Emergence of order in quantum extensions of the classical quasispecies evolution

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We study evolution equations which model selection and mutation within the framework of quantum mechanics. The main question is to what extent order is achieved for an ensemble of typical systems. As an indicator for mixing or purification, a quadratic entropy is used which assumes values between zero for pure states and $(d-1)/d$ for fully mixed states. Here, $d$ is the dimension. Whereas the classical counterpart, the quasispecies dynamics, has previously been found to be predominantly mixing, the quantum quasispecies (QS) evolution surprisingly is found to be strictly purifying for all dimensions. This is also typically true for an alternative formulation (AQS) of this quantum mechanical flow. We compare this also to analogous results for the Lindblad evolution. Although the latter may be viewed as a simple linear superposition of the purifying QS and AQS evolutions, it is found to be predominantly mixing. The reason for this behavior may be explained by the fact that the two subprocesses by themselves converge to different pure states, such that the combined process is mixing. These results also apply to high-dimensional systems.

I. INTRODUCTION

We consider evolution equations familiar from various fields such as chemistry, biology, population dynamics, or financial mathematics. The basic question is whether, in the course of time, the system evolves toward a pure state characterized by a minimum value of the entropy $S$, or toward a mixed state with a large (or possibly even maximum) value of $S$. As a measure for this tendency we use the quadratic entropy, which vanishes for pure states, and which approaches $(d-1)/d$ for the fully mixed state. Here, $d$ is the dimension of the probability space.

Various models for such evolutions have been proposed [1,2]. Recently, we have considered the—arguably—simplest model for such a dynamics [3], the so-called quasispecies equation introduced by Eigen and Schuster [1,4]. In the biological context, a quasispecies is an ensemble of similar genomes, which are formed by an evolutionary mutation-selection process modeled according to chemical reaction kinetics [5,6]. As shown below, these evolution equations, which are purely classical, are formulated in terms of a matrix $\alpha$ of rate constants, whose elements are assumed to be strictly positive $\alpha_{ij}>0$ but possibly very small. Here, $\alpha$ does not depend on time and represents a static environment. Since we are interested only in the general features and not in the individual evolution of a particular system, the matrix elements are taken to be equally distributed random numbers with a specified upper bound. The upper bounds may differ for the elements belonging to the three parts spanning the matrix space, namely, the diagonal matrices (DMs), the upper triangular matrices (UTMs), and the lower triangular matrices (LTM). It is concluded in Ref. [3] that the matrices $\alpha$ taken predominantly from one of these three subalgebras (with the matrix elements from the two other subalgebras being negligibly small) give a predominantly purifying dynamics. If, however, the mixed-in amount from another part exceeds a certain threshold, the dynamics becomes predominantly mixing. Various variants of this classical model have been studied extensively in the past, both in static [7–10] and fluctuating [11] environments.

In this paper we extend these considerations to the quantum-mechanical setting where the state corresponds to a density matrix. The physical system we have in mind is a quantum system that models, for example, kaon decay or the decay of a radioactive substance. The Hamiltonian describing the time evolution is extended to a non-Hermitian operator representing the decay. As for the classical evolution, the basic growth term is linear and conservation of probability is restored by a quadratic term corresponding to a normalization. This distinguishes the quasispecies approach from other master equations, for which the growth term is already strictly nonlinear [12].

There is also the alternative to imbed the system in a larger but still finite system [13,14] and extend the evolution to a Lindblad equation, which has the advantage that it can be obtained in an appropriate scaling limit. Below we discuss the asymptotic behavior of the entropy for the quasispecies and Lindblad equations and observe that they behave quite differently.

To provide a comparison with the classical case, we first specify in Sec. II the classical model and summarize our results of Ref. [3]. A quantum-mechanical generalization of the quasispecies equation is given in Sec. III, which defines a time evolution both forward and backward in time. We analyze the convergence properties for the general solutions and find that the dynamics is (almost) always purifying. In Sec. IV we present an alternative formulation of this quantum dynamics, for which the time evolution is defined only for positive time. Again, we conclude that the modified dynamics is generally purifying. These findings apply to all dimensions $d$ and vastly differ from the classical case. In Sec. III we illustrate our general result for the simplest two-dimensional case, both theoretically and by computer simulations.
The corresponding Lindblad dynamics is treated in Sec. V. This dynamics may be viewed as a linear combination of the two versions of the quasispecies evolution discussed in the previous sections. From the physics point of view, the advantage of this model lies in the fact that it can be justified as the limit of a time evolution of a subsystem suitably embedded in a larger system. It constitutes the most general form of a quantum dynamical semigroup. Its advantage from the mathematical point of view lies in the fact that it is a linear equation and, therefore, the evolution can be characterized by its eigenvalues and eigenfunctions. We concentrate on this fact and characterize the possible eigenvalues and asymptotic solutions, theoretically and by computer simulations. In Sec. V A we illustrate our results for the two-dimensional case. Numerical examples for dimensions up to eight are provided in Sec. V B. We conclude in Sec. VI with a summary of our results.

II. CLASSICAL EVOLUTION

Classically, the state of a system is described by the $d$-dimensional positive vector

$$p = \{p_i\}, \quad 0 \leq p_i \leq 1; \quad i = 1, 2, \ldots, d,$$

which evolves according to the so-called quasispecies equation

$$\frac{dp_i}{dt} = \sum_{j=1}^{d} \alpha_{ij} p_j - p_i \sum_{k=1}^{d} \alpha_{ik} p_k.$$  \quad (1)

The coefficients $\alpha_{ij}$ are elements of a $d \times d$ matrix $\alpha$ and are assumed to be strictly positive random variables. From the general solution

$$p(t) = \frac{\exp(at)p(0)}{\sum_{i=1}^{d} \exp(at)p(i)},$$ \quad (2)

it follows that the vector $p$ is constrained to the simplex $S_d$,

$$\sum_{i=1}^{d} p_i = 1$$ \quad (3)

provided the initial point is also contained in $S_d$. The state $p$ may then be regarded as a $d$-dimensional probability distribution. One can easily show [3] that for strictly positive matrix elements $\alpha_{ij}$ the stationary asymptotic solution $p = \lim_{t \to \infty} p(t)$ is stationary and unique, i.e., nondegenerate, and is determined by the eigenvector associated with the maximum eigenvalue of $\alpha$.

