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## Steepest-Entropy-Ascent Quantum Thermodynamic Non-equilibrium Modeling of Decoherence of a Composite System of Two Interacting Spin- $\frac{1}{2}$ Systems

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### ABSTRACT

The equation of motion of steepest-entropy-ascent quantum thermodynamics (SEA-QT) was first postulated in the early 1980s with the intent of modeling the non-linear dynamic behavior encountered in nature, which the unitary (linear) dynamics of the Schrödinger-von Neumann equation cannot. The SEA-QT equation is used here to model the decoherence phenomenon between two distinguishable and indivisible elementary constituents of type spin- $\frac{1}{2}$  (e.g., quantum bits or qubits). The resulting set of non-linear, first-order differential equations is solved with a fourth-order-Runge-Kutta routine provided by Matlab<sup>®</sup>. The time evolution of the state of the composite system as well as that of the reduced and locally-perceived states of the two constituents are traced from an initial non-equilibrium state of the composite along its relaxation towards stable equilibrium at constant system energy. An entangled and generally coherent, initial non-equilibrium state of the composite quantum system is prepared using a heuristic approach, which consists of randomly and homogeneously generating an initial point on the Bloch sphere for each of the constituents and then using a weighted average of their projections to arrive at an initial state for the composite. Results show how the initial entanglement and coherence between the two spin- $\frac{1}{2}$  constituents are reduced during relaxation towards a state of stable equilibrium. When the two particles are non-interacting, the initial coherence is lost once stable equilibrium is reached. When they are interacting, the coherence in the final stable equilibrium state is only that due to the interaction.

**Keywords:** non-equilibrium thermodynamics, steepest-entropy-ascent modeling, maximum-entropy-production modeling, entanglement, decoherence.

### 1. Introduction

Non-equilibrium thermodynamics is an important field of study within the scientific community and has as its general aim the development of a deeper understanding of how nature behaves and as a consequence, how new technologies can be more effectively developed. This applies at all spatial and temporal scales of analysis. Lately, of particular interest has been a consideration of the non-equilibrium phenomena which occur at the nanoscale, particularly in relation to quantum computing and nanometric devices [1-4] where entanglement, coherence, and decoherence are of great importance. The entanglement of zero-entropy states or the coherence of non-zero-entropy states is present when the local state of one constituent is correlated to that of another. The loss of correlation among the local states of the constituents of a composite system is known as decoherence.

The analysis (both experimental and numerical) of the creation and loss of correlations has significance for explaining the transition between the microscopic and macroscopic worlds [5, 6]. In addition, the manipulation of these communication-type phenomena can be used for the development of nanometric devices, which rely for their operation (e.g., a quantum computer [7]) on the correlation of states among the different subsystems, which make up the composite system.

A common approach to modeling these phenomena is to use linear Markovian quantum master equations (i.e., those of the Lindblad type [8-10]), which are based on the so-called “open-system model”, which assumes that the system is attached to (and weakly interacts with) a thermal bath or reservoir (environment). It is assumed that entanglement or coherence continually builds up due to the weak interactions between the system and the reservoir, while at the same time decoherence results from a dissipation or loss of quantum entanglement or coherence. Of course, under this assumption, the dissipation

phenomenon is the result of a loss of information. Although as is widely known these Markov quantum master equations fit the dissipative behavior of such simple systems well, they fail among other things to provide a proper description of the time evolution of the state of the system for more general or strongly coupled (and, thus, complicated) microscopic systems [11, 12].

In this paper, an alternative and comprehensive model is presented based on SEA-QT and its dynamical law of time evolution along the locally perceived direction of SEA, which effectively implements on a local basis the maximal entropy production (LMEP) [13]. This is used to model the non-linear dynamic behavior of a general (closed and adiabatic) microscopic system as its state evolves in time towards stable equilibrium, resulting in the loss of correlations among the constituents of the composite microscopic system. In general, the non-linear SEA-QT equation of motion consists of two terms, the first of which captures the unitary, Hamiltonian dynamics of the Schrödinger-von Neumann equation, and the second which models the non-linear dynamics of dissipative evolution in state based on the principle of SEA subject to the relevant dynamical constraints [14-17]. In particular, for the case of a system composed of two or more distinguishable (separable or non-separable, i.e., interacting or non-interacting) subsystems, we adopt the form of the SEA-QT equation which ensures that the evolution in state follows in correlated or uncorrelated local states the path of locally-perceived SEA [18].

