Temperature of a finite-dimensional quantum system

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A general expression for the temperature of a finite-dimensional quantum system is deduced from thermodynamic arguments. At equilibrium, this magnitude coincides with the standard thermodynamic temperature. Furthermore, it is well-defined even far from equilibrium. Explicit formulas for the temperature of two and three-dimensional quantum systems are presented, and some additional relevant aspects of this quantity are discussed.

I. INTRODUCTION

One of the main concerns of quantum thermodynamics is the correct identification of quantum analogues of relevant thermodynamic magnitudes. Our experience with the macroscopic world induces us to express the results of our research in this area in terms of concepts like free energy, work, or entropy production, which are well-defined in the classical world. However, the connection between both worlds (classical and quantum) has been shown not to be trivial, often counterintuitive, and in some cases, traumatic [1]. As a consequence, after almost a century of existence of quantum theory, and despite the enormous progress of quantum thermodynamics in recent years [2–7], most classical thermodynamic magnitudes are still waiting for an universally accepted quantum definition.

As an example, let us examine the two basic mechanisms of energy exchange: heat and work. Early works in quantum thermodynamics were based on the idea that heat is related to changes in the state $\rho$ of the system, while work is linked to the time variation of its Hamiltonian $H$, controllable by the experimenter [8]. This point of view leads to the following straightforward partition of the energy change, $d\langle H \rangle$:

$$d\langle H \rangle = \text{tr}[H d\rho] + \text{tr}[\rho dH]$$

(1)

where $\text{tr}$ denotes the trace operation. Under this perspective, the two terms on the r.h.s. of Eq. (1) can be clearly identified as heat and work, respectively, so the above equation can be considered to be an statement of the first law of thermodynamics.

This point of view has been widely employed during the last four decades, leading to very interesting results in matters such as the characterization of entropy production [9], or the deduction of the Landauer limit [10]. Nevertheless, several alternative definitions of heat and work have been used [11–14]. In particular, very recently two independent groups placed attention on the fact that certain changes in the state of the system are not accompanied by an entropy change, and argue that this fact implies that the part of the term $\text{tr}[H d\rho]$ which is not related to the change in the eigenvalues of $\rho$, but in its eigenvectors, should not be considered as heat, but as work. As a consequence, new definitions of both magnitudes were proposed [15, 16].

Considering this new perspective, in this work we focus on the study of the concept of temperature, which, except for a few special cases, has been elusive to an extension to the quantum regime. Our approach is based on the fact that both entropy and energy have well accepted definitions in the quantum case, so the application of the standard definition of temperature,

$$\frac{1}{T} = \frac{\partial S}{\partial E}$$

(2)

is, at least in principle, plausible.

This will also lead to the concept of temperature for a system out of equilibrium. Although temperature is clearly an equilibrium property, "effective temperatures" and similar concepts have proven to be very useful in their respective contexts [17–23], so the idea of an out-of-equilibrium temperature should not be discarded without a more profound exploration. One step in that direction is given in the present work.

The remainder of this paper is organized as follows. In Section II, we apply Eq. (2) in order to find the temperature of a two-level system. This particular case is interesting in its own right, and gives some insight on the general situation. In Section III, we deduce an expression for the temperature of a generic $N$-dimensional quantum system. Using this result, an explicit formula for the temperature of a qutrit is obtained, and shown to be consistent with the classical case. Conclusions and final remarks are presented in Section IV.

II. TWO-LEVEL SYSTEM

A. Temperature

In order to find the temperature of the system, we start by assuming that the von Neumann entropy $S_{vN}$ is a valid extension of the thermodynamic entropy in the quantum regime. This is based on the fact that in, thermal equilibrium, both entropies coincide. For a two-level system, $S_{vN}$ can be expressed in terms of the natural populations, i.e., the eigenvalues $\{\lambda_1, \lambda_2\}$ of the density matrix of the system, as [24]:

$$S_{vN} = -\lambda_1 \ln \lambda_1 - \lambda_2 \ln \lambda_2,$$

(3)
Then, applying the usual definition of temperature (using \( S e N \) instead of the thermodynamic entropy \( S \)), we obtain:

\[
\frac{1}{k_B T} = \frac{\partial S_{e N}}{\partial E} = \frac{\partial S_{e n}}{\partial \lambda_1} \frac{\partial \lambda_1}{\partial E} + \frac{\partial S_{e n}}{\partial \lambda_2} \frac{\partial \lambda_2}{\partial E}.
\]

