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Quantum Thermodynamics of Time Evolving Networks

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***Abstract*—In this paper, we present a novel thermodynamic framework for graphs that can be used to analyze time evolving networks, relating the thermodynamics variables to macroscopic changes in network topology, and linking major structural transition to phase changes in the thermodynamic picture. We start from a recent quantum-mechanical characterization of the structure of a network relating the graph Laplacian to a density operator and resulting in a characterization of the network's entropy. Then we adopt a Schrödinger picture of the dynamics of the network, resulting in an estimation of a hidden time-varying Hamiltonian from the data, from which we derive a measure of Energy exchange. From these variables, using the thermodynamic identity, we obtain temperature under the assumption of constant volume of the system. Evaluation of real-world data shows that the thermodynamic variables thus extracted are effective in detecting critical events occurring during network evolution.**

I. Introduction

Networks arise naturally in several fields as a characterization of complex phenomena. Examples can be found in biology, ecology, epidemiology, social sciences, to name a few, with notable examples such as the World Wide Web, metabolic reaction networks, financial market stock correlations, scientific collaboration, coauthorship and citation relations, and social interactions [1].

For such reason, investigating the properties of these networks has become increasingly crucial. In particular, the study of their evolution mechanisms plays an increasingly crucial role in science. This follows a recent shift in focus of network analysis from a rather unrealistic static view of the networks to the characterization of the dynamics of the system, in an attempt to understand, describe and predict their behavior and the behavior of the processes that act over the networks. Whereas in the past the effort has been focused on the representation problem, i.e. the characterization of network structure, now, the main focus has shifted to how the structure affects the network performance and how the network evolves with time to respond to such needs [2].

Statistical physics and thermodynamics offer an excellent framework for the analysis of complex networks, relating the behavior of microscopic particles to the macroscopic properties of a system [3], [4], [5]. Specifically, thermodynamics casts these macroscopic properties in terms of variables - that are subject to constraints imposed by the four laws of thermodynamics. For instance, in the case of graph representation of complex networks, Escolano et al. [6] provide a thermodynamic characterization based on the variation of local histories over graphs.

In this paper, we present a novel quantum thermodynamic framework for graphs where the graph Laplacian of each time slice is seen as a quantum mixed state undergoing free evolution through the Schrödinger equation under an unknown time-dependent Hamiltonian representing the change in potential due to external factors, and entropy and energy changing direct interaction with the environment. From the evolution of the network we estimate the Hamiltonian and the Energy-exchange at each time interval, as well as the variation in entropy of the underlying structure. From these we derive all the thermodynamic variables of networks, including the free energy and temperature.

The resulting characterization is applied to the characterization of two real-world time-varying networks: the price correlation of selected stocks in the New York Stock Exchange (NYSE) [7], and the gene expression of the life cycle of the the *Drosophila melanogaster* (fruit fly) [8] [9].

II. Quantum Thermodynamics of the Network

Let $G(V, E)$ be an undirected graph with node set V and edges set $E \subseteq V \times V$ and let $A = a_{ij}$ be the adjacency matrix, where

$$a_{ij} = \begin{cases} 1, & v_i \sim v_j, \\ 0, & \text{otherwise.} \end{cases}$$

The degree d of a node is the number of edges incident to the node and it can be represented through the degree matrix $D = (d_{ij})$ which is a diagonal matrix with $d_{ii} = \sum_i a_{ij}$. The graph Laplacian is then defined as $L = D - A$, and it can be interpreted as a combinatorial analogue of the discrete Laplace-Beltrami operator. The normalized Laplacian matrix $\tilde{L}$ is defined as

$$\tilde{L} = D^{1/2}(D - A)D^{1/2} \quad (1)$$

If we divide the normalized Laplacian by the number of vertices in the graph we obtain a unit-trace positive semidefinite matrix that Passerini and Severini [10] suggest can be seen as a density matrix in a quantum system representing a quantum

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superposition of the transition steps of quantum walk over the graph.

The *continuous-time quantum walk* is the quantum counterpart of the continuous-time random walk, and it is similarly defined as a dynamical process over the vertices of the graph [11]. Here the classical state vector is replaced by a vector of complex amplitudes over V, and a general state of the walk is a complex linear combination of the basis states $|v\rangle, v \in V$, such that the state of the walk at time t is defined as

$$|\psi_t\rangle = \sum_{u \in V} \alpha_u(t) |u\rangle \tag{2}$$

where the amplitude $\alpha_u(t) \in \mathbb{C}$ and $|\psi_t\rangle \in \mathbb{C}^{|V|}$ are both complex. Moreover, we have that $\alpha_u(t)\alpha_u^*(t)$ gives the probability that at time t the walker is at the vertex u, and thus $\sum_{u \in V} \alpha_u(t)\alpha_u^*(t) = 1$ and $\alpha_u(t)\alpha_u^*(t) \in [0,1]$, for all $u \in V$, $t \in \mathbb{R}^+$.