Within the SEA-QT model, the dissipative aspects of the time evolution emerge from the non-Hamiltonian term in the SEA-QT equation of motion. Thus, instead of focusing on the non-Hamiltonian effects of the interactions between the microscopic system and its surroundings, the SEA-QT description assumes the composite system to be isolated and its time evolution to be intrinsically non-Hamiltonian. In so doing, the equation predicts a loss of quantum entanglement or coherence consistent with that observed in recent experiments [19-22]. This is illustrated here via the evolution in state of a microscopic system composed of two spin-1/2 particles. Direct comparisons with experiments are given in [23, 24].

## 2. Model description

### 2.1. Two spin-1/2-particles composite system

The composite system considered here is depicted in Figure 1. It consists of two interacting, spin-1/2-type particles. This represents the smallest composite system that can be formed in Nature and can, for example, be used to analyze the entangled or coherent states obtained when physically measuring the state of an atom in which one constituent represents the particle and the other the measuring device treated as a two-level-type subsystem [25].

For the analysis here, the state of constituent A and that of B are fully represented in subspaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively. The Hilbert space corresponding to the composite system is given as the outer product of the two subspaces such that

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \quad (1)$$

When the particles interact, their states become correlated and the state (density) operator  $\rho$  for the composite system may be written as

$$\rho = \rho_A \otimes \rho_B + \zeta \quad (2)$$

Here  $\rho$  is formed from the outer product of the local state operators represented by the reduced state operators  $\rho_A \equiv \text{Tr}_B \rho$  and  $\rho_B \equiv \text{Tr}_A \rho$ , and a correlation operator,  $\zeta$ , which is the null operator only in the absence of correlations.

The Hamiltonian operator on  $\mathcal{H}$ , representing the total energy of the composite system, is

$$H = H_A \otimes I_B + I_A \otimes H_B + V \quad (3)$$

where the operators

$$H_A = \frac{1}{2} \hbar \omega_0 \sigma_A^z \quad (4a)$$

$$H_B = \frac{1}{2} \hbar \omega_0 \sigma_B^z \quad (4b)$$

are the Hamiltonians on subspaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively,  $\omega_0$  is the transition frequency between the excited and ground energy levels of each constituent, and  $\hbar$  is the reduced Planck constant. The coupling operator on  $\mathcal{H}$ , given by

$$V = -\Gamma (\vec{\sigma}_A \otimes \vec{\sigma}_B) \quad (5)$$

represents the interaction between constituents,  $\vec{\sigma}_i$  ( $i = A, B$ ) are three-dimensional vectors of Pauli operators, and  $\Gamma$  is the strength of the coupling between the subsystems. For the system under consideration, the Hamiltonian of Eq. (3) becomes

$$H = -m (\sigma_A^z \otimes I_B + I_A \otimes \sigma_B^z) - \Gamma (\vec{\sigma}_A \otimes \vec{\sigma}_B) \quad (6)$$

where  $m = (1/2) \hbar \omega_0$  is the unit strength of a uniform externally applied magnetic field in the  $z$ -direction. The strength of the field given by  $M = m \hat{z}$  is small with respect to the Zeeman interaction splitting effects. For simplicity and without loss of generality,  $m$  and  $\hbar$  are set to 1, while  $\Gamma$  is set to 0.02.

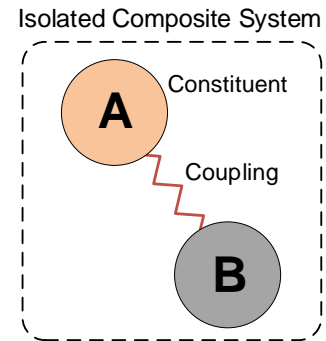


Figure 1. Schematic representation of a composite system in which the constituents interact with each other.

