Entanglement in thermal equilibrium states

O. Osenda* and G.A. Raggio†

FaMAF-UNC, Córdoba, Argentina

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Abstract

We revisit the problem of entanglement of thermal equilibrium states of composite systems. We introduce characteristic, viz. critical, temperatures –and bounds for them–marking transitions from entanglement to separability or vice versa. We present examples for the various possible thermal entanglement scenarios in bipartite qubit/qubit and qubit/qutrit systems.

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*Electronic address: osenda@famaf.unc.edu.ar

†Electronic address: raggio@famaf.unc.edu.ar

I. INTRODUCTION

Since the work of Nielsen [1] and Arnesen et al., [2] the issue of entanglement in thermal equilibrium states has been the subject a number of papers [3–15] dealing with different aspects of the problem. Since formulas which allow one to decide whether a given state is entangled or not are available only for a bipartite qubit/qubit or qubit/qutrit system, the quantitative entanglement studies presented in the literature have, perforce, been restricted to investigations of the entanglement of the Gibbs-state reduced to the possible two-component subsystems, or to the study of particular so called entanglement witnesses or other entanglement monotone functions (e.g. [10]). Among the physically more relevant are the studies of the different spin 1/2 one-dimensional chain models (Heisenberg [2, 8], Ising [3, 7], XX [6], XY [7], XXZ [9]) where the two-component subsystem entanglement issue is studied in dependence of the length of the chain and/or parameters entering the Hamiltonian. All studies identify a threshold temperature above which thermal states restricted to bipartite subsystems are separable. Although many of the available studies, e.g. [1, 2, 5–7, 11, 14], observe that the bipartite subsystem entanglement of thermal states need not be monotone in temperature, it is not at all clear what entanglement behaviour is to be expected for Gibbs states with temperatures below the threshold temperature. Moreover it is not clear which qualitative features of the entanglement of the Gibbs state (of the specific Hamiltonians studied) reduced to two-component subsystems, carry over to global entanglement properties of the thermal states of multipartite systems. To clarify these points was one of our basic motivations. The other basic motivation comes from certain problems addressed in [16] that will be briefly discussed below.

In this report we revisit the global entanglement problem of thermal equilibrium states of arbitrary composite quantum systems. We give precise definitions and basic properties for two characteristic, viz. critical, temperatures: the upper entanglement temperature T_E below which the corresponding thermal equilibrium states are entangled, and the lower separability temperature T_S above which the corresponding Gibbs states are separable. One has generally $0 \leq T_E \leq T_S$ and various entanglement scenarios can be distinguished depending on whether the two inequalities are equalities or not. We provide bounds on these two critical temperatures. We also show that when $T_E < T_S$ then there can be many transitions from entanglement to separability for the thermal states with temperatures in the interval $[T_E, T_S]$. We exhibit examples of the different scenarios for two qubits and a qubit/qutrit system.