The motion equations are linear in $\alpha$ and of second order in $p$. Other models also discussed in the literature are of third order in $p$ [2]. Here, we restrict ourselves to the simpler case of Eq. (1).

The quadratic entropy $S$ [17]

$$S = \sum_{i=1}^{d} p_i(1 - p_i).$$ \quad (4)

provides a convenient measure for the purifying or mixing tendency of Eq. (1) [3]. Classically, a pure state is not decomposable and corresponds to a point measure in phase space. $S$ vanishes for a pure state, it is $(d-1)/d$ for the completely mixed state and it is in between otherwise. It is readily obtained for the asymptotic state $p(\infty)$.

To understand the general behavior, it is useful to separate the matrix space for $\alpha$ into three parts, the DMs, and the UTM's and LTM's, respectively. The rates $\alpha_{ij}$ are taken to be equally distributed random variables with upper bounds which may differ for DMs, UTM's, and LTM's. For each choice of upper bounds, one obtains an ensemble of matrices $\alpha$ and, hence, asymptotic states, from which a normalized distribution of entropies $\pi(S)$ may be constructed.

The following general picture emerges for the classical case [3], which persists also for large dimensions: If the dynamics of the system is dominated by the elements of only one of the three subalgebras (which means that the upper bounds of the elements belonging to the other two parts are still positive but negligibly small), the normalized entropy distribution for the asymptotic states develops a maximum near or at $S=0$ and the evolution is predominantly purifying. If, however, the upper bound for the elements belonging to any of the other subalgebras is raised beyond a few percent, the entropy distribution exhibits peaks somewhere in the allowed interval $0 \leq S \leq (d-1)/d$ away from zero and possibly near the mixing limit $(d-1)/d$. The evolution becomes mixing.

III. QUANTUM PURIFICATION FOR THE QUASISPECIES DYNAMICS

In the quantum mechanical setting, the distribution $\rho(t)$ in Eq. (1) is replaced by a density matrix $\rho(t)$, which evolves according to

$$d\rho(t)/dt = h\rho(t) + \rho(t)h^\dagger - \rho(t)Tr[h\rho(t) + \rho(t)h^\dagger].$$ \quad (5)

$h$ is a sort of Hamilton operator which, generally, is not Hermitian, and $h^\dagger$ is its Hermitian adjoint. The general solution of this equation is almost the same as in the classical quasispecies case

$$\rho(t) = \frac{\exp(ht)\rho(0)\exp(th^\dagger)}{Tr[\exp(ht)\rho(0)\exp(th^\dagger)]},$$ \quad (6)

but now the noncommutativity of the operators has to be observed. The map $h \rightarrow h + c1$ does not change $\rho(t)$, thus we may assume $Trh = 0$. The quadratic entropy, which in quantum information theory is also known as the linear entropy, becomes

$$S(t) = Tr[\rho(t)[1 - \rho(t)]]/2.$$ \quad (7)

Now a pure state is a projection onto a general vector in Hilbert space. As in the classical case $S=0$ indicates a pure state and $S=(d-1)/d$ a completely mixed state. In the fol-
following, $S$ always refers to the asymptotic limit $t \to \infty$ if not stated otherwise.

We now show that—in contrast to the classical case—the quantum quasispecies dynamics is generally purifying. Let $\{|i\rangle: i = 1, \ldots, d\}$ be an orthonormal basis in Hilbert space, such that the unity is decomposed according to

$$1 = \sum_i Q_i, \quad Q_i Q_j = \delta_{ij} Q_i, \quad Q_i^* = Q_i,$$

where $Q_i = |i\rangle\langle i|$ projects onto $|i\rangle$. The classical dynamics is a special case, for which $\rho = \Sigma_i \rho_i Q_i$ and $h Q_i = \Sigma_i a_i Q_i$. With these properties, the classical quasispecies Eq. (1) is recovered from Eq. (5), and the dynamics is purifying if $\rho$ converges to any particular $Q_i$. In quantum dynamics, however, any pure state $|\beta\rangle$ is a superposition of the states $|i\rangle$, and purification is already achieved, if $\rho$ converges to any (much more general) one-dimensional projector $P_\beta$ obeying $P_\beta = P_\beta^* = P_\beta^2$.

In the following we use a generalization of Hermitian matrices, which is more convenient for our purpose. It is the class $\mathcal{J}$ of $d \times d$ matrices $A$, which are diagonal in the Jordan form and, therefore, have eigenvectors forming a linear basis. This class is (i) dense, (ii) setwise invariant under similarity transformations $A \to MAM^{-1}$, and (iii) invariant under the transformation $A + c I$, $c \in \mathbb{C}$, $\mathcal{J}$ has the following properties. (1) If $a_i$ denotes the eigenvalues and $|\varphi_i\rangle$ the corresponding eigenvectors of $A$, for which $\langle \varphi_i | \varphi_j \rangle = 1$, there exists another basis $|\psi_j\rangle$, which generally is not normalized, such that $A = \Sigma_i a_i |\varphi_i\rangle \langle \varphi_i|$ and $\langle \psi_i | \psi_j \rangle = \delta_{ij}$. (2) The quantities $P_i = |\varphi_i\rangle \langle \psi_i|$ are projectors, $P_i^2 = P_i$, which are not necessarily Hermitian. They decompose the unity $\Sigma_i P_i = 1$. Their trace is unity, $\text{Tr} P_i = \langle \psi_i | \varphi_i \rangle = 1$. Therefore, $\text{Tr} A = \Sigma_i \langle \psi_i | A | \varphi_i \rangle$. (3) Since $A^2 = \Sigma_i a_i a_i |\varphi_i\rangle \langle \varphi_i| \psi_i\rangle \langle \psi_i| = \Sigma_i a_i^2 |\varphi_i\rangle \langle \psi_i|$, it follows for any analytic function $f$

