omega_2(1 + 0.4) \\
\rho_2(\omega_3) &= \omega_3(1 - 0.2) \\
\rho_2(\omega_4) &= \omega_4(1 - 0.2) \\
\rho_2(\lambda) &= \lambda(1 - 0.4) \\
\rho_2(v_1^{(1)}) &= v_1^{(1)}(1 + 0.4) \\
\rho_2(v_2^{(1)}) &= v_2^{(1)}(1 + 0.4) \\
\end{align*}
\]

with \(k = 1, 2, \ldots\) The graphs plotted in Figure 7 represent an evidence of how, even for small values of \(\tau\), the proposed approach, combining the action of the Hamiltonian \(H\) with a suitable rule able to adjust the model to the evolution of the system, provides a valuable description of what is observed in bacterial population in a closed environment. Even in the event that some stress factor is introduced for the scarcely recyclable garbage, the step–wise linear model employing the rule \(\rho_2\) proves to be efficient in describing the expected behavior, characterized by a gradual decay of the densities of all the compartments of the system, as visible in Figure 8.
Figure 8. Time evolution of the densities of all the compartments of the ecosystem (a) and of the bacteria (b) using the stepwise linear model in the non-conservative case and imposing the rule $\rho_2$ after a time interval of length $\tau = 10$.

Table 2. Stepwise linear model using the rule $\rho_1$ with $\tau = 10$: values of the parameters in the various time intervals.

<table>
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<th>[0,10]</th>
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<th>[30,40]</th>
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<td>0.180</td>
<td>0.252</td>
<td>0.353</td>
<td>0.212</td>
<td>0.296</td>
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<td>0.107</td>
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<tr>
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<td>0.200</td>
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<td>0.099</td>
<td>0.059</td>
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4. Conclusions

In this paper, we have considered a theoretical model of closed ecosystems based on fermionic operators, and applied the operatorial techniques of quantum physics with the aim of describing the long-term survival of bacteria in a batch culture. The dynamics is ruled by either a self-adjoint or not self-adjoint Hamiltonian operator whose definition expresses the various interactions occurring among the compartments of the system.

In order to avoid the complexity limitations imposed by the fast growth of the size of the problem in the case of nonlinear models, we have combined the usual quantum definition of the dynamics governed by a quadratic Hamiltonian with the action of specific rules periodically modifying the parameters involved in the Hamiltonian in order to adjust them according to the state of the system. Specifically, we have defined a suitable quadratic functional form for the Hamiltonian operator and two different rules $\rho_1$ and $\rho_2$ changing the values of the parameters entering the model (as reported in Tables 2 and 3); the rules are intended to account for the changes of the metabolic activity of bacteria (and hence in their interaction parameters) due to the increased density of the scarcely recyclable garbage or to a lack of nutrients.

The numerical simulations obtained by considering the evolution of the system for consecutive time intervals in accordance with the Heisenberg representation and repeatedly imposing the rules have shown the validity of the proposed stepwise method in describing
ON FERMIONIC MODELS OF A CLOSED ECOSYSTEM

<table>
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<tr>
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<td>0.038</td>
<td>0.023</td>
<td>0.032</td>
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</tr>
</tbody>
</table>

TABLE 3. Stepwise linear model using the rule $\rho_2$ with $\tau = 10$: values of the parameters in the various time intervals.

*Figure 9.* Time evolution of the density of the bacteria using the linear model with the final values of the parameters obtained applying either the rule $\rho_1$ (a) or the rule $\rho_2$ (b) after 10 time intervals of length $\tau = 10$.

The behavior of the bacteria, differently from what happens by adopting the standard linear model, even when we use the final values for the parameters deriving from several applications of the rule (as shown in Figure 9).

The stepwise linear model we have proposed requires the formulation of a reduced strategy to efficiently deduce the time evolution of the components of the operators representing the observables of the system. The equivalence of the obtained results with the ones computed using the classical approach is proved here only from a numerical point of view. However, a formal proof of the correctness of our reduced method exists and will be contained in a forthcoming paper.

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References


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