Evaluation of Eq. (4) requires to express the natural populations in terms of the energy, which, as usual, is defined as the expected value of the local Hamiltonian in the actual state:

\[
E = \langle H_S \rangle = \text{tr}[\rho_S H_S].
\]

Expanding the density matrix \( \rho_S \) in its instantaneous eigenbasis \( \{|\psi_i\rangle, |\psi_2\rangle\} \):

\[
\rho_S = \lambda_1 |\psi_1\rangle\langle \psi_1 | + \lambda_2 |\psi_2\rangle\langle \psi_2 |,
\]

replacing Eq. (6) in Eq. (5), and using that \( \text{tr}[|\psi_j\rangle\langle \psi_j | H_S] = \langle \psi_j | H | \psi_j \rangle \), we obtain:

\[
E = \lambda_1 \langle \psi_1 | H_S | \psi_1 \rangle + \lambda_2 \langle \psi_2 | H_S | \psi_2 \rangle.
\]

Eq. (7) together with the fact that the density matrix has a trace equal to one

\[
\text{tr}(\rho_S) = \lambda_1 + \lambda_2 = 1,
\]

allows us to find \( \lambda_1 \) as a function of the energy:

\[
\lambda_1 = \frac{E - \langle \psi_2 | H_S | \psi_2 \rangle}{\langle \psi_1 | H_S | \psi_1 \rangle - \langle \psi_2 | H_S | \psi_2 \rangle},
\]

and from the above equation we obtain

\[
\frac{\partial \lambda_1}{\partial E} = \frac{1}{\langle \psi_1 | H_S | \psi_1 \rangle - \langle \psi_2 | H_S | \psi_2 \rangle},
\]

and a similar expression for \( \frac{\partial \lambda_2}{\partial E} \). On the other hand:

\[
\frac{\partial S_{e N}}{\partial \lambda_i} = -\text{ln} \lambda_i + 1, \quad i = 1, 2.
\]

From Eqs. (10), (10) and (11), we obtain the final expression:

\[
T = \frac{\langle \psi_1 | H_S | \psi_1 \rangle - \langle \psi_2 | H_S | \psi_2 \rangle}{k_B \text{ln}(\lambda_2/\lambda_1)}.
\]

**B. Discussion**

We first compare the above result with the well-known relation between the temperature and the populations in thermal equilibrium \( P_g \) and \( P_e \) of the ground and excited states, respectively, with corresponding energies \( E_g \) and \( E_e \):

\[
T = \frac{E_e - E_g}{k_B \ln(P_g/P_e)}.
\]

Since in this particular case the density matrix and the Hamiltonian commute, both are diagonal in the same basis, and, as a consequence the above expressions become identical. Thus Eq. (12) is a natural extension of Eq. (13) for the out-of-equilibrium case.

Let us now consider the (possibly time-dependent) Hamiltonian:

\[
H_S = \epsilon |e\rangle\langle e| - \epsilon |g\rangle\langle g|.
\]

Using Eq. (14), the terms in the numerator of Eq. (12) are:

\[
\langle \psi_i | H_S | \psi_i \rangle = \epsilon [\langle \psi_i | e \rangle^2 - |\psi_i | g \rangle^2], \quad i = 1, 2.
\]

The density operator, Eq. (6), can also be expressed in the energy basis in terms of the components of the Bloch vector \( \vec{B} = (u, v, w) \), which are a measure of the magnetization of the system, since they are proportional to the expected values of the spin operators. The expression is:

\[
\rho_S = \frac{1}{2} [ (1 + w) |g\rangle\langle g| + (u - iv) |e\rangle\langle e|]
\]

\[
+ (u + iv) |e\rangle\langle g| + (1 - w) |e\rangle\langle e|].
\]