$$f(A) = \sum_i f(a_i) P_i = \sum_i f(a_i) |\varphi_i\rangle \langle \psi_i|.$$

To illustrate this construction, we give a simple two-dimensional example: Let $A$, with eigenvalues $a_i$ and eigenvectors $|\varphi_i\rangle$, be given by

$$A = \begin{pmatrix} \epsilon_1 & 1 \\ 0 & \epsilon_2 \end{pmatrix}; \quad a_i = \epsilon_i, \quad i = 1, 2,$$

$$|\varphi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad |\varphi_2\rangle = \begin{pmatrix} 1 \\ \epsilon_2 - \epsilon_1 \end{pmatrix} a,$$

where $a = \sqrt{1 + (\epsilon_2 - \epsilon_1)^2}$, then the vectors $|\varphi_i\rangle$ and the projectors $P_i$ become

$$|\varphi_i\rangle = \begin{pmatrix} 1 \\ 1/(\epsilon_1 - \epsilon_2) \end{pmatrix}; \quad |\psi_i\rangle = \begin{pmatrix} 0 \\ 1/(\epsilon_2 - \epsilon_1) \end{pmatrix} a;$$

For the following we consider operators $h$ from this class $\mathcal{J}$, whose eigenvalues $a_j$ are all different (which is true for a dense set). Since Eq. (8) applies, the time evolution of the density matrix Eq. (6) becomes

$$\rho(t) = \sum_{j,k} e^{(a_j - a_k)t} |\varphi_j\rangle \langle \psi_j| \rho(0) |\varphi_k\rangle \langle \varphi_k| \langle \psi_k|.$$

For large $t$, this sum is dominated by the term with the eigenvalue $a_j$, for which $a_j + a_j^*$ is maximal. Thus,

$$\rho(t) \to \frac{1}{d} |\varphi_j\rangle \langle \varphi_j|$$

and the density matrix projects onto the corresponding eigenvector $|\varphi_j\rangle$. The dynamics is purifying.

In the exceptional case where this term coincides for different eigenvalues, we remain with a density matrix that changes periodically in time. We have to consider also the case that the set of eigenvectors do not form a basis. This may happen if $\text{det}(h - a I) = 0$ has degenerate solutions. Considering such an operator as a limit of operators from the class $\mathcal{J}$, this corresponds to the fact that different $|\varphi_j\rangle$’s converge to the same vector, whereas the corresponding $|\psi_j\rangle$’s diverge. However, the details of convergence are of no importance because of the modifying influence of the norm in the denominator. Typically, the limiting density matrix is $|\varphi_j\rangle \langle \varphi_j|$ and the system is purifying.

One notices that $\rho(0) \to \rho(t)$ is a one-parameter group of positive maps. Thus, one may ask what happens for negative $t$. For $t \to -\infty$, $P_i$ for the eigenvalue with the maximum real part is replaced by $P_j$, belonging to the eigenvalue $a_j$ with the minimum real part. Attractors are replaced by repellors and vice versa.

One may look at the quasispecies dynamics as a description of decaying states. If, for example, there is some distribution of uranium isotopes at present, the isotope with the longest lifetime will dominate in the far future, whereas in the far past there must have been a domination by the isotope with the shortest lifetime. Both limiting states may be considered to be pure.

*Quasispecies dynamics in two dimensions.* We illustrate the general results for the quasispecies dynamics by restricting ourselves to quantum states in two dimensions (qubits). In this case, the density matrix for any mixed state may be written as

$$\rho(t) = \frac{1}{2} \begin{pmatrix} 1 + \sigma \cdot n(t) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + n_1 & n_3 - n_1 \n_3 + n_1 & 1 - n_3 \end{pmatrix},$$

where we have used the notation $\sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
Here, 
\[ \sigma = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \]
are the Pauli matrices, and the Bloch vector \( n = \{ n_1, n_2, n_3 \} \) is a real vector taken from \( \mathbb{R}^3 \) such that \( n^2 \leq 1 \). As required, \( \text{Tr}p = 1 \). The quantity
\[ M(t) = e^\mathbf{ht} e^{\mathbf{h}^\dagger t} \tag{12} \]
is always Hermitian even if \( h \) is not. Therefore, it may be represented as
\[ M(t) = c(t)[1 + \sigma \cdot m(t)], \tag{13} \]
where \( m = \{ m_1, m_2, m_3 \} \) is a positive vector from \( \mathbb{R}^3 \) such that \( m^2 \leq 1 \). \( c \) is a factor which drops out in the expression for the entropy
\[ S(t) = 1 - \text{Tr}p^2(t) = 1 - \frac{\text{Tr}[M\rho(0)M\rho(0)]}{\text{Tr}[M\rho(0)]^2}. \]
With the help of Eqs. (11) and (13), this expression may be cast into
\[ S(t) = \frac{1}{2} \frac{[1 - m^2(t)]^2}{[1 + (m(t) \cdot n(0))]} \tag{14} \]
Whenever \( m^2 \) approaches unity, the dynamics is strictly purifying and independent of the initial conditions \( n(0) \). However, for a mixing dynamics, for which \( m^2 < 1 \), the entropy also depends on the initial conditions. This seems to be a serious deficiency.