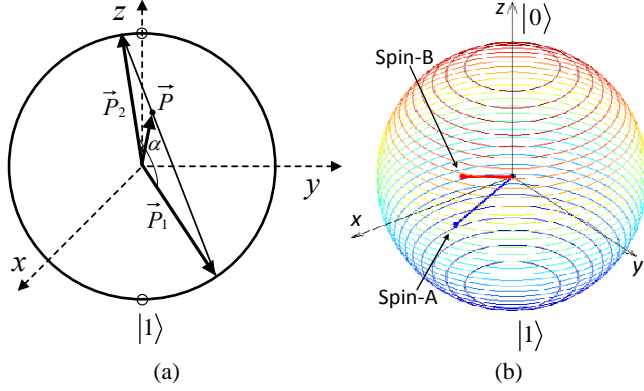


Figure 2. Bloch sphere representation of a qubit. (a) Construction of a non-zero-entropy state and (b) initial state for the system under analysis.

Important ingredients of the SEA-QT model are the local observables given by the linear local operators defined as follows [18]

$$(H)^A \equiv \text{Tr}_B [(I_A \otimes \rho_B) H] \quad (7a)$$

$$(H)^B \equiv \text{Tr}_A [(\rho_A \otimes I_B) H] \quad (7b)$$

which represent the “local effective perception” of the overall Hamiltonian operator and whose local mean values can be interpreted as the overall system’s energy as “locally perceived” by each constituent, and the local observables given by the nonlinear local operators defined as follows [18]

$$(S)^A \equiv -k_B \text{Tr}_B [(I_A \otimes \rho_B) B \ln \rho] \quad (8a)$$

$$(S)^B \equiv -k_B \text{Tr}_A [(\rho_A \otimes I_B) B \ln \rho] \quad (8b)$$

which represent the “local effective perception” of the overall  $-k_B \ln \rho$  operator and whose local mean values can be interpreted as the overall system’s entropy as “locally perceived” by each constituent.

The entropy of the overall, composite, microscopic system is given by the von Neumann entropy relation [26]

$$S = -k_B \text{Tr}(\rho \ln \rho) \quad (9)$$

where  $k_B$  is Boltzmann’s constant.

## 2.2. Construction of the initial entangled and correlated density operators in non-equilibrium states

Let us consider Figure 2a for visualization purposes where the state (either of zero entropy or of non-zero entropy) of a spin- $\frac{1}{2}$  particle is represented as a vector in the Bloch sphere [7]. If the state is a zero-entropy state, the tip of its vector representation,  $\vec{P}_1$ , is on the surface of the sphere ( $|\vec{P}_1| = 1$ ). A non-zero-entropy state, on the other hand, lies within the sphere and can, for example, be constructed as a statistical mix of two zero-entropy states [25] such that

$$\rho = \frac{1}{2} [I + \lambda \vec{P}_1 \cdot \vec{\sigma} + (1 - \lambda) \vec{P}_2 \cdot \vec{\sigma}] \quad (10)$$

where the tip of the non-pure vector state,  $\vec{P}$ , is on a line connecting the tips of the two unit-norm pure vector states,  $\vec{P}_1$  and  $\vec{P}_2$ , and  $|\vec{P}| < 1$ .  $\lambda$  is a real constant satisfying  $0 < \lambda < 1$ . Note that Eq. (10) represents the density operator for a single qubit. However, if instead of a single qubit two distinguishable qubits, A and B, on  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively, are considered, a state operator on  $\mathcal{H}$  may be obtained by using a development similar to that for Eq. (10), i.e., by employing the weighted sum of the outer products of sets of local pure (zero-entropy) state operators, namely,

$$\rho = \omega_1 \rho_1^A \otimes \rho_1^B + \omega_2 \rho_2^A \otimes \rho_2^B + \omega_3 \rho_1^A \otimes \rho_2^B + \omega_4 \rho_2^A \otimes \rho_1^B \quad (11)$$

where  $\rho_1^A$  and  $\rho_2^A$  for constituent A (or  $\rho_1^B$  and  $\rho_2^B$  for constituent B) are two pure (zero-entropy) state operators whose vector tips on the respective Bloch spheres are  $P_1(\theta, \phi)$  and  $P_2(\theta + \pi, \phi + \pi)$ , and are in opposite directions along a diameter of the Bloch sphere. We generate random initial states by randomly choosing the real positive constants,  $\omega_i$ , such that

$$\sum_i \omega_i = 1 \quad \text{and} \quad 0 < \omega_i < 1 \quad (12)$$

In an attempt to preserve the generality of the approach, random points with equal probability density are selected from the surface of the unit sphere [27] to represent the pure states  $P_i(\theta, \phi)$  for  $i=1,2$  where  $\theta$  and  $\phi$  are the rotational and azimuthal angle, respectively. Figure 2b shows the initial vector states representing the reduced density operator on  $\mathcal{H}_A$  and  $\mathcal{H}_B$  for particles A and B, respectively, obtained for the particular case provided in this paper.

