How two spins can thermalize a third spin

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We consider thermalization of a microscopic quantum system by interaction with a thermal bath. Our interest is the minimal size the bath can have while still being able to thermalize the system. Within a specific thermalization scheme we show that a single spin-1/2 can be fully thermalized by interaction with a bath that consists of just two other spin-1/2. The two bath spins are initially in a pure, entangled state, and the thermalizing interaction is a Heisenberg exchange-interaction of the system-spin with one of the bath spins. The time dependent coupling strength has to obey a single integral constraint. We also present a simple generalization of this minimal model in which the bath consists of an arbitrary number of spin-1/2 pairs.

Our topic is thermalization of a system by means of an interaction with a bath, as specified in detail below. A bath that is suitable for that purpose has to exhibit certain features. Particularly, the standard textbook discussion explicitly or tacitly assumes that some kind of thermodynamic limit regarding the bath has to be taken in order to guarantee perfect thermalization of the system. The bath is assumed to be macroscopic in a certain sense, also if the system to be thermalized is a microscopic one.

The purpose of this brief note is to challenge the view that the bath should always be a macroscopic one. To this end we present a simple quantum-mechanical model in which the system is a single spin-1/2, and the bath consists of only two other spin-1/2. Initially, the two bath spins are in an entangled, pure state. The system spin is shown to perfectly thermalize by means of a finite-time exchange interaction with one of the bath spins. As will be shown below, the mechanism at work is essentially swapping the states of system spin and one bath spin by the exchange interaction. As a result, the entangled initial state of the two bath spins becomes the final entangled state of the system spin and the second bath spin. Tracing out the bath spin yields the final thermal state of the system. This mechanism is neither new nor particularly intriguing. However, to the best of our knowledge, it has not yet been discussed in the context of thermalization. Doing so may help to gain further insights in this problem: as simple as our model is, it very clearly points out the important role entanglement can play in the thermalization of a system. We note that this aspect is crucial in modern theoretical approaches to the phenomenon of thermalization in general.

We will discuss thermalization by a bath within the following general scheme. A closed quantum system $A$, the system, is initially prepared in an arbitrary state associated with a density operator $\rho_A$. Aside $A$ there is another closed quantum system, the bath $B$. Irrespective of the system’s state $\rho_A$, initially the bath is always in a certain state associated with a density operator $\rho_B$. The third ingredient of the scheme is a time dependent interaction that is supposed to establish thermal contact between system $A$ and bath $B$ during a finite period of time $[0, T]$. Particularly, this means that the interaction vanishes for $t < 0$ and $t > T$. By the interaction and the internal dynamics of $A$ and $B$, the initial state $\rho_A \otimes \rho_B$ of the joint system at time $t = 0$ evolves to a final joint state $\rho'_{AB}$ at time $t = T$. We say that the scheme thermalizes system $A$ at some temperature $\beta^{-1}$, if for any initial state $\rho_A$ of $A$ the final reduced state of $A$,

$$\rho_A' = \text{tr}_B \rho'_{AB},$$

is the thermal state $\tau = e^{-\beta H_A}/Z$ of the canonical ensemble. Here, $H_A$ is the Hamiltonian of system $A$ and $Z = \text{tr}e^{-\beta H_A}$ is its partition sum.

The above scheme is idealistic as it requires the system to be fully thermalized after an interaction during a finite period of time, $[0, T]$. To obtain a more realistic scheme one could demand that $\rho_A'$ reaches the thermal state $\tau$ within some meaningful approximation, if necessary, for $T \to \infty$. Here we stay with the idealized scheme simply because our model meets its stronger conditions.

Admittedly, our scheme uses the notion bath in a loose way. For instance, it is not required that the bath itself is in some thermal equilibrium, we do not demand that it is able to thermalize an entire class of (microscopic) systems, and we also do not insist that the bath is suitable for thermalizing the system by an entire class of system-bath interactions. Significantly strengthening the scheme in this point will probably make it impossible to construct a microscopic bath. On the other hand, we think that the presented scheme still captures essential features of a general thermalization process.