For the computation of \( m(t) \) we note that any non-Hermitian Hamiltonian \( h \) (with \( \text{Tr}h \) up to a multiple of unity) may be represented as
\[ h = \sigma \cdot (r + ij), \tag{15} \]
where \( r \) and \( j \) are three-dimensional vectors in \( \mathbb{R}^3 \). Note that the dynamics Eq. (1) is not affected by a multiple of unity in \( h \). In the next sections we shall encounter evolutions, where this is not true any more. It follows from Eq. (15) that
\[ h^2 = r^2 - j^2 + 2i(r \cdot j) = \omega^2, \tag{16} \]
where \( \omega = \sqrt{\omega^2} \) is given by
\[ \omega = \sqrt{\frac{1}{2}[(r^2 - j^2) + \sqrt{(r^2 - j^2)^2 + 4(r \cdot j)^2}]^{1/2} + \frac{i}{2}[-(r^2 - j^2) + \sqrt{(r^2 - j^2)^2 + 4(r \cdot j)^2}]^{1/2}. \]
Furthermore,
\[ e^{\mathbf{ht}} = 1 + \mathbf{ht} + \frac{\mathbf{h}^2 t^2}{2} + \frac{\mathbf{h}^3 t^3}{6} + \cdots = \cosh(\omega t) + \frac{h}{\omega} \sinh(\omega t) \]
\[ = \cosh(\omega t)(1 + \sigma \cdot v), \tag{17} \]
where because of Eq. (15) the (complex) vector \( v \) becomes
\[ v = \frac{\tanh(\omega t)}{\omega}(r + ij). \tag{18} \]
If this expression is inserted into Eq. (12), one obtains
\[ M(t) = c'[1 + (\sigma \cdot v)][1 + (\sigma \cdot v^*)] \]
\[ = c'[\{1 + (v \cdot v^*) + \sigma \cdot (v + v^* + iv \times v^*)\}], \]
where for the second step the identity \[ (\sigma \cdot a)(\sigma \cdot b) = a \cdot b - i\sigma \cdot (a \times b) \]
has been used. All common factors are included in a constant \( c' \). Casting this expression into the canonical form of Eq. (13), we obtain after some manipulations
\[ M(t) = c \frac{1 + \sigma \cdot (v + v^* + iv \times v^*)}{1 + (v \cdot v^*)}. \tag{19} \]
As already mentioned before, the common factor \( c \) does not concern us here. A comparison with Eq. (13) provides an explicit expression for the vector \( m(t) \):
\[ m(t) = \frac{v + v^* + iv \times v^*}{1 + (v \cdot v^*)}. \tag{20} \]
Together with \( v \) and \( \omega \) given above, this equation may be used for the numerical computation of the entropy, Eq. (14).

Extending the general vector identity
\[ (a \times b)^2 = a^2 b^2 - (a \cdot b) \]
to complex vectors, one further obtains
\[ m^2(t) = 1 - \frac{(1 - v^2)(1 - v^*)}{[1 + (v \cdot v^*)]^2}. \tag{20} \]
From Eqs. (16) and (18) we infer \( v^2 = \tanh^2(\omega t) \) and \( (v \cdot v^*) = |\tanh(\omega t)|^2 |r^2 + j^2| \), and we finally get
\[ 1 - m^2(t) = \frac{1 - v^2}{1 + (v \cdot v^*)} = \frac{|\sinh(\omega t)|^2}{\sqrt{(r^2 + j^2)^2 + 4(r \cdot j)^2}}. \tag{21} \]
We are actually interested in the asymptotic solution for \( t \to \infty \). For \( r = 0 \), the Hamiltonian \( h \) is anti-Hermitian, \( \omega \) is purely imaginary, and the cosh function in Eq. (21) is periodic. However, the factor of sinh becomes unity and, as a consequence, \( m^2(\infty) = 0 \). It follows from Eq. (14) that the entropy becomes constant in agreement with the fact that \( e^h \) is unitary for an anti-Hermitian \( h \).

If \( j = 0 \), \( h \) is Hermitian, and \( \omega \) is real. According to Eq. (21), \( m^2(\infty) = 1 \), and the entropy vanishes asymptotically. The system is purifying.

In the general case, for which the vectors \( r \) and \( j \) in the representation of the Hamiltonian do not vanish, it follows from Eq. (21) that \( m^2(t) \) asymptotically approaches unity:

\[ \text{The system is strictly purifying. This is demonstrated in Fig. 1, where we show the time-dependent entropies for 100 realizations of the Hamiltonian} \ h \ \text{according to Eq. (15). The components of} \ r \ \text{and} \ j \ \text{are selected from uniform random} \]

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distributions and are bounded according to \(0 < r_a < R\) and \(0 < j_a < J\), \(a \in \{1, 2, 3\}\). In Fig. 1, \(R=1\) and \(J=1\). The evolution Eqs. (5) for \(d=2\) are directly integrated for uniform random initial conditions \(\rho(0)\) representing mixed states \(0 < n_a(0) < 1\), \(a \in \{1, 2, 3\}\), such that \(\sum_{a=1}^{3} n_a^2 < 1\) [see Eq. (11)]. Starting from the same initial conditions, the integration is performed both forward and backward in time. Clearly, pure states act as attractors for the dynamics regardless of the direction of time.

The convergence to a pure state may be slow, if the components of \(r\) are small and the Hamiltonian is “nearly” anti-Hermitian. To be independent of the initial conditions, we demonstrate this by computing the normalized distribution \(\pi(m^2(t))\) of \(m^2\) at fixed times \(t>0\) for an ensemble of random Hamiltonians similar to that used for Fig. 1, but with upper bounds \(R<1\) and \(J=1\). In the top panel of Fig. 2, distributions \(\pi(m^2(t))\) for various \(R\) are shown for the fixed time \(t=10\). For \(R=1\), the system has enough time to reach a pure state as is indicated by the distribution resembling \(\delta(m^2-1)\). This is in full agreement with Fig. 1. For smaller bounds \(R\), however, the distributions are peaked for smaller values of \(m^2\) indicating still partial or even full mixing. In the lower panel of the figure, the same distributions are shown at a time \(t=10,000\). For \(R \approx 10^{-3}\) we already find pure states, whereas mixed states still persist for smaller \(R\). According to the general considerations of Sec. III the distributions \(\pi(m^2)\) become \(\delta\) functions at unity and the dynamics is strictly purifying.