II. GENERAL RESULTS

Consider a finite composite quantum system described by the complex Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$, which is the tensor product of N (≥ 2) finite dimensional Hilbert spaces $\mathcal{H}_j$ of dimension $d_j \geq 2$ ($j = 1, 2, \cdots, N$); and has dimension $D = d_1 d_2 \cdots d_N$. Given any Hamiltonian $H = H^*$ acting on $\mathcal{H}$, the thermal equilibrium (or Gibbs) state ρ_T for temperature T is given by the density matrix $\rho_T = \exp(-H/T)/tr(\exp(-H/T))$.
We recall that an arbitrary state (mixed or pure) of the composite system is said to be *separable* or *unentangled* if it can be written as a mixture (finite convex sum) of pure product states. If this is not the case, the state is said to be *entangled*.
The rest of this section collects basic information which is generally valid, i.e., for any N and D, and every Hamiltonian. If the Hamiltonian is a real multiple of the identity, $H = c \cdot \mathbf{1}$, then $\rho_T = \mathbf{1}/D$ for all T,and the state is the normalized trace or the completely mixed state, which we denote by τ. Since $\mathbf{1}/D = (\mathbf{1}/d_1) \otimes (\mathbf{1}/d_2) \otimes \cdots \otimes (\mathbf{1}/d_N)$ the normalized trace τ is a separable state. We assume henceforth that the Hamiltonian H is not a multiple of the identity, and let P_- be the spectral projection associated with the minimal (ground-state energy) eigenvalue h_{min} whose multiplicity we denote by m_-. For the ground-state $\rho_0 = P_-/m_-$, one has $\lim_{T\to 0} \rho_T = \rho_0$ where the limit can be taken in various ways. As the limit of matrix elements in any orthonormal basis you wish; or $\lim_{T\to 0} tr(\mid \rho_T - \rho_0 \mid) = 0$ where $\mid X \mid$ denotes the absolute value of the operator X; etc. Moreover $\lim_{T\to\infty} \rho_T = \tau$ in the same sense, and the map $0 \leq T \mapsto \rho_T$ is continuous.
For what follows it will be important to observe that the energy $U(T) = tr(\rho_T H)$ as a function of temperature, is a monotone increasing continuous function with $\lim_{T\to 0} U(T) = h_{min}$ and $\lim_{T\to\infty} U(T) = tr(\tau H) = tr(H)/D$.

Various "critical" temperatures. As mentioned, a critical or threshold temperature above which entanglement is impossible has been observed in all cited studies. It is shown in [16] that for every Hamiltonian there exists a finite critical temperature T_S which satisfies: (i) $0 \leq T_S < \infty$; (ii) ρ_T is separable for every $T \in [T_S, \infty]$; and (iii) for every $0 \leq T < T_S$ there are entangled thermal states with temperatures in the interval $[T, T_S)$. We call T_S the *lower separability temperature*. Even if H is not a multiple of the identity, it could still be trivial in the sense that it contains no interactions whatsoever between the component subsystems, $H = \sum_{n=1}^{N} H^{(n)}$, $H^{(n)}$ acting only on the n-th component. In this case $\rho_T = \rho_T^{(1)} \otimes \rho_T^{(2)} \otimes \cdots \otimes \rho_T^{(N)}$ is a product-state, hence unentangled and $T_S = 0$.

It is important to stress the fact that the convex set of separable states is closed, and this implies that the set of non-negative temperatures T for which ρ_T is unentangled, is closed. Accordingly, the non-negative temperatures T for which ρ_T is entangled is an open set in $[0, T_S)$.

By their very definition, entanglement witnesses or entanglement monotone functions will always provide temperatures for which the thermal states are entangled and these temperatures are lower bounds on T_S. A particularly simple witness is the energy itself as observed in [11–13]. Let $\eta = \inf\{tr(\omega H) : \ \omega \text{ is separable}\}$, that is the lowest energy expectation value obtainable with an unentangled state. The infimum is assumed, and since the map $\omega \mapsto tr(\omega H)$ is convex-linear, it can be taken over the pure product-states. η can be calculated or estimated in general as soon as the Hamiltonian is known.