The state operator obtained with Eq. (11) is for the initial non-equilibrium state of the composite microscopic system given by Eq. (2) [28]. In contrast, the final stable equilibrium state, reached at the end of the relaxation evolution, takes the canonical form

$$\rho_{se} = \frac{e^{-H/kT}}{\text{Tr}(e^{-H/kT})} \quad (13)$$

where the Hamiltonian operator is given by Eq. (6). The energy eigenlevel occupation probabilities showing the energy redistribution within the energy eigenlevels of the system

$$p_j = \langle \phi_j \rangle = \text{Tr}(\phi_j \rho) \quad (14)$$

are obtained in accordance with the eigenprojectors of the Hamiltonian operator,  $\phi_j = |\varepsilon_j\rangle\langle\varepsilon_j|$ .

## 2.3. Locally SEA state evolution dynamics

The generators of the motion for the isolated two-particle spin- $\frac{1}{2}$  composite system are given by the set  $R = \{I, H\}$  with the identity operator  $I$  expressed as  $I = I_A \otimes I_B$  and the

Hamiltonian operator by Eq. (6). The locally SEA-QT equation of motion is [18]

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \left( \frac{1}{\tau_A} D_A \otimes \rho_B + \frac{1}{\tau_B} \rho_A \otimes D_B \right) \quad (15)$$

where the first term on the right-hand side describes the unitary Hamiltonian dynamics of the system and the second the non-Hamiltonian dissipation dynamics. The operator  $[H, \rho] = H\rho - \rho H$  is the commutator between the Hamiltonian and density or state operator.  $\tau_A$  and  $\tau_B$  are internal-relaxation times particular to each constituent, considered to be real constants or functionals. For the case presented here, they are assumed to be real constants with a value of  $\tau_A = \tau_B = 1$ . The operators  $D_J$  ( $J = A, B$ ) are the nonlinear functions of the overall density operator defined explicitly in [18] and take the form

$$D_J = \frac{1}{2} \left( \sqrt{\rho_J} \tilde{D}_J + (\sqrt{\rho_J} \tilde{D}_J)^\dagger \right) \quad (16a)$$

$$\tilde{D}_J = \begin{bmatrix} \sqrt{\rho_J} (B \ln \rho)^J & \sqrt{\rho_A} (I)^J & \sqrt{\rho_A} (H)^J \\ (I, B \ln \rho)^J & (I, I)^J & (I, H)^J \\ (H, B \ln \rho)^J & (H, I)^J & (H, H)^J \end{bmatrix} \quad (16b)$$

$$\begin{bmatrix} (I, I)^J & (I, H)^J \\ (H, I)^J & (H, H)^J \end{bmatrix}$$

where  $B$  is the idempotent operator obtained by substituting unity for each nonzero eigenvalue of  $\rho$ ,  $|\cdot|$  denotes a determinant,  $(F, G)^J = (\sqrt{\rho_J} (F)^J | \sqrt{\rho_J} (G)^J)^J$ , and  $(F_J | G_J)^J = \frac{1}{2} \text{Tr}_J (F_J^\dagger G_J + G_J^\dagger F_J)$ .

## 2.4. Measures of correlation and entanglement

Since our scope is to model decoherence, we need to adopt some measure of entanglement and correlation. There are several options in the literature. For example, a correlation functional, which in this case is the entropy correlation function, is [18]

$$\sigma_{AB}(\rho) = \text{Tr}(\rho \ln \rho) - \text{Tr}_A(\rho_A \ln \rho_A) - \text{Tr}_B(\rho_B \ln \rho_B) \quad (17)$$

Another measure of the coherence between the constituents of the system is the norm of the commutator operator

$$\|C\| = \text{Tr}(CC^\dagger) \quad (18)$$

where  $C = i[H, \rho]$ . It can be used as an indicator of how the off-diagonal elements of the matrix representing the state operator evolve towards zero. It can, thus, also be thought of as a measure of the evolution of the coherence of the constituents.