It is instructive to view the thermalization of system $A$ formally as a (rather simple) quantum operation $T$ that maps an arbitrary initial state $\rho_A$ onto the thermal state $\tau$. Being a proper quantum operation $T$, $T$ can be represented by an isometry $V : \mathcal{H}_A \to \mathcal{H}_A \otimes \mathcal{H}_B$ that is followed by taking the partial trace with respect to $\mathcal{H}_B$, i.e., $T(\rho_A) = \text{tr}_B V_{\rho_A} V^\dagger$. Here, $\mathcal{H}_A$ denotes the Hilbert space of system $A$, and $\mathcal{H}_B$ is some appropriate ancilla Hilbert space. Since $T$ describes thermalization into $\tau$, we have

$$\text{tr}_B V_{\rho_A} V^\dagger = \tau$$

for any initial state $\rho_A$. This relation can be phrased in more physical terms if the isometry $V$ is expressed via an
unitary operator \( U \) on \( \mathcal{H}_A \otimes \mathcal{H}_B \) and a normalized vector \( |\psi\rangle \in \mathcal{H}_B \) as
\[
V|\phi\rangle = U|\phi\rangle \otimes |\psi\rangle .
\]
Then, Eq. (1) becomes
\[
\text{tr}_B U \rho_A \otimes \psi U^\dagger = \tau , \tag{2}
\]
where \( \psi \) denotes the projection \( |\psi\rangle \langle \psi| \). This relation might be interpreted within our thermalization scheme as follows: \( \mathcal{H}_B \) is the Hilbert space of a certain bath system \( B \), \( \psi \) is its initial pure state, and \( U \) is the joint quantum-mechanical time-evolution of \( A \) and \( B \).

Thus far, mathematical objects have been merely named with physical terms. The question is whether there is a \( T \) representing isometry \( V \) such that the associated \( \mathcal{H}_B \), \( U \) and \( \psi \) have a physically meaningful interpretation. A quite simple answer to that question is suggested if one looks at the dimensions \( d_A \) and \( d_B \) of the involved Hilbert spaces \( \mathcal{H}_A \) and \( \mathcal{H}_B \). Assuming that \( d_A \) is finite, it is known that \( V \) can be realized as long as \( d_B \geq d_A^2 \). Hence, it is possible to find an isometry \( V \) for the choice \( \mathcal{H}_B = \mathcal{H}_A \otimes \mathcal{H}_A \), which means that in this case the bath can be thought of as consisting of just two copies \( A_1 \) and \( A_2 \) of the system \( A_0 \equiv A \). This, in turn, suggests to chose the initial pure state \( |\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_A \) as a purification of the thermal state \( \tau \) of \( A_1 \). I.e., for energy eigenstates \( |0\rangle_1, |1\rangle_1, \ldots, |d_A - 1\rangle_1 \) of \( A_1 \) with energies \( E_0, \ldots, E_{d_A - 1} \), and for arbitrary orthogonal states \( |0\rangle_2, |1\rangle_2, \ldots, |d_A - 1\rangle_2 \) of \( A_2 \) let
\[
|\psi\rangle = \frac{1}{\sqrt{2}} \sum_k e^{-\beta E_k} |k\rangle_1 \otimes |k\rangle_2 , \tag{3}
\]
which clearly satisfies \( \text{tr}_{A_2} |\psi\rangle \langle \psi| = \tau \). As a consequence of this choice the joint unitary time evolution must be a product of a swap operation \( W \) on \( A_0 \) and \( A_1 \),
\[
W|k\rangle_0 \otimes |k'\rangle_1 = |k'\rangle_0 \otimes |k\rangle_1 , \tag{4}
\]
and an arbitrary unitary operation \( U_2 \) on \( A_2 \),
\[
U = W \otimes U_2 . \tag{5}
\]
The effect on \( A_0 \) in an arbitrary initial state \( \rho_A \) is
\[
\text{tr}_B (W \otimes U_2) \rho_A \otimes \psi (W \otimes U_2)^\dagger = \text{tr}_{A_1} W (\rho_A \otimes \text{tr}_{A_2} (1 \otimes U_2^\dagger) \psi (1 \otimes U_2^\dagger)) W^\dagger = \text{tr}_{A_1} W (\rho_A \otimes \text{tr}_{A_2} \psi W^\dagger = \text{tr}_{A_1} W (\rho_A \otimes \tau) W^\dagger = \text{tr}_{A_1} \tau \otimes \rho_A = \tau .
\]
This is the desired thermalization of \( A_0 \).