If for some $T_1 \geq 0$ we have $\rho_{T_1}(H) < \eta$, then ρ_{T_1} is entangled. By the monotone increase of $U(T)$ and the intermediate-value theorem there is a unique $T_H > T_1$ such that $U(T_H) = \eta$ and all Gibbs states with temperatures in $[0, T_H)$ are entangled (in particular ρ_0 is entangled). In [12], T_H is denoted by T_E and called the entanglement-gap temperature. It follows that $T_H \leq T_S$. It does not follow that Gibbs states with temperatures (immediately) above T_H are necessarily separable. Although $T_H > 0$ does indeed signal the presence of thermal entanglement at low enough temperatures, its importance should not be overrated. The correct critical value is: $T_E = \inf\{T \geq 0 : \ \rho_T \text{ is separable}\}$; for which one can prove, as in [16], that: (i) $0 \leq T_E \leq T_S$, and ρ_{T_E} is separable; and (ii) $T_E > 0$ if and only if ρ_0 is entangled, and in this case all thermal states with temperatures in $[0, T_E)$ are entangled. Alternatively, T_E could be defined as the greatest temperature such that all Gibbs-states with temperatures below it are entangled; we call T_E the *upper entanglement temperature*. Obviously, $T_H \leq T_E$, but one should expect that, in general, T_H can be a rather poor lower bound on T_E. The following example should serve as illustration. Consider two qubits; and suppose the minimal energy h_{min} of your Hamiltonian is doubly degenerate with ground-state vectors $\psi_1 = \alpha \otimes \alpha$, and $\psi_2 = (\alpha \otimes \beta + \beta \otimes \alpha)/\sqrt{2}$ where α (resp. β) is an eigenstate of σ_3 to the eigenvalue 1 (resp. -1) for one qubit. Then the ground-state is $\rho_0 = (1/2) \mid \psi_1\rangle\langle\psi_1 \mid +(1/2) \mid \psi_2\rangle\langle\psi_2 \mid$, and it is entangled (the partial transpose of ρ_0 has a negative eigenvalue); $\eta = h_{min} = \langle\psi_1, H\psi_1\rangle$ and thus $T_H = 0$; but $T_E > 0$.

The "more mixed than" ordering of thermal states. Upper bounds on T_S. The proof of existence of T_S given in [16] proceeds via an upper bound which turns out to be very poor. The theory of the "more mixed than"partial ordering of states of a quantum system, [17], can be put to use in the discussion of entanglement of Gibbs states, and provides upper bounds on T_S. It is a result of Wehrl and Uhlmann (cf. Refs. [17, 18]), that $0 \leq T < T' \leq \infty$ implies $F(\rho_T) \leq F(\rho_{T'})$, for every unitarily invariant, concave, continuous real-valued functional F defined on states. It is shown in [16], that for every such functional F, for which $F(\omega) = F(\tau)$ implies $\omega = \tau$, there is a critical constant $C_F < F(\tau)$ such that: (i) If the state ω satisfies $F(\omega) \geq C_F$ then ω is separable; and (ii) For every possible value C of F below C_F there is an entangled state ϕ with $F(\phi) = C$. There is an analogous version of this for unitarily invariant, convex, continuous real-valued functionals. Thus, every unitarily invariant, continuous real-valued functional which isolates τ and is either convex or concave, acts as a separability detector and can be used to obtain an upper bound on T_S. Indeed, take such a concave separability detector F. Then, $T \mapsto F(\rho_T)$ is a non-decreasing continuous function for which $\lim_{T\to\infty} F(\rho_T) = F(\tau) > C_F$. By the intermediate-value theorem there is $T_F < \infty$ such that $F(\rho_{T_F}) = C_F$ and all Gibbs states with temperatures in $[T_F, \infty]$ are unentangled. It follows that $T_S \leq T_F$.

The map $\omega \mapsto tr(\omega^2)$ is strictly convex (cf. Ref. [18], p. 47), unitarily invariant and is easily seen to isolate τ. It turns out to be a rather useful separability detector because it is easy to calculate. Furthermore, the critical values for the trace of the square are known for bipartite systems, and lower bounds for the critical values are known for the general case [16, 19, 20]. This allows one to obtain upper bounds on T_S.

Thermal entanglement scenarios. The above results allow one to distinguish various entanglement scenarios. The uninteresting scenario occurs when $T_E = T_S = 0$ as happens when the Hamiltonians present no interactions whatsoever. But this scenario is possible even when interactions are present, cf. Section III.

The next scenario is that in which the ground-state is separable, i.e., $T_E = 0$, but $T_S > 0$. Then as temperature increases away from zero, separability is lost at some temperature $0 < T_1 < T_S$. For temperatures in the "separable segment" $[0, T_1]$ all Gibbs states are unentangled, and the segment (T_1, T_S) contains temperatures for which the corresponding thermal states are entangled. The possibility arises for various closed "separable segments" $([0, T_1], [T_2, T_3], \cdots [T_n, T_{n+1}])$ alternating with open "entanglement segments" $((T_1, T_2), \cdots (T_{n+1}, T_S))$. We will present examples for this "abnormal" scenario in section III.