The rate of change of the correlation functional given by Eq. (17) is expressed as

$$\frac{d(\sigma_{AB}(\rho))}{dt} = \dot{\sigma}_{AB}|_H - \dot{\sigma}_{AB}|_D \quad (19)$$

where the first term on the right-hand side represents the

contribution, which the Hamiltonian term of Eq. (15) makes to the rate of change of the correlation functional. The second term on the right-hand side represents the contribution of the dissipative term of Eq. (15). Based on the characteristics of Eq. (15), it has been conjectured [18] that  $\dot{\sigma}_{AB}|_D$  only destroys correlations between the constituents, namely, it should be non-negative at all times.

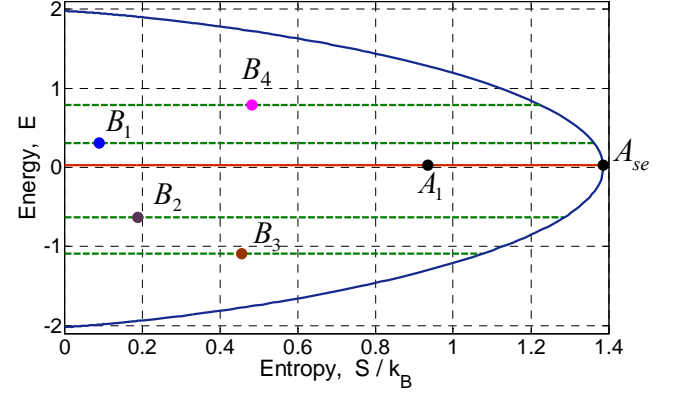


Figure 3. Energy-entropy diagram for the state evolution of the composite two spin-1/2-particles system. States  $A$  are for the particular case presented in this paper, while states  $B$  are other possible initial non-equilibrium states.

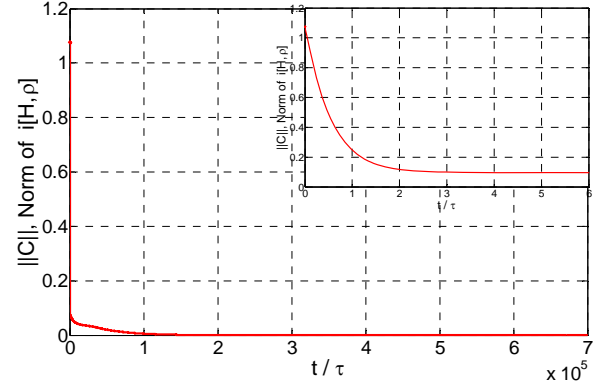


Figure 4. Evolution of the norm  $\|C\|$  of the commutator term.

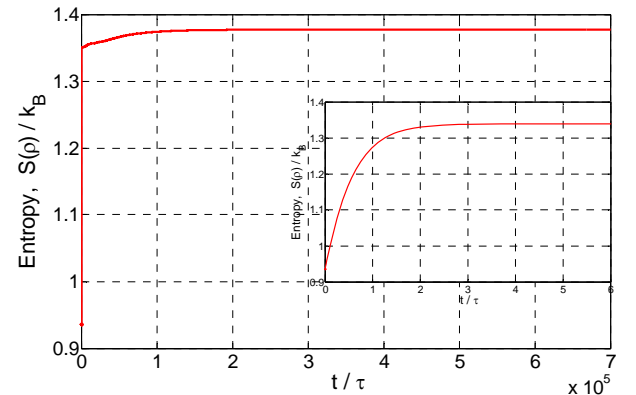


Figure 5. Entropy evolution of the composite system.

### 3. Results

Figure 3 shows an energy-entropy (E-S) diagram for the state evolution of the system. The four points depicted inside the curve are possible initial non-equilibrium states obtained with the approach described in Section 2.2 and illustrate the fact that any non-equilibrium state can be modeled with the approach used in this paper. Although state  $A_1$  together with states  $B_1$ ,  $B_2$ ,  $B_3$  and  $B_4$  were all modeled in terms of their evolution towards a state of stable equilibrium, the focus here is on the evolution in state  $A$  only for which a complete set of results is presented. With this in mind, the system evolves at constant energy from state  $A_1$  towards the state of stable equilibrium at  $A_{se}$  that for this case just happen to have a high negative temperature. When the state of the system reaches  $A_{se}$ , the density operator takes the canonical form of Eq. (13).