For the remaining task of finding a physically meaningful Hamiltonian that generates the above dynamics we restrict ourself to the simple case of system \( A_0 \) being a spin-1/2 in a magnetic field. It is a well-known fact that then the swap \( W \) can be generated by the Heisenberg-exchange interaction \( S^0 \cdot \vec{S} \) with an appropriate time-dependent coupling \( J(t) \). [We use standard physics notation in units where \( \hbar = 1 \), i.e. \( \vec{S} = (S_x, S_y, S_z) \equiv \frac{1}{2}(\sigma_1, \sigma_2, \sigma_3) \), \( S^0 = S^0_1 \otimes 1^1 \otimes 1^2 \), etc.] In the end, this leads to a Hamiltonian
\[
H(t) = c S^0_1 + c S^2_2 + J(t) \vec{S} \cdot \vec{S}^1 + H_2 , \tag{6}
\]
where \( \epsilon \) denotes the common spin-splitting energy for the spins \( A_0 \) and \( A_1 \), and \( H_2 \) is an arbitrary Hamiltonian for the second bath spin \( A_2 \). Making use of the identity
\[
W = 2S^0_0 \cdot \vec{S}_1 + 1/2 \text{ it is straight forward to check that the time evolution } U = T_e \exp -i \int_0^T H(t) dt \text{ generated by } H(t) \text{ over the time period } [0,T] \text{ can be written as}
\]
\[
U = (\cos \alpha + i W \sin \alpha) \otimes U_2 , \tag{7}
\]
where the phase \( \alpha \) is given by
\[
\alpha = \frac{1}{2} \int_0^T J(t) dt , \tag{8}
\]
and the unitary \( U_2 \) describes the time evolution of the second bath spin. Provided the time-dependent coupling \( J(t) \) is such that the phase \( \alpha \) is an odd multiple of \( \pi/2 \), the entire time evolution \( U \) is precisely of the form Eq. (5) that we aimed for.

The minimal thermalization model thus obtained is summarized in Fig. 1. It is worth emphasizing that the two bath spins in the pure state \( \psi \) together with the proposed interaction always lead to complete thermalization of the system spin, irrespective of the initial state \( \rho_A \) of the system spin. Also, the interaction is physical in the sense that it is a simple two-spin interaction; a three-spin interaction would comply with the mathematical formalism as well but is actually not required. Owing to the fact that the bath is microscopic its dynamics has to match the dynamics of the system to be thermalized. For this reason the spin-splitting energy of the system spin must equal the one of the first bath spin. In contrast to that, the local dynamics of the second bath

![FIG. 1: A system spin (A) in an arbitrary initial state \( \rho \) interacts with two bath spins (B) in a pure, entangled initial state \( \psi \). By the interaction the entanglement is swapped to the upper spin and the reduced state of the upper spin becomes a thermal state \( \tau \).](image-url)
spin generated by $H_2$ does not change the entanglement with the two other spins and therefore is irrelevant for the thermalization. This offers a trivial interpretation of our model: Since the second bath spin is actually not involved in the system-bath interaction it can be traced out right from beginning. This leaves us with the first bath spin in the thermal state $\tau$, which by the exchange interaction is then simply transferred to the system spin.