The other scenarios occur when the ground-state ρ_0 is entangled, i.e., $T_E > 0$. The normal case is $T_E = T_S$ and this is what has been observed in most studies we know of. The abnormal scenario is $0 < T_E < T_S$, and then there is a temperature T_1 with $T_E \leq T_1 < T_S$ such that for $T \in [T_E, T_1]$, ρ_T is unentangled but there are temperatures $T' \in (T_1, T_S)$ for which $\rho_{T'}$ is entangled. Again the way is open for closed separable segments alternating with open entanglement segments. Examples of this behaviour are given in section III.

Measuring entanglement: the modulus of separability. Consider any state ω of the composite system and consider the segment joining the normalized trace τ to ω, i.e., $\omega_t = t \cdot \omega + (1 - t) \cdot \tau$ with $0 \leq t \leq 1$. Since $\omega_0 = \tau$ is separable, one will ask in case $\omega_1 = \omega$ is entangled: when as t increases does one lose separability? This question has been analyzed by many authors, notably by Życzkowski, et al., [21], who develop it to obtain a method of estimating the "size" of the separable states; by Vidal , and Tarrach, [22], who give a virtually complete treatment of formal aspects of the problem; and by Gurvits and Barnum [19, 20] who obtain the best bounds. In Ref. [16], the modulus of separability of ω was defined as $\ell(\omega) = \sup\{0 \leq t \leq 1 : \omega_t \text{ is separable }\}$, whereas the quantity considered by Vidal and Tarrach is $R(\omega \,||\, \tau) = (\ell(\omega))^{-1} - 1$ and called by them *the random robustness of entanglement*. The modulus of separability has an inmediate geometric interpretation; it tells you how far along the segment with end points τ and ω you can go starting from τ until you lose separability. Here we only need to observe that $0 < \ell(\omega) \leq 1$, with $\ell(\omega) = 1$ if and only if ω is separable. Moreover, the upper-semicontinuity property of ℓ obtained in [16], guarantees that the map $T \mapsto \ell(\rho_T)$ is continuous. This in turn, proves the claims about the sets of temperatures where the Gibbs state is separable, respectively entangled.

III. THERMAL ENTANGLEMENT IN QUBIT/QUBIT AND QUBIT/QUTRIT SYSTEMS

In dealing with two qubits one may use the well-known concurrence or the entanglement of formation to characterize separability. For two qubits or a qubit/qutrit system one could use the negativity to characterize separability via the positive partial transpose criterion. Nevertheless in the graphs we will present we stick to ℓ, in part because it appears naturally as a tool in various proofs suggested above and in those given in [16]. Fortunately, Vidal and Tarrach, [22] have computed the modulus of separability for a qubit/qubit ($D = 4$) or a qubit/qutrit ($D = 6$); their beautiful formula is

$$\ell(\omega) = \frac{1}{1 + D \mid \min\{\lambda(\omega), 0\} \mid} ,$$

where $\lambda(\omega)$ is the minimal eigenvalue of the partial-transpose of ω with respect to the qubit. The plots which we will exhibit show $T \mapsto \ell(\rho_T)$ for selected Hamiltonians which exemplify the distinct scenarios.