Figure 4 shows the norm of the commutator operator defined by Eq. (18). The evolution of the norm is taken as an indicator of how the off-diagonal elements of the matrix representing the density or state operator decay; and as a result, it is also an indicator of how the coherence of the system disappears as the state of the system evolves towards  $A_{se}$ . A drastic descent is observed at the beginning of the evolution because the local coherence within each constituent is being annihilated by the dissipative term of the equation of motion. This drastic descent is in accordance with the locally-perceived steepest entropy ascent ansatz upon which the dynamic model is constructed. As seen in Figure 5 where the evolution of the composite system entropy is given, the entropy increases very rapidly at the beginning of the evolution and then quickly slows its increase, asymptotically approaching its stable equilibrium value.

Figure 6 shows the x-, y-, and z-components of the vector state representation for both constituents. It can be seen that constituent A starts its evolution closer to the surface of its corresponding unit sphere than constituent B (also see Figure 2b). The red line corresponds to the z-component of the vector, which shows how the two constituents are coherently exchanging energy, i.e., when the energy of constituent A decreases, that of constituent B increases. The x- and y-components evolve very fast towards a value of zero, which is reached at a dimensionless time of about 10. This evolution towards the center of the local-Bloch sphere represents the loss of local-coherence of the constituents. In contrast, the non-local coherence belonging to the off-diagonal elements of the density matrix of the system continues its decay but at a very gradual rate until it reaches a value of zero at which point the Hamiltonian and density operators commute and the state of the composite system is that of stable equilibrium (see Figure 4 above). During this slow, non-linear and non-local decay, the constituents continue exchanging energy with each other.

Figure 7 shows the evolution in time of the energy eigenlevel occupation probabilities given by Eq. (14). As can be seen, the largest redistribution of system energy takes place primarily between two of the four energy eigenlevels of the system, the

majority of which occurs during a short non-dimensional time interval corresponding to the decay of the local-coherence of the constituents. After this fast initial redistribution, the redistribution of energy represented by changes in the eigenlevel occupation probabilities occurs at a much slower rate.

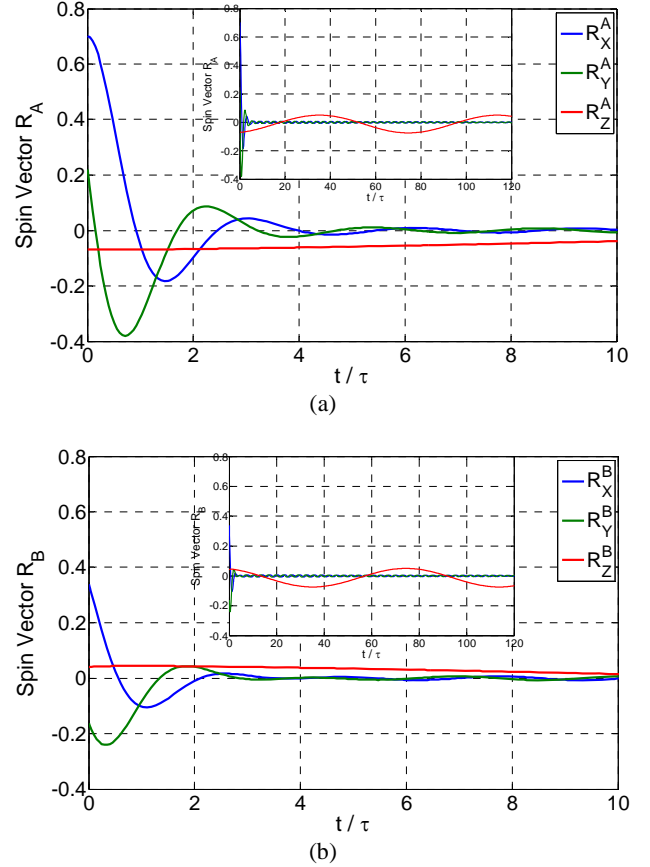


Figure 6. Evolution of the components of the state vector for (a) constituent A and (b) constituent B.