### IV. ALTERNATIVE QUASISPECIES EVOLUTIONS

In Eq. (5) we used an additive generalization of the dynamics to preserve the Hermiticity of the density matrix. As a consequence, the quasispecies dynamics is purifying both forward and backward in time. Alternatively, we consider

\[
dp(t)/dt = hp(t)\h^1 - \rho(t)\text{Tr}[hp(t)\h^1].
\]

This equation is not invariant under \(h \to h+c\), but under \(h \to e^{\gamma h}, \gamma \in \mathbb{R}\). To control conservation of positivity and of the trace, we write \(\rho(t) = C(t)/\text{Tr}C(t)\), where \(C(t)\) is a solution of the linear part

\[
dC(t)/dt = hC(t)\h^1.
\]

Since \(hC(t)\h^1 \geq 0\), \(C(t)\) remains positive for positive times. Analyzing the time evolution for \(C\), we may take advantage of the fact that it is linear in \(C\). We consider the operators \(C\) as vectors in a linear Hilbert space equipped with the Hilbert-Schmidt norm

\[
\langle C|D \rangle = \text{Tr} C^D.
\]

Operators on this extended Hilbert space are linear combinations of operators \(A \otimes B\) acting as

\[
A \otimes B(C) = |ACB^T|,
\]

where \(B^T\) is the transpose of \(B\). With this notation and with \(A^T = \tilde{A}\), Eq. (23) becomes
\[
\frac{d}{dt}|C\rangle = h \otimes \vec{h}|C\rangle.
\]

With
\[
h = \sum_k a_k |\varphi_k\rangle \langle \varphi_k|,
\]
where, as before, \(a_k\) and \(|\varphi_k\rangle\) denote the eigenvalues and eigenvectors of \(h\), respectively, we obtain
\[
\frac{d}{dt}|C\rangle = \sum_{k,l} a_k a_l^* |\varphi_k\rangle \langle \varphi_l| |\varphi_l\rangle \langle \varphi_k| |C\rangle
\]

or, using Eq. (8) again,
\[
|C(t)\rangle = \sum_{k,l} e^{i\alpha_{kl}} |\varphi_k\rangle \langle \varphi_l| |\varphi_l\rangle \langle \varphi_k| |C\rangle.
\]

After normalization, the dominating term for large \(t\) is \(|\varphi_k\rangle \langle \varphi_k|\) for that particular \(k\), for which \(|a_k|\) is maximal. Written as a density matrix in the original \(d\)-dimensional Hilbert space, one explicitly obtains
\[
\rho(t) = \sum_{k,l} e^{i\alpha_{kl}} P_k \rho(0) P_l / \sum_{k,l} \text{Tr}(e^{i\alpha_{kl}} P_k \rho(0) P_l)
\]

and
\[
\rho(t) \rightarrow_{t \rightarrow \infty} |\varphi_k\rangle \langle \varphi_k|.
\]

if \(a_k a_l^*\) is maximal. Since \(|\varphi_k\rangle \langle \varphi_k|\) corresponds to a projector, it follows that also in this evolution, for almost all \(h\), the density matrix converges to a pure state. However, the map \(\rho(0) \rightarrow \rho(t)\) is only a semigroup and remains positive only for positive times, as one also sees in the simulation.

An exception occurs, if \(a_k a_l^* = a_l a_k^*\) for some pair \((a_k, a_l)\) of eigenvalues of \(h\), which happens if \(a = e^{i\gamma} a_l\), where \(\gamma\) is some angle. Then the evolution leads to a mixed state, although \(h\) is not degenerate.

Different from the previous cases, there is also the possibility of a further variation by considering several Hamiltonians \(h^{(a)}\) acting simultaneously, such that the evolution equation becomes
\[
d\rho(t)/dt = \sum_a h^{(a)} \rho(t) h^{(a)\dagger} - \rho(t) \text{Tr} \left( \sum_a h^{(a)} \rho(t) h^{(a)\dagger} \right).
\]

Again we can solve this equation in the extended Hilbert space. However, we lose the easy passage from the representation of \(h\) to the evolution operator. Due to linearity we can still conclude that almost surely the density matrix will converge, but in general not to a pure state.

**Alternative quasispecies dynamics in two dimensions.** As an illustration we show the purifying properties of the alternative quasispecies Eq. (22) in the top panel of Fig. 3. There, 100 realizations of Hamiltonians \(h \in \mathcal{H}\) are used to compute time-dependent entropies by numerical integration of Eq. (22). The elements of \(h\) are taken as complex random numbers, where the real and imaginary parts are uniformly distributed between zero and unity. Initial conditions \(\rho(0)\) were constructed from Eq. (11), where the random vector components of \(n\) are assumed to be uniformly distributed between zero and unity. The integration is performed both forward and backward in time. For negative \(t\) the nonpositivity of \(S\) is apparent, stressing the semigroup nature of this dynamics. For positive times, the entropy asymptotically vanishes, indicating strict purification as required by Eq. (30).