We denote by T_*, the numerically obtained value of T_F –recall §II– for F equals minus the trace of the square. The critical values for the trace of the square are 1/3 for two qubits and 1/5 for the qubit/qutrit case. The eigenvalues of the Hamiltonian counting multiplicities are given as a row-vector $\mathbf{h}$. Since in our definition of ρ_T we have incorporated Boltzmann's constant in the Hamiltonian, the components of $\mathbf{h}$ have the same dimension as the temperature. Since thermal equilibrium states are invariant with respect to addition of a multiple of the identity to the Hamiltonian, we choose $h_{min} = 0$, and use T/h_{max} as the temperature scale. The eigenvector to the j-th eigenvalue h_j is listed as a row vector e_j, where the coordinates are with respect to the canonical orthonormal tensor-product basis built from the orthonormal basis $\{(1,0),(0,1)\}$ of $\mathbb{C}^2$, and $\{(1,0,0),(0,1,0),(0,0,1)\}$ of $\mathbb{C}^3$. The Hamiltonians to be presented are specifically chosen to exhibit transitions from entanglement to separability below T_S, that is in the interval $[0, T_S)$. The general idea is, obviously, to choose the eigenvector associated with the non-degenerate ground-state energy to be either separable or entangled and then the eigenvector associated to the first excited state to be, correspondingly, either entangled or separable; etc.

qubit/qubit: The minimal value of the separability modulus for two qubits is 1/3. The scenarios $0 < T_E = T_S$ and $0 = T_E < T_S$ have been observed before; e.g. in [1, 4, 5, 14]. Figure 1, shows the $0 = T_E < T_S$ scenario with a separable segment $[0, T_1]$ followed by an entanglement segment (T_1, T_S). Using the very same eigenvectors as those of Fig. 1, but with $\mathbf{h} = (0, 1.5, 2, 3)$, ρ_T is unentangled for every $T \geq 0$, that is $T_S = 0$.
In the qubit/qubit system, we have not found the scenario where $0 < T_E < T_S$ (cf. Figure 2 for a qubit/qutrit). The suggestion is that the dimension is too small to accomodate this case, but we have no precise arguments for or against this.

qubit/qutrit: The minimal value of the separability modulus for a qubit/qutrit systems is 1/4. Figure 2 shows the $0 < T_E < T_S$ scenario; the entanglement segment $[0, T_E)$ is followed by a separability segment $[T_E, T_1]$ and a second entanglement segment (T_1, T_S). In this an further examples not shown here, we have found that once a region of the **h**-space is found where the pertinent scenario is present, the values T_E, T_1, T_S are quite stable with respect to changes in **h** which are large with respect the temperature values. The inset of Figure 2 shows this effect for which we have no physical rationalization and needs to be studied further. Moreover, the same eigenvectors used in Fig. 2, but with $\mathbf{h} = (0, 1.7, 1.75, 2, 3, 4)$ give $T_E = T_S = 0.699$.
Figure 3 shows the $0 = T_E < T_S$ scenario (cf. Figure 1 for the two qubit system) with four transitions: $[0, T_1]$, and $[T_2, T_3]$ are separable segments alternating with entanglement segments (T_1, T_2) and (T_3, T_S).

IV. CONCLUDING REMARKS

We have introduced two characteristic temperatures T_E and T_S which organize the entanglement behaviour of the thermal state associated to any Hamiltonian of an arbitrary composite system. For qubit/qubit and qubit/qutrit systems, we have exemplified the possibility of various transitions from entanglement to separability as temperature increases from zero to T_S, above which entanglement is impossible. One could expect that the features found here will persist and be enhanced as N or D increase (although at present there is no manageable criterion to decide when a given state is entangled or not). Thus, in general, there will be many separable temperature segments alternating with entangled ones for multipartite systems of higher dimensions.

In the general case if one is able to obtain the bounds T_H and T_* then one has a rough idea of the location of the interval $[T_E, T_S]$. For temperatures between T_H and T_* one can use some appropiate entanglement monotone to try to detect the entanglement segments, if one is lucky (recall that an entanglement monotone can be zero for entangled states).

One of the main motivations for the present study came from certain problems posed in Ref. [16]. From that point of view, the main conclusion to be drawn from our findings here are theoretical and concern the results briefly mentioned in §II. It was asked in Ref. [16]: given a separable state ω which is not pure, does there exist a unitarily invariant, concave, continuous real-valued functional F defined for the states of the composite system which isolates the trace and such that $F(\omega) \geq C_F$? The answer given here is definitely no! Take any unentangled thermal state ρ_{T_1} such that for some $T_2 > T_1$ the Gibbs state ρ_{T_2} is entangled. Then there cannot exist an F with $F(\rho_{T_1}) \geq C_F$ because by Wehrl's result (cf. §II), $F(\rho_{T_2}) \geq C_F$ and by [16], the separability of ρ_{T_2} would follow.