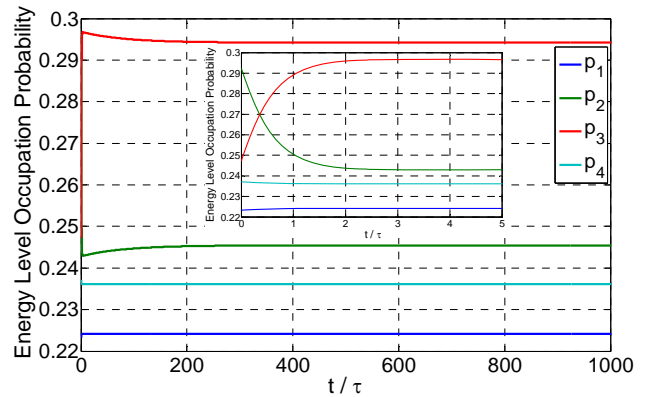


Figure 7. Evolution of the energy eigenlevel occupation probabilities of the composite system.

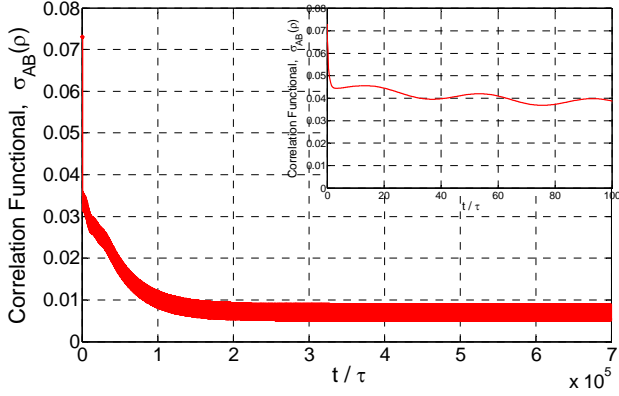


Figure 8. Evolution of the entropy correlation functional.

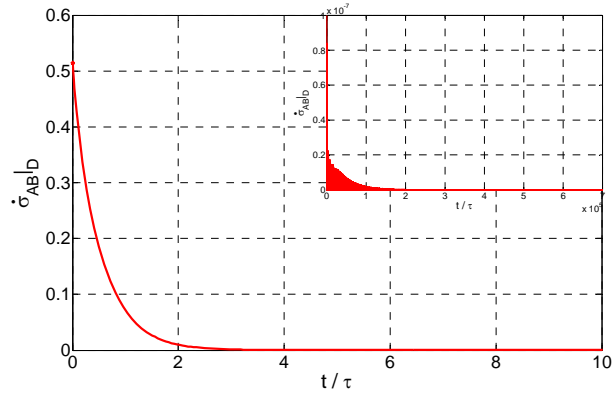


Figure 9. Rate of change of the contribution of the dissipative term to the rate of change of the entropy correlation functional.

Figure 8 depicts the evolution in time of the entropy correlation functional, which is a measurement of how the correlation between the constituents disappears when the composite system evolves towards a state of stable equilibrium. The correlation functional effectively reaches zero (within a certain convergence criterion) at stable equilibrium which occurs at about  $7 \times 10^5$  dimensionless time units and at which the value of the correlation functional is  $\sigma_{AB} = 0.0051$ .

Figure 9 shows the rate of change of the dissipation term of the equation of motion and confirms the conjecture that it can only destroy and never create correlations between constituents. Indeed, the rate of change of the entropy correlation is always non-negative, and this result is reproduced in all other simulations performed (but not reported here) obtained by randomly varying the initial state. In an attempt to generalize the validity of this statement, many different initial non-zero-entropy states randomly generated as discussed above were tested ( $\sim 100$ ) and in each case always resulted in non-negative values of  $\dot{\sigma}_{AB|D}$ . The cloud of initial points tested is depicted in Figure 10 for constituents A and B.