It is easy to see that the eigenvalues of \( \rho_S \) can be expressed in terms of the modulus of the Bloch vector \( B = (u^2 + v^2 + w^2)^{1/2} \) as:

\[
\lambda_{1/2} = \frac{1}{2} (1 \pm B).
\]

Using this result and Eqs. (15) and (11), we obtain:

\[
\begin{align*}
\left| \langle \psi_1 | g \rangle \right|^2 - \left| \langle \psi_2 | g \rangle \right|^2 &= \frac{w}{B} \\
\left| \langle \psi_1 | e \rangle \right|^2 - \left| \langle \psi_2 | e \rangle \right|^2 &= -\frac{w}{B}
\end{align*}
\]

Finally, from Eqs. (12), (15) and (18), we obtain a compact expression for the temperature of the two-level system:

\[
T = \frac{\epsilon w}{k_B B \text{tanh}^{-1}(B)},
\]

which is discussed in more detail in Appendix A, together with other properties of the system that emerge from this equation.

**III. GENERAL CASE**

**A. Temperature**

In this section, we will show that it is possible to generalize Eq. (12) to any arbitrary finite dimension. First, let us consider what happens in the classical case.

In classical equilibrium thermodynamics, the macrostate of a system is determined when the
values of a reduced set of extensive quantities are known. For some systems, a common selection of these quantities is the triplet \( E, V, N \) (energy, volume, and particle number). This means that any other property is a function of this fundamental set.

In the quantum case, the state of the system is determined by the density matrix, which, expressed in its natural basis is:

\[
\rho_S = \sum_{j=1}^{N} \lambda_j |\psi_j\rangle \langle \psi_j|.
\]  

(20)

This means that given its eigenvectors, and assuming that their change is not related to heat transfer, a set of \( N \) parameters is required to determine the state. Taking into account the normalization condition, and the restriction imposed by the energy

\[
E = \sum_{j=1}^{N} \lambda_j \langle \psi_j | H_S | \psi_j \rangle,
\]  

(21)

it is clear that \( N - 2 \) independent quantities should be specified to define the quantum state.

A second observation is that in the classical case, temperature is defined as the inverse of the partial derivative of the entropy with respect to the energy, keeping the other quantities of the fundamental set fixed. Since in the quantum case these quantities are not specified, and in order to keep the discussion as general as possible, we shall consider a set of \( N - 2 \) observables \( \{O^1, ..., O^{N-2}\} \), such that their expected values, together with the energy and the normalization condition, determine the state, and which will play the role of the complementary thermodynamic quantities that will be kept constant when defining the temperature. We should note that in the two-level case there was no need to introduce such additional quantities because the energy and the eigenvectors of \( \rho_S \), suffice to completely determine the state. The expected values of these observables are,

\[
\langle O^k \rangle = \sum_{j=1}^{N} \lambda_j \langle \psi_j | O^k | \psi_j \rangle, \quad k = 1, ..., N-2.
\]  

(22)

To simplify the notation, in what follows we denote the matrix elements of a local operator \( X \) in the diagonal basis of \( \rho_S \) as \( \langle \psi_j | X | \psi_j \rangle = X_{jj} \). From Eqs. (21), (22) and the normalization condition, we see that we can find the natural populations \( \lambda_j \) by solving the linear system \( M \Lambda = \Gamma \), with

\[
M = \begin{pmatrix}
H_{11} & H_{22} & \cdots & H_{NN} \\
O_{11}^1 & O_{22}^1 & \cdots & O_{NN}^1 \\
O_{11}^2 & O_{22}^2 & \cdots & O_{NN}^2 \\
\vdots & \vdots & \ddots & \vdots \\
O_{11}^{N-2} & O_{22}^{N-2} & \cdots & O_{NN}^{N-2} \\
1 & 1 & \cdots & 1
\end{pmatrix},
\]  