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[1] M.A. Nielsen: *Quantum Information Theory.* Ph.D. Thesis, University of New Mexico, Albuquerque, New Mexico, USA 1998.

[2] M.C. Arnsen, S. Bose, and V. Vedral, Phys. Rev. Lett. **87**, 017901 (2001).

[3] D. Gunlycke, V.M. Kendon, and V. Vedral, Phys. Rev. A **64**, 0423021 (2001).

[4] X. Wang, Phys. Lett. A **281**, 101 (2001).

[5] X. Wang, Phys. Rev. A **64**, 0123131 (2001).

[6] X. Wang, Phys. Rev. A **66**, 0343021 (2002).

[7] T.J. Osborne, and M.A. Nielsen, Phys. Rev. A **66**, 0321101 (2002).

[8] X. Wang, Phys. Rev. A **66**, 0443051 (2002).

[9] U. Glaser, H. Büttner, and H. Fehske, Phys. Rev. A **68**, 0323181 (2003).

[10] G.K. Brennen, and S.S. Bullock, Phys. Rev. A **70**, 052303 (2004).

[11] G. Toth, Phys. Rev. A **71**, 0103011 (2005).

[12] M.R. Dowling, A.C. Doherty, and S.D. Bartlett, quant-ph/0408086 (v3).

[13] L.-A. Wu, S. Banyopadhyay, M.S. Sarandy, and W.A. Lidar, quant-ph/0412099.

[14] H. Fu, A.I. Solomon, and X. Wang, quant-ph/0401015 (v1).

[15] I. Bose, and A. Tribedi, quant-ph/0503170 (v2).

[16] G.A. Raggio, quant-ph/0505044 (v3).

[17] P.M. Alberti, and A. Uhlmann: *Stochasticity and Partial Order.* VEB Deutscher Verlag der Wissenschaften, Berlin 1982.

[18] M. Ohya, and D. Petz: *Quantum Entropy and its Use.* Springer-Verlag, Berlin 1993.

[19] L. Gurvits, and H. Barnum, Phys. Rev. A **68**, 042312 (2003).

[20] L. Gurvits, and H. Barnum, quant-ph/0409095.

[21] K. Życzkowski, P. Horodecki, A. Sanpera, and M. Lewenstein: Phys. Rev. A **59**, 141-155 (1999).

[22] G. Vidal, and R. Tarrach, Phys. Rev. A **59**, 141 (1999).