Another important point is that the coupling $J(t)$ has to be chosen such that the associated phase $\alpha$ must be an odd multiple of $\pi/2$. Here it is to mention that also in case of a macroscopic bath an interaction that is able to thermalize will have to obey conditions. For instance, a system-bath coupling that is instantaneously switched off will almost never leave the system in a thermal state. Yet, it seems to be clear that a macroscopic bath allows for more freedom in the choice of a thermalizing interaction. To illustrate the latter point we briefly discuss a simple generalization of the above minimal model.

The generalized model consists of a system spin $A_0$ and $n$ pairs of bath spins denoted by $A_{\nu 1}$ and $A_{\nu 2}$ with $\nu = 1, \ldots, n$. Initially, each spin pair $A_{\nu 1}A_{\nu 2}$ of the bath is in the kind of pure state Eq. (3) as in the minimal model. This defines an initial bath state $\psi_n$ as a product of $n$ entangled two-spin states, each being a purification of $\psi_{A_{\nu}}\psi_{A_{\nu}}$. The exchange interactions $\bar{\mathcal{S}}^{0}, \bar{\mathcal{S}}^{\nu 1}$ do not commute among each other. To allow for an analytical treatment we therefore assume that the couplings $J_1(t), \ldots, J_n(t)$ are supported on disjoint time intervals $[0, t_1], [t_1, t_2], \ldots, [t_n, T]$. With this assumption the time evolution operator on $A_0, A_{11}, \ldots, A_{n1}$ can be written as the ordered product

$$H = \epsilon \bar{\mathcal{S}}^{0} + \epsilon \sum_{\nu=1}^{n} \bar{S}_{z}^{\nu 1} + \sum_{\nu=1}^{n} J_{\nu}(t) \bar{S}^{0} \cdot \bar{S}^{\nu 1} + \sum_{\nu=1}^{n} H^{\nu 2},$$

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$$\prod_{\nu} (\cos \alpha_{\nu} + i W_{0\nu} \sin \alpha_{\nu}),$$

where $W_{0\nu}$ is the swap operation on $A_0, A_{\nu 1}$, and $\alpha_{\nu} = \frac{1}{2} \int_{0}^{T} J_{\nu}(t) dt$. The effect of the entire time evolution on the system spin $A_0$ can be easily computed if first all spins $A_{12}, \ldots, A_{n2}$ are traced out and then successively the partial traces over the bath spins $A_{11}, A_{21}, \ldots, A_{n1}$ are taken. This is conveniently done by representing the density operators as matrices w.r.t. to the energy eigenstates $|0\rangle, |1\rangle$. In this way we find that an initial state of the system spin $A_0$

$$\rho_0 = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix}$$

becomes a final state

$$\rho'_{0} = \left( \begin{array}{cc} p a_{00} & \lambda a_{01} \\ \lambda^{*} a_{10} & p a_{11} \end{array} \right) + (1 - p)\tau,$$

where $\tau$ is the thermal state, and the parameters $p$ and $\lambda$ are given by

$$p = \prod_{\nu=1}^{n} p_{\nu}, \quad \lambda = \prod_{\nu=1}^{n} \lambda_{\nu},$$

with

$$p_{\nu} = \cos^{2} \alpha_{\nu},$$

$$\lambda_{\nu} = \cos^{2} \alpha_{\nu} + i \cos \alpha_{\nu} \sin \alpha_{\nu} \tanh \frac{\beta e}{2}.$$
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[6] Here, the equivalence of $\rho'_{AB}$ and $\rho'_A \otimes \rho'_B$ means that for any local operators $O_A, O_B$ $\text{tr} O_A \otimes O_B \rho'_{AB} = \text{tr} O_A \rho'_A \text{tr} O_B \rho'_B$. 