(23)

and \( \Lambda = (\lambda_1, ..., \lambda_N)^T \), \( \Gamma = (E, \langle O^1 \rangle, ..., \langle O^{N-2} \rangle, 1)^T \). If \( M \) satisfies \( \det(M) \neq 0 \), the system has the solution

\[
\lambda_j = M^{-1}_j \Gamma.
\]  

(24)

Therefore the natural populations are lineal functions of the thermodynamic quantities, plus a constant term:

\[
\lambda_j = M^{-1}_j E + \sum_{i=2}^{N-1} M^{-1}_j \langle O^{i-1} \rangle + M^{-1}_j N.
\]  

(25)

It is now possible to obtain the temperature. The von Neumann entropy is given, in the present case, by

\[
S_{vN} = - \sum_{j=1}^{N} \lambda_j \ln \lambda_j,
\]  

(26)

so we can define the temperature as

\[
\frac{1}{k_B T} = \frac{\partial S_{vN}}{\partial E} \bigg|_{\langle O^1 \rangle, \ldots, \langle O^{N-2} \rangle} = \sum_j \frac{\partial S_{vN}}{\partial \lambda_j} \bigg|_{\lambda_k \neq \lambda_j} \frac{\partial \lambda_j}{\partial E} \bigg|_{\langle O^1 \rangle, \ldots, \langle O^{N-2} \rangle}
\]  

(27)

The partial derivatives needed are

\[
\frac{\partial S_{vN}}{\partial \lambda_j} \bigg|_{\lambda_k \neq \lambda_j} = -(\ln \lambda_j + 1),
\]  

(28)

and

\[
\frac{\partial \lambda_j}{\partial E} \bigg|_{\langle O^1 \rangle, \ldots, \langle O^{N-2} \rangle} = M^{-1}_j 1
\]  

(29)

From Eqs. (27), (28) and (29), we obtain

\[
T = - \left[ \frac{1}{k_B} \sum_{j=1}^{N} M^{-1}_j (\ln \lambda_j + 1) \right]^{-1}
\]  

(30)

A further simplification is possible. Since the last row of \( M \) has equal elements, each one of the first \( N - 1 \) columns of \( M^{-1} \) verifies that the sum of its entries is zero. Thus, \( \sum_{j=1}^{N} M^{-1}_j 1 = 0 \), and

\[
T = - \frac{1}{k_B \sum_{j=1}^{N} M^{-1}_j \ln \lambda_j},
\]  

(31)

which is the main result of this paper.

As an example, we can write an explicit formula for the temperature of a three-level system. Once the second relevant observable \( O \) is selected, in order to find the temperature we must invert the matrix

\[
M = \begin{pmatrix}
H_{11} & H_{22} & H_{33} \\
O_{11} & O_{22} & O_{33} \\
1 & 1 & 1
\end{pmatrix},
\]  