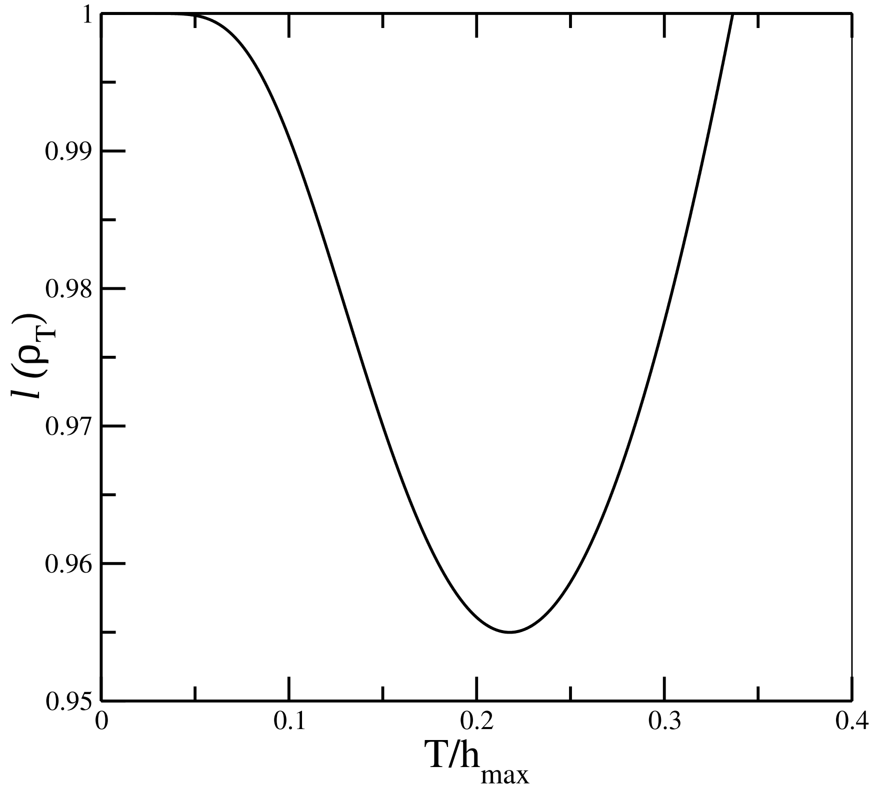

FIG. 1: $e_1 = (1, 0, 0, 0)$, $e_2 = (0, x, y, 0)$, $e_3 = (0, x, -x^2/y, z/y)$, $e_4 = (0, z, -xz/y, -x/y)$, where $x = 0.5$, $y = \sqrt{1-x^2}$ and $z = \sqrt{1-2x^2}$; $\mathbf{h} = (0, 1.5, 7, 8)$. $T_H = T_E = 0$, $T_1 = 0.159$, $T_S = 2.356$, and $T_* = 5.40$.