In the bottom panel of Fig. 3 we consider the exceptional case \(|a_1|^2 = |a_2|^2\) for the eigenvalues of \(h\), which, according to the general treatment, gives a mixing dynamics. In two dimensions, Hamiltonians with a vanishing trace such as given in Eq. (15) have this property. 100 random realizations of \(h\), where the real and imaginary parts of the complex vector \(r\) are uniformly distributed between zero and unity, and with initial conditions \(\rho(0)\) identical to those for the top panel, yield time-dependent entropies, which do not converge to zero and, hence, indicate partial mixing for positive times. Clearly, adding to \(h\) a multiple of unity gives purification again.
V. Lindblad Dynamics

A consistent description of a dissipative quantum system is provided by the Lindblad dynamics [19–22], which is commonly written as [16]

\[
\frac{d\rho(t)}{dt} = \sum_\alpha h^{(\alpha)} \rho(t) h^{(\alpha)\dagger} - \frac{1}{2} \sum_\alpha \left( h^{(\alpha)\dagger} h^{(\alpha)} \rho + \rho h^{(\alpha)} h^{(\alpha)\dagger} \right) - i[H, \rho],
\]

where \( H = H^0 \) represents an inner Hamiltonian, whereas all the other terms containing \( h^{(\alpha)} \), \( \alpha = 1, 2, \ldots \), are due to a coupling to the surrounding. In the following we consider only a single coupling Hamiltonian, which makes the upper index \( \alpha \) superfluous. Furthermore, we neglect any internal dynamics \( H = 0 \) such that the Lindblad equation becomes

\[
\dot{\rho} = h h^{\dagger} - \frac{1}{2} (h^{\dagger} h \rho + \rho h^{\dagger} h),
\]

which is used in the following.

Equation (32) may be viewed as a linear combination of two quasispecies evolutions, namely, the alternative quasispecies (AQS) equation (22), from which a term (QS) resembling the original quasispecies dynamics Eq. (5) is subtracted:

\[
\frac{d\rho(t)}{dt} = \text{AQS} - \frac{1}{2} \text{QS},
\]

\[
\text{AQS} = h \rho(t) h^{\dagger} - \rho(t) \text{Tr}[h \rho(t) h^{\dagger}],
\]

\[
\text{QS} = \frac{1}{2} h^{\dagger} h \rho(t) + \rho(t) h^{\dagger} h - \rho(t) \text{Tr}[h^{\dagger} h \rho(t) + \rho(t) h^{\dagger} h].
\]

In addition, the operator \( h \) in QS has been replaced by an operator \( h^\dagger h \), such that the normalization terms of AQS and QS containing the trace cancel and the Lindblad Eq. (32) is recovered. The Lindblad evolution is linear in \( \rho \). It generates a semigroup [15], giving nonpositive \( \dot{\rho} \) if followed for negative times. It is interesting to note that this is a consequence of AQS, which has the same property, whereas for the quasispecies dynamics QS the density operator and the entropy remain positive both forward and backward in time (see Fig. 1). Considering the interpretation of the Lindblad evolution in terms of a piecewise deterministic process [16], the alternative quasispecies term corresponds to the contributions given by the quantum jumps, whereas the regular quasispecies term is contributed by the deterministic time evolution of this non-Hermitian process [23].

Similar to Eq. (26), we rewrite Eq. (32) according to

\[
\frac{d\rho}{dt} = \mathcal{L} \rho \tag{35}
\]

and represent the Lindblad operator \( \mathcal{L} \) in the \( d^2 \)-dimensional extended Hilbert space

\[
\mathcal{L} = h \otimes h - \frac{1}{2} (h^{\dagger} h \otimes 1 + 1 \otimes h h^{\dagger}).
\]

Its eigenvalues \( \lambda_k \), and eigenvectors \( |\phi_k\rangle \), \( k = 1, \ldots, d^2 \) characterize the evolution. Of course, these are special operators in the extended Hilbert space, which map the cone corresponding to positive matrices into itself. We may apply Eq. (36) also to \( \mathcal{L} \) and find

\[
\frac{d^2}{dt^2} = \sum_k \lambda_k |\phi_k\rangle \langle \phi_k|.
\]

Since \( \lim_{t \to \infty} e^{Lt} \rho \neq 0 \), there exist eigenvalues \( \lambda_k \) with \( \text{Re}(\lambda_k) \geq 0 \). Since \( \| e^{Lt} \rho \| \) remains bounded, \( \text{Re}(\lambda_k) \leq 0 \) for all \( k \). Since \( \langle 1 | e^{Lt} \rho | 1 \rangle = 1 \) for all \( t \), there must be at least one vanishing eigenvalue, say \( \lambda_0 = 0 \), which determines the asymptotic time dependence. Its corresponding eigenvector, normalized such that its trace in the original \( d \)-dimensional Hilbert-space representation becomes unity, is the density matrix for the asymptotic state. This forms the basis of our numerical computations of the asymptotic entropy in Sec. V B. All other eigenvectors satisfy

\[
\langle 1 | e^{Lt} \phi_k | 1 \rangle = \langle e^{L\lambda_k} | \phi_k \rangle = \langle e^{L1} | \phi_k \rangle = \langle 1 | \phi_k \rangle = 0 \quad \text{and correspond to traceless operators.}
\]

A. Lindblad dynamics in two dimensions

In two dimensions, the Lindblad Eq. (32) can be explicitly solved. Excluding the trivial case \( h = e_1, e \) const, for which \( \rho = 0 \), and choosing an appropriate basis and phase, the operator \( h \) can be written

\[
\begin{pmatrix} a & b \\ 0 & c \end{pmatrix},
\]

where \( \{ a, c \} \in \mathbb{C} \) and \( b \geq 0 \). With this \( h \), the evolution equation for the density matrix becomes

\[
\frac{dp_{12}}{dt} = \left( a^2 - \frac{|a|^2 + |c|^2 + b^2}{2} \right) p_{12} + 2 b^2 c - a b \frac{a b}{2} p_{21} - \frac{a b}{2} p_{11},
\]

\[
\frac{dp_{22}}{dt} = - \left( b^2 p_{21} + a b p_{12} + b^2 p_{22} \right).
\]

If \( b = 0 \), “dephasing” occurs and the off-diagonal elements of the density matrix decay exponentially, \( \rho_{12}(t) = e^{-b^2 t/2} \rho(0) \). If \( b \neq 0 \), where \( \beta = |a| - |c|^2/2 \) and \( \delta = \text{Im} (ac^*) \). The entropy rises accordingly [24], and the system is mixing. The diagonal elements \( \rho_{11} = 1 - \rho_{22} \) and \( \rho_{22} \) are constant in time. Thus, any diagonal density matrix is constant. For negative times the off-diagonal elements increase exponentially with time, and the positivity of \( \rho \) gets lost.