(32)
It is straightforward to see that its inverse exists provided that the condition
\[ \det(M) = H_{11}(O_{22} - O_{33}) + H_{22}(O_{33} - O_{11}) + H_{33}(O_{11} - O_{22}) \neq 0 \]
is satisfied. If we now consider the first column of \( M^{-1} \),
\[
\begin{align*}
M_{11}^{-1} &= [O_{22} - O_{33}]\det(M)^{-1}, \\
M_{21}^{-1} &= [O_{33} - O_{11}]\det(M)^{-1}, \\
M_{31}^{-1} &= [O_{11} - O_{22}]\det(M)^{-1},
\end{align*}
\]
from Eqs. (31), (33) and (34), we obtain an explicit expression for the temperature of a three-level system:
\[ T = \frac{O_{11}(H_{33} - H_{22}) + O_{22}(H_{11} - H_{33}) + O_{33}(H_{22} - H_{11})}{k_B[O_{11}\ln(\lambda_2/\lambda_3) + O_{22}\ln(\lambda_3/\lambda_1) + O_{33}\ln(\lambda_1/\lambda_2)]} \]
where the eigenvalues \( \lambda_i \) are
\[
\begin{align*}
\lambda_1 &= \frac{H_{22}O_{33} - H_{33}O_{22} + E(O_{22} - O_{33}) + \langle O \rangle(H_{33} - H_{22})}{\det(M)}, \\
\lambda_2 &= \frac{H_{33}O_{11} - H_{11}O_{33} + E(O_{33} - O_{11}) + \langle O \rangle(H_{11} - H_{33})}{\det(M)}, \\
\lambda_3 &= \frac{H_{11}O_{22} - H_{22}O_{11} + E(O_{11} - O_{22}) + \langle O \rangle(H_{22} - H_{11})}{\det(M)},
\end{align*}
\] and \( I^n \) is the identity operator in \( \mathcal{H}_n \). Thus, the global state at time \( t \) is given by
\[ |\psi(t)\rangle = U^t|\psi(0)\rangle, \]
where \( |\psi(0)\rangle \) can be written as
\[ |\psi(0)\rangle = \sum_n |n\rangle \otimes |a_n(0)|R + b_n(0)|N + c_n(0)|L| \]
with \( a_n(0), b_n(0) \) and \( c_n(0) \) satisfying the normalization condition \( \sum_n (|a_n(0)|^2 + |b_n(0)|^2 + |c_n(0)|^2) = 1 \).

We now focus on the evolution of the coin, which can be considered as a three-level system in interaction with a large environment, represented by the position Hilbert space \( \mathcal{H}_n \). To make sure that the environment is effectively large at any time, we restrict the study to Gaussian position distributions that span a large number of sites, i.e. with a standard deviation \( \sigma \gg 1 \). For convenience we take equal initial amplitudes for the left and right states,
\[
\begin{align*}
a_n(0) &= c_n(0) = \frac{e^{-\frac{x^2}{2\sigma^2}}}{\sqrt{2\pi\sigma^2}} a_0, \\
b_n(0) &= e^{-\frac{x^2}{2\sigma^2}} b_0.
\end{align*}
\]
As in the quantum walk with two internal states described in Refs. [28, 29], in this case the open evolution of the coin, starting from the initial condition given by Eq. (42), consists of an unitary part described by the effective local Hamiltonian \( G \), and a dissipative contribution due to interactions with the environment. In particular, in the asymptotic regime, the coin reaches an equilibrium state characterized by its reduced density matrix \( \rho_S^\infty \), which adopts the general form:
\[ \rho_S^\infty = \frac{1}{3} \begin{pmatrix} x & x & x \\ x & 1/3 & x \\ x & x & 1/3 \end{pmatrix}, \]
where \( x \) depends on the initial state, and, for physical states, it satisfies the inequality \(-1/6 < x < 1/3\). On the other hand, a simple calculation shows that the thermal state associated to the local Hamiltonian \( H_S = G \) at a given inverse temperature \( \beta \), i.e. \( e^{-\beta G}/tr[e^{-\beta G}] \), has exactly the form of Eq. (43), with
\[ x = -\frac{2 \sinh \beta}{3(3 \cos \beta + \sinh \beta)} \]
This implies that the equilibrium state can be considered a thermal state, and from the above equation we can obtain the corresponding equilibrium temperature \( (k_B = 1) \):
\[ T_{eq} = \frac{1}{2} \ln \left( \frac{1 - 3x}{1 + 6x} \right). \]
As the observable \( O \), we choose one represented by one of the Gell-Man matrices, which, together with the
curse with the observables to the same behavior of the temperature. The same expected value during the entire evolution, leading independent of the observable chosen, as they converge to a constant.