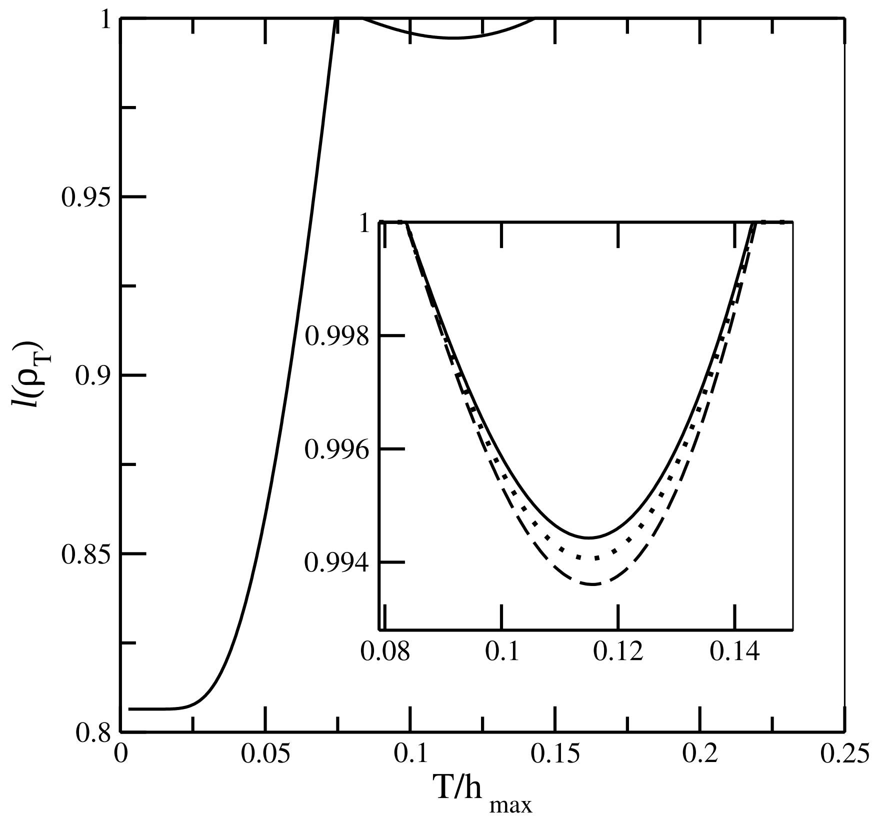

FIG. 2: $e_1 = (0,0,x,0,x,y)$,$e_2 = (1,0,0,0,0,0)$, $e_3 = (0,0,1/\sqrt{2},0,-1/\sqrt{2},0)$, $e_4 = (0,1/\sqrt{2},0,1/\sqrt{2},0,0)$, $e_5 = (0,1/\sqrt{2},0,-1/\sqrt{2},0,0)$, $e_6 = (0,0,y/\sqrt{2},0,y/\sqrt{2},-x\sqrt{2})$, where $x = 0.2$ and $y = \sqrt{1-2x^2}$; $\mathbf{h} = (0,0.75,0.75,2,3,4)$. $T_H = 0.13$, $T_E = 0.296$, $T_1 = 0.334$, $T_S = 0.571$, and $T_* = 2.76$. Inset: using the same eigenvectors and eigenvalues except, from top to bottom, $h_2 = 0.75, 1$ and 1.5

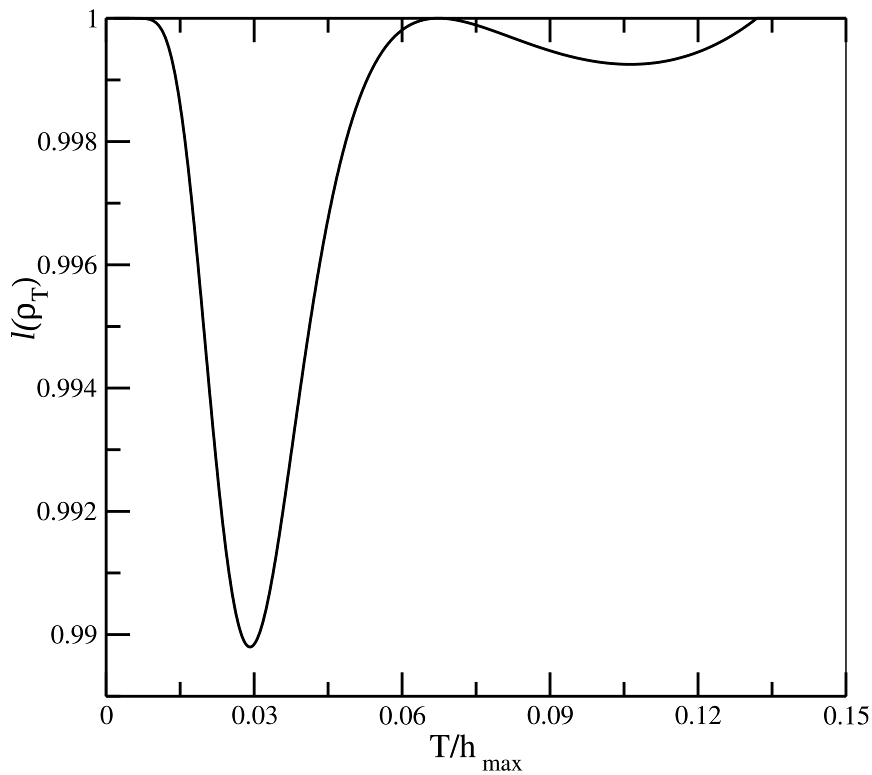

FIG. 3: $e_1 = (1,0,0,0,0,0)$, $e_2 = \frac{1}{2}(0,1,0,1,1,1)$, $e_3 = \frac{1}{2}(0,1,0,1,-1,-1)$, $e_4 = \frac{1}{2}(0,1,0,-1,1,-1)$, $e_5 = \frac{1}{2}(0,-1,0,1,1,-1)$, $e_6 = (0,0,1,0,0,0)$; $\mathbf{h} = (0,0.7,0.9,1,1.5,7)$. $T_H = T_E = 0$, $T_1 = 0.0355$, $T_2 = 0.467$, $T_3 = 0.476$, $T_S = 0.923$, and $T_* = 2.645$.