Finally, additional possible measures of decoherence are given in Figures 11 and 12, which show the evolution of the difference in the locally perceived energies and the energy of the composite system and the difference in the locally perceived

entropies and the entropy of the composite system, respectively. As can be seen, these differences decay very quickly at first and then very gradually, effectively going to zero at stable equilibrium, which occurs at about  $7 \times 10^5$  dimensionless time units (not depicted in the figures).

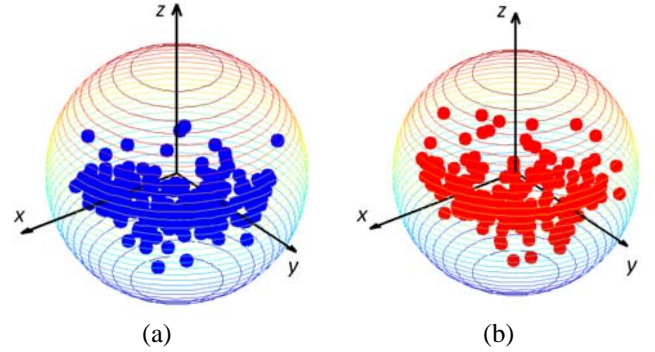


Figure 10. Bloch sphere representation of different random initial states for (a) spin-A and (b) spin-B.

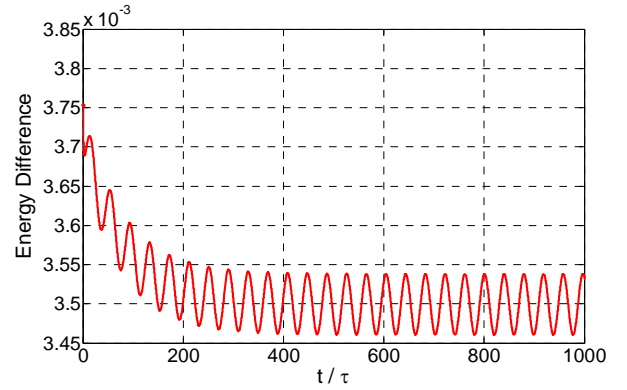


Figure 11. Evolution of the difference in the locally perceived energies and the energy of the composite system.

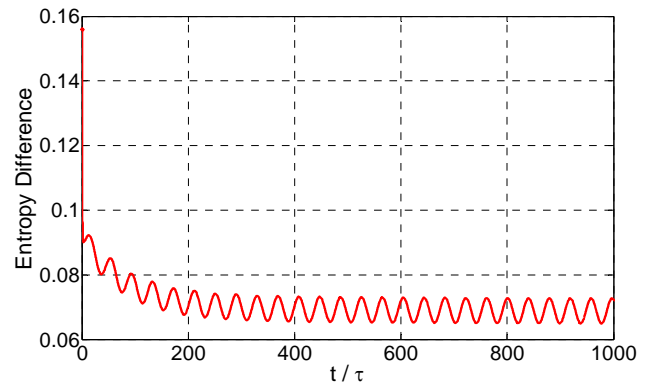


Figure 12. Evolution of the difference in the locally perceived entropies and the entropy of the composite system.

## 4. Conclusions

In this paper, an approach based on the steepest-entropy-ascent principle is used in which a non-linear model dynamics of

the state evolution is embedded in the equation so as to describe in a thermodynamically consistent way the decoherence which occurs during relaxation to equilibrium of a simple but realistic quantum system consisting of two interacting, correlated particles of type spin- $\frac{1}{2}$ . The results show that the local coherence within each constituent (particle) disappears in a very short period of time, whereas the non-local coherence belonging to the composite system takes a very long time to disappear. This suggests that at least one way of controlling decoherence may be to judiciously choose the initial state in such a way that the spontaneous loss of correlations between constituents is so slow as to be almost negligible. Another possibility as suggested by Levin *et al.* [29] may be to induce a steady state of the composite system via a set of constant energy fluxes with the environment. Limits to this control or any other must also be understood [30]. Of course, the first step in any control is the ability to simulate the process of loss of coherence, something for which we have demonstrated in the present paper that the SEA modeling concept could be used with profit.

Finally, as shown here, the dissipation term of the proposed model equation of motion is capable of destroying but never creating correlations between constituents. In addition, the results obtained demonstrate that the dynamic approach utilized in this paper is a robust and comprehensive framework for simulating the non-linear dynamics encountered in complex quantum systems.

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