Fig. III B. We note that as time increases, thermal equilibrium is reached with an environment at temperature $T_E = 1/\beta E$, we have that:

$$\lambda_j = \frac{e^{-\beta E_j}}{Z} \tag{47}$$

where $Z$ is the partition function and $\{E_j\}$ is the set of eigenenergies of the system Hamiltonian. Using Eq. (47), and the fact that $\sum_{j=1}^N M_{j1}^{-1} = 0$, the denominator of Eq. (31) reads:

$$\sum_{j=1}^N M_{j1}^{-1} \ln(\lambda_j) = -\beta E \sum_{j=1}^N M_{j1}^{-1} E_j. \tag{48}$$

On the other hand, since in thermal equilibrium $[H_S, \rho_S] = 0$, the instantaneous eigenstates of $\rho_S$ coincide with the energy eigenstates $\{|E_j\rangle\}$, so the diagonal elements of the Hamiltonian in the eigenbasis of $\rho_S$ are, in this case, the eigenenergies:

$$\langle \psi_j | H_S | \psi_j \rangle = E_j \tag{49}$$

so the first row of the matrix $M$ verifies that $M_{1j} = E_j$. As a consequence,

$$\sum_{j=1}^N M_{j1}^{-1} E_j = 1 \tag{50}$$

Therefore, from Eqs. (31), (48) and (50), we obtain,

$$T = T_E \tag{51}$$

showing that the consistency of our temperature with the thermodynamic temperature in thermal equilibrium,
is independent of the choice of the complementary properties.

Regarding the behavior of the temperature, note that as the state of system becomes closer to a pure state, \(N - 1\) of its eigenvalues tend to zero, so the denominator of Eq. (51) diverges and the temperature takes the value \(T = 0\). In the opposite case of a maximally mixed state, since the eigenvalues are equal, we can factorize \(\ln(1/N)\) in the denominator and the temperature diverges due to the condition \(\sum_{j=1}^{N} M_{jj} = 0\).

Finally, we would like to compare the present results with a related concept, the spectral temperature [17], which is a commonly employed definition of temperature for out-of-equilibrium quantum systems [37, 43].

For a non-degenerate \(N\)-level system, the spectral temperature \(\tau\) is defined as,

\[
\frac{1}{\tau} = \left(1 - \frac{P_1 + P_N}{2}\right)^{-1} \sum_{j=1}^{N-1} \left[\frac{P_{j+1} + P_j}{2}\right] \frac{\ln(P_j / P_{j+1})}{E_{j+1} - E_j},
\]

where \(E_j\) are the eigenenergies, and \(P_j\) the corresponding probabilities under projective measurements in the energy eigenbasis. It can be shown that this expression, as it is the case with the one we propose in this work, reduces to the ordinary temperature in thermal equilibrium. In addition, it has the advantage of being easy to calculate, unlike Eq. (31), which requires the inversion of a potentially large matrix. Nevertheless, a critical observation can be made considering the simple case of a two-level system, situation in which Eq. (52) becomes

\[
\tau = \frac{E_2 - E_1}{\ln(P_1 / P_2)}.
\]

Recalling Eq. (13), we see that this expression has the same structure than the equilibrium temperature, but considering the out-of-equilibrium populations. Although this strategy is commonly employed to assign a temperature to two-level systems \[43, 15\], it is possible to see that it represents the change in entropy associated to a change in the energy only in some special cases. For instance, an unitary (isentropic) process in which the populations change in time can be implemented using a time-dependent Hamiltonian. In that case, the derivative of entropy with respect to energy is zero, while the spectral temperature is not. Our proposal does not suffer from this problem since, by construction, the temperature defined in this work is, precisely, the derivative of the entropy with respect to energy.

This can be confirmed by analyzing the same situation but employing Eq. (12), instead of Eq. (55). Since the system remains in a pure state, one of its eigenvalues is 1 and all others are 0, and therefore the denominator diverges, leading to \(T = 0\). Furthermore, while the temperature in thermal equilibrium depends only on the populations, it would be reasonable to think that in the out-of-equilibrium situation, other aspects of the quantum state play a role. This is so because the energy, Eq. (21), is a function of the eigenvalues and the eigenstates of \(\rho_S\). Spectral temperature, as defined through Eq. (52), does not meet this expected behavior.