If \( b > 0 \), we have convergence to a unique density matrix

\[
\lim_{t \to \infty} \rho_{12}(t) = \frac{|a|}{|a|^2 + b^2 + |c|^2}, \quad \lim_{t \to \infty} \rho_{22}(t) = \frac{|a|^2}{|a|^2 + b^2 + |c|^2}.
\]

It commutes with \( h \). For the asymptotic entropy one finds

\[
\rho_{12}(t) = \frac{|a|}{|a|^2 + b^2 + |c|^2}.
\]
We conclude that the Lindblad dynamics in two dimensions is purifying if and only if $\det h = 0$. The respective initial conditions $\rho(0)$ are obtained from Eq. (11), where the $n_a$ are uniformly distributed random numbers such that $0 < n_a(0) < 1$, $\alpha \in \{1, 2, 3\}$, and $\sum \rho_n^2 < 1$. They correspond to mixed states for which $0 < S(0) < 1/2$. Starting at time $t=0$, the Lindblad Eqs. (32) are integrated both forward in time (positive $t$) and backward in time (negative $t$).

$$S(\infty) = \text{Tr}[\rho(\infty)[1 - \rho(\infty)]] = 2 \det \rho(\infty) = \frac{2|a|^2|c|^2}{(|a|^2 + |b|^2 + |c|^2)^2}.$$ 

We illustrate the time dependence of the entropy in Fig. 4 for the same choice of Hamiltonians and for the same initial conditions $\rho(0)$ as in Fig. 1 for the quasispecies dynamics.

The appearance of mixed states is also apparent in Fig. 5, where in the top and middle panels we show the probability distributions $p(S)$ of the asymptotic entropy for random matrices $h$ represented by Eq. (38). In the top panel all matrix elements are assumed to be positive and uniformly distributed random numbers, where the diagonal elements are bounded from above by $D$ and the off-diagonal element by unity. In the middle panel the diagonal elements are taken to be complex and random, with positive real and imaginary parts bounded by $D$, whereas for the off-diagonal element $b$ we still have $0 < b < 1$.

In the panel at the bottom of Fig. 5 we consider a more general case, where all four elements of $h$ do not vanish and are complex. The real and imaginary parts of the diagonal elements are assumed to be positive and random and bounded by $D$. Similarly, the off-diagonal elements are taken as complex and random with an upper bound unity for their real and imaginary parts.

We immediately infer from these figures that, whenever $h$ is dominated by the diagonal elements, a sharp peak at $S = 1/2$ emerges, indicating the appearance of maximally mixed asymptotic states. There are, however, significant differences between the various panels. Before we comment on them we ask the question, how do these features survive in higher dimensions? This is addressed in the following section.

**B. Lindblad dynamics in higher dimensions**

In Sec. V we have shown that the asymptotic solution of Eq. (32) is determined by the maximum (vanishing) eigenvalue of the Lindblad operator $L$ in the extended Hilbert space $\lambda_0=0$. The associated eigenvector, rewritten as an operator in the original $d$-dimensional Hilbert space and normalized such that its trace becomes unity, is the asymptotic density matrix, from which the asymptotic entropy is computed.
FIG. 6. (Color online) Entropy distributions $\pi(S)$ for the Lindblad dynamics in four dimensions $d=4$. Top: All elements of $h$ are real with upper bounds for DMs, UTMs, and LTMs given by $D$, 1, and 0, respectively. Middle: All elements of $h$ are complex with bounds for the real and imaginary parts for DMs, UTMs, and LTMs given by $D$, 1, and 0, respectively. Bottom: All elements of $h$ are complex with bounds for the real and imaginary part of DMs, UTMs, and LTMs given by $D$, 1, and 1, respectively.

In the following we consider ensembles of operators $h$ from the class $\mathcal{J}$ of Sec. III and compute asymptotic entropy distributions $\pi(S)$ for such ensembles. Each distribution is constructed from two million points. Similar to the classical case in Ref. [3], the matrix elements of $h$ are separated into three parts, the DMs and the UTMs and LTMs. The real and imaginary parts of all elements are positive uniformly distributed random variables bounded from above as specified below.

We first consider the four-dimensional case. If all elements of $h$ are considered to be real, uniformly distributed random numbers with upper bound $D$ for the DMs, unity for the UTMs, and zero for the LTMs, we obtain the entropy distributions shown in the top panel of Fig. 6 for various $D$. If all elements are complex with upper bounds for the real and imaginary parts of DMs, UTMs, and LTMs equal to $D$, unity, and zero, respectively, the entropy distributions in the middle panel are obtained. Finally, if the real and imaginary parts of the lower triangular elements are also bounded by unity, the resulting distributions are shown in the bottom panel of this figure. The general appearance of these curves closely resembles that of the two-dimensional case of Fig. 5.

Finally, in Fig. 7 we show analogous distributions for the eight-dimensional Lindblad system. Again, in the top panel $h$ is assumed to be real, and the upper bounds for DMs, UTMs, and LTMs are given by $D$, unity, and zero, respectively. For complex elements with the upper bounds for the real and imaginary parts of DMs, UTMs, and LTMs given by $D$, unity, and zero, respectively, the distributions in the middle panel are obtained. And for the most general case, where also the real and imaginary parts of LTMs are bounded by unity instead of vanishing as before, the distributions in the lower panel are obtained.