IV. FINAL REMARKS AND CONCLUSIONS

In this work we have shown that it is possible to define the notion of temperature for finite-dimensional quantum systems, in a way such that the consistency with the classical definition is preserved. Our proposal is based on the fact that the von Neumann entropy and the internal energy are well-defined functions of the state of the system, even far from equilibrium. We have presented explicit formulas for the temperature of low-dimensional systems (\(\dim(H_S) = 2, 3\)), but similar expressions exist for higher dimensional systems.

An important aspect of our method is that, in order to define the temperature, one is required to select a set of observables such that their expected values are kept fixed when performing the partial derivative calculations. They play an analogous role to volume and particle numbers in classical thermodynamics, and this degree of freedom in the definition allows to adapt the application of the formula to the context, selecting those properties that are most convenient to keep fixed. Possible restrictions on the choice of these observables that ensure that the matrix \(M\) is invertible require a more profound study. Further aspects of the present definition, such as its relation with the direction of the heat flow, are currently under investigation.

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Appendix A: Comments on Eq. (19)

In Ref. [20] an expression for the temperature of a two-level system similar to Eq. (19) was found, but in which the factor \(w/B\) appears inverted. In order to help understand the origin of this difference, we first briefly present the arguments used in that work.

We note that since the state of a two-level system is completely defined by the components of the Bloch vector \((u, v, w)\), any thermodynamic property can be expressed in terms of these three components. In particular, as shown in Ref. [20], the entropy is a function of the modulus \(B\) of the Bloch vector:

\[
S_{vN} = -\left(\frac{1 + B}{2}\right) \ln \left(\frac{1 + B}{2}\right) - \left(\frac{1 - B}{2}\right) \ln \left(\frac{1 - B}{2}\right).
\]  
(A1)
Choosing the $z$ axis in the direction of $\{|q\rangle, |\epsilon\rangle\}$, the internal energy associated to the Hamiltonian (14) is:

$$E = -\varepsilon B \cos \theta = -\varepsilon w$$  (A2)

where $\theta$ is the polar angle of $\vec{B}$ in spherical coordinates. Then, Ref. [20] defines the inverse temperature as the partial derivative of the entropy with respect to the energy in a zero work process from the standard point of view [8], i.e. fixing the Hamiltonian, which in this case means fixing the $z$ axis and $\varepsilon$:

$$\frac{1}{k_B T} = \frac{\partial S_{vN}}{\partial E} \bigg|_\varepsilon$$  (A3)

Since entropy depends on the three components of the Bloch vector, but energy depends only on the $z$ component, applying the chain rule we obtain:

$$\frac{1}{k_B T} = \frac{\partial S_{vN}}{\partial E} \bigg|_\varepsilon \frac{\partial w}{\partial B} \frac{\partial E}{\partial w}$$  (A4)

Finally, using Eqs. (A1) and (A2), the expression for the temperature of the two-level obtained in reference [20] is:

$$T = \frac{\varepsilon B}{k_B w \tanh^{-1}(B)}$$  (A5)

Observe the different position of the factors $B$ and $w$ with respect to Eq. (19).

The previous argument was based on the hypothesis that the work done on the system is exclusively related to the changes in the local Hamiltonian. In the present work, we have adopted the new point of view presented in [15, 16]. This new perspective can be illustrated by considering the infinitesimal energy change obtained by differentiating Eq. (7):

$$dE = d\lambda_1 \langle \psi_1 | H_S | \psi_1 \rangle + \lambda_1 d\langle \psi_1 | H_S | \psi_1 \rangle + d\lambda_2 \langle \psi_2 | H_S | \psi_2 \rangle + \lambda_2 d\langle \psi_2 | H_S | \psi_2 \rangle$$  (A6)

Since entropy depends only on the eigenvalues of $\rho_S$, only the first and third terms of Eq. (A6) contribute to the entropy change of the system. As a consequence, they are the only terms which should be considered as heat. This implies that work can be performed on the system even in the case that the Hamiltonian is kept fixed, as long as the eigenvectors of $\rho_S$ change in time.

The adoption of this point of view implies that in the attempt of defining temperature by analogy with the classical case, the restriction of keeping the equivalent to the volume fixed in the partial derivative, i.e. zero work, implies that in the differentiation not only the Hamiltonian is kept fixed, as in Ref. [20], but also the eigenstates of the reduced density matrix are kept fixed. Since an instantaneous eigenstate of $\rho_S$ in the Bloch sphere is defined by the pair of angles $(\theta, \varphi)$, the definition of temperature from this new perspective becomes:

$$\frac{1}{k_B T} = \frac{\partial S_{vN}}{\partial E} \bigg|_{\varepsilon, \theta, \varphi} = \frac{dS_{vN}}{dB} \frac{\partial E}{dB} \bigg|_{\varepsilon, \theta, \varphi}$$  (A7)

The two factors in the above equation can be obtained from Eqs. (A1) and (A2):

$$\frac{dS_{vN}}{dB} = -\tanh^{-1}(B), \quad \frac{\partial E}{\partial E} \bigg|_{\varepsilon, \theta, \varphi} = -\frac{1}{\varepsilon \cos(\theta)}$$  (A8)

Finally, from the above equations and using that $\cos \theta = w/B$, we arrive at Eq. (19). It is clear that the adoption of Eq. (19) or Eq. (A5) as the qubit’s temperature is directly linked to a more fundamental question, which is, what are the most appropriate definitions of heat and work in the quantum regime? Perhaps the exploration of the corresponding temperatures can help to shed light on this matter.

In that sense, one fundamental difference between both approaches is related to the existence of an intrinsic entropy production. In [20] it was shown that the adoption of Eq. (A5) as the qubit’s temperature implies the existence of an entropy production which represents a measure of the loss of internal coherence by the qubit. In this new approach employed in this work, it is straightforward to verify that $dS_{vN} = \delta Q/T$, which implies no internal entropy production, as reported in [27]. Of course, since in the general case the system is in an out-of-equilibrium state, the temperatures of the system and the environment may not coincide, so a boundary contribution of entropy production due to the possibly finite temperature difference is expected.

Equation (19) can be used to analyze the properties associated to the temperature obtained in the present approach. Note that, since $w$ is the component of the Bloch vector parallel to the effective magnetic field, the temperature defined in Eq. (19) is positive when the scalar product between the magnetization and the field is positive. On the other hand, we can see that pure states ($B = 1$) and those with $w = 0$ have zero temperature, except for the maximally mixed state ($B = 0$), for which $T = \infty$. To illustrate this, two isothermal surfaces in the Bloch sphere, one associated with a positive and another with a negative temperature, are represented in Fig. (2).

As an application of the concept of temperature of a two level system employed in the present work, we will obtain the expression of the heat capacity of a qubit. In classical thermodynamics, the heat capacity is defined as the derivative of the energy with respect to temperature in a zero work process. Thus we define:

$$C = \frac{\partial E}{\partial T} \bigg|_{\varepsilon, \theta, \varphi}$$  (A9)

Using Eqs. (19) and (A2), we have that,

$$E = -\varepsilon \cos \theta \tanh \left( \frac{\varepsilon \cos \theta}{k_B T} \right)$$  (A10)
FIG. 2: Isothermal surfaces in the Bloch sphere, corresponding to the temperature values $k_B T_1 = 0.5 \varepsilon$ (red, northern hemisphere) and $k_B T_2 = -2 \varepsilon$ (blue, southern hemisphere).

And therefore:

$$C = \left[ \frac{\varepsilon \cos \theta / k_B T}{\cosh (\varepsilon \cos \theta / k_B T)} \right]^2 \quad (A11)$$

Clearly the heat capacity $C$ is non-negative, and since in thermal equilibrium the Bloch vector is parallel to the magnetic field, which is along the $z$-axis, and the temperature is equal to the equilibrium temperature $T_E$, Eq. (A11) reduces to the classical expression for the heat capacity:

$$C = \left[ \frac{\varepsilon / k_B T}{\cosh (\varepsilon / k_B T)} \right]^2. \quad (A12)$$
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