In all cases, if different upper bounds for the real and imaginary parts of the elements are used, nearly identical
distributions are obtained by interchanging the bounds for the real and imaginary parts of DMs, UTM, and/or LTMs. Furthermore, interchanging the bounds for UTM and LTMs also leaves the distributions unaffected.

In spite of differences in detail, a comparison of Figs. 5–7 reveals striking similarities. For purely real Hamiltonians and with vanishing elements below (as is assumed for all the top panels in the figures) or above the diagonal, the systems are strictly purifying, as long as the diagonal elements are much smaller than the off-diagonal elements in UTM (or LTMs if the roles of UTM and LTMs are interchanged). However, if the diagonal elements start to dominate, the system becomes mixing with asymptotic entropies distributed over the whole allowed range \(0 \leq S \leq (d-1)/d\). A spike at \(S=0\) still remains. If we consider a more general case, where the DMs and one of the triangular submatrices either above or below the diagonal are complex, the probability for strict purification becomes small for large DMs. This may be inferred from the middle panels of Figs. 5–7. If all matrix elements are allowed to contribute to the evolution, as is shown in the bottom panels of these figures, strict purification is almost completely lost even for very small elements of DMs.

C. Lindblad dynamics with normal operators

In Ref. [20] it was observed that for \(\Sigma_{d} h^{(a)} h^{(a)\dagger}\), the entropy is monotonically increasing in time. (This was actually shown for the entropy \(S=-\text{Tr} \rho \ln \rho\), but the proof can easily be carried over to our entropy.) Therefore, it is natural to look what are the eigenvalues and eigenvectors of \(L\) in this situation. We start with a single \(h^{(a)} = \Sigma_{a} a_{k} |\phi_{a}\rangle \langle \phi_{a}|\). The evolution equation becomes

\[
\frac{d}{dt} |\phi_{a}\rangle = \left( h|\phi_{a}\rangle \langle \phi_{a}| - \frac{1}{2} (h^\dagger h|\phi_{a}\rangle \langle \phi_{a}| + |\phi_{a}\rangle \langle \phi_{a}| h^\dagger h) \right)
\]

\[
= \left( a_{k} a_{k} - \frac{1}{2} |a_{k}|^2 \right) |\phi_{a}\rangle \langle \phi_{a}| + \delta_{k-1} a_{k} |\phi_{a}\rangle \langle \phi_{a}|.
\]

Therefore, the \(|\phi_{a}\rangle \langle \phi_{a}|\) are time invariant density matrices, whereas \(|\phi_{k}\rangle \langle \phi_{l}|, \) with \(k \neq l\), are eigenvectors of \(L\), whose eigenvalues have a strictly negative real part, such that their contributions to the density matrix \(\rho(t)\) tend to zero. Strict periodicity cannot occur.

If we have several Hermitian operators \(h^{(a)}\), then the Lindblad operator \(L\) in the extended Hilbert space is also Hermitian. Therefore we can find its eigenvectors with a variational principle: the eigenvectors have to be also eigenvectors of the individual \(L^{(a)}\). It follows that the time invariant density matrices have to commute with all \(h^{(a)}\), which in general will reduce the possible solutions to \(\rho = \frac{1}{d} I\), the maximally mixed state.

VI. CONCLUSION

In this paper we ask the question if order may emerge accidentally in dynamical evolution equations which model selection and mutation. As an indicator for order we use the quadratic entropy \(S\) and say the system is purifying if \(S\) tends to zero, and mixing if it tends to its maximum value. The system is said to be partially mixing if \(S\) approaches a value between these two extremes. This paper extends our previous work on the classical quasispecies dynamics to the quantum-mechanical setting, where the probabilities are now given by a density matrix \(\rho\). For its time evolution we start with a straightforward generalization of the classical evolution equations, which incorporate mutation and selection and are determined by a rate matrix \(\alpha\). “Accidental” means that not a single fixed matrix, but a whole ensemble of matrices is considered, and the dynamics is solved for each member of the ensemble. In this way we ignore exceptional cases and ask whether, typically, mixing or purification prevails.

Here we meet a first surprise. Whereas, as is shown in Ref. [3], the classical system is mixing unless order is brutally enforced, the corresponding quantum generalization is strictly purifying. This means that the quantum quasispecies evolution freezes anything completely within a few time units (which may correspond to a few nanoseconds in reality). This is independent of the dimension of the system. Even a variation of that quantum-mechanical quasispecies dynamics, which for lack of a better term we refer to as alternative quasispecies dynamics, is generally purifying. Only a negligible subclass of Hamiltonians gives partial mixing in the latter case. The mathematical reason is the minimal entropy principle. Every density matrix \(\rho\) gives a probability distribution \(p = \{p_{i}\}\) for any observable \(Q\) with projections \(Q_{i}\), such that \(p_{i} = \text{Tr}(\rho Q_{i})\). According to this principle, \(S(\rho) = \min_{Q} S(p_{i})\). Thus, the entropy of \(\rho\) is the minimum of the entropy as it appears to different observers. Our result says there is always one observer to whom the final state appears as pure.

In order to gain some physical insight, we compare these models with the Lindblad equation, which describes the dynamics of a system interacting with its surrounding in a limit, where the interaction proceeds on a much faster time scale than the dynamics itself. The Lindblad equation turns out to be the linear superposition of the two models treated previously, namely, the quasispecies equation and its alternative formulation. Each of the two subprocesses has been shown to be purifying by itself but, in combination, the Lindblad dynamics turns out to be mixing. The explanation for this second surprise is found by noting that the two subprocesses will generally tend to different pure states and, hence, their combined effort gives a partially mixing evolution.

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