The evolution of the walk is then given by the Schrödinger equation, where we denote the time-independent Hamiltonian as $\mathcal{H}$.

$$\frac{\partial}{\partial t} |\psi_t\rangle = -i\mathcal{H} |\psi_t\rangle \ . \tag{3}$$

Given an initial state $|\psi_0\rangle$, we can solve Equation (3) to determine the state vector at time t

$$|\psi_t\rangle = e^{-i\mathcal{H}t} |\psi_0\rangle \ . \tag{4}$$

The *density operator* (or *density matrix*) is introduced in quantum mechanics to describe a system whose state is an ensemble of pure quantum states $|\psi_i\rangle$, each with probability p_i. The density operator of such a system is a positive unit-trace matrix defined as

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i| \ . \tag{5}$$

The *von Neumann entropy* [12] H_N of a mixed state is defined in terms of the trace and logarithm of the density operator ρ

$$H_N = -\operatorname{Tr}(\rho \log \rho) = -\sum_i \xi_i \ln \xi_i \tag{6}$$

where $\xi_1, \ldots, \xi_n$ are the eigenvalues of ρ. The von Neumann entropy is related to the distiguishability of the states, *i.e.*, the amount of information that can be extracted from an observation on the mixed state

The observation process for a quantum system is defined in terms of projections onto orthogonal subspaces associated with operators on the quantum state-space called *observables*. Let O be an observable of the system, with spectral decomposition

$$O = \sum_i a_i P_i \tag{7}$$

where the a_i are the (distinct) eigenvalues of O and the P_i the orthogonal projectors onto the corresponding eigenspaces. The outcome of an observation, or projective measurement, of a quantum state $|\psi\rangle$ is one of the eigenvalues a_i of O, with probability

$$P(a_i) = \langle\psi| P_i |\psi\rangle \tag{8}$$

After the measurement, the state of the quantum systems becomes

$$|\bar{\psi}\rangle = \frac{P_i |\psi\rangle}{||P_i |\psi\rangle ||} , \tag{9}$$

where $|| |\psi\rangle || = \sqrt{\langle\psi | \psi\rangle}$ is the norm of the vector $|\psi\rangle$.

Density operators play an important role in the quantum observation process. The observation probability of a_i is $P(a_i) = \operatorname{Tr}(\rho P_i)$, with the mixed state being projected by the observation process onto the state represented by the modified density matrix $\rho' = \sum_i P_i \rho P_i$. The expectation of the measurement is $\langle O\rangle = \operatorname{Tr}(\rho O)$. The projective properties of quantum observation means that an observation actively modifies the system, both by altering its entropy and forcing an energy exchange between quantum system and observer.

Thermodynamics describes the behavior of a composite system in terms of macroscopic variables such as energy, entropy and temperature. These are linked together by the thermodynamic identity

$$dU = TdS - PdV \tag{10}$$

where U is the internal energy, S the entropy, V the volume, T the temperature, and P the pressure.

Following Passerini and Severini [10] in their use of the normalized Laplacian matrix as a density operator defining the current state of the network, we derive the network entropy in terms of the von Neumann entropy

$$S_{VN} = -\sum_{i=1}^{|V|} \frac{\tilde{\lambda}_i}{|V|} \ln \frac{\tilde{\lambda}_i}{|V|} \tag{11}$$

With this we can measure dS the change in entropy as the network evolves. Previous work used similar entropic measure to define thermodynamic variables on networks, but linked energy to the number of edges in the graph [13] or derived it through the Boltzmann partition function of the network [14]. However, in these approaches the structure of the graph has the dual function of state (determining the density operator) and operator. Here we opt for an different approach that does away with this duality, assuming that the energy operator is unknown and estimated from the evolution. We assume that the dynamics of the network is governed by a free evolution following the Schrödinger equation under an unkown time-varying Hamitonian $\mathcal{H}_t$, and an interaction with the outside world which acts as an observer. The free evolution does not change the thermodynamic variables, while the cause of the variation in Entropy has to be sought from the interaction process which also causes an energy exchange.

To measure the energy exchange we need to recover the potential term expressed by the unknown Hamiltonian. In fact, the Hamiltonian acts as an energy operator, resulting the following expression for the change in energy between state ρ_t and ρ_{t+1}

$$dU = \operatorname{Tr}(\mathcal{H}_t \rho_{t+1}) - \operatorname{Tr}(\mathcal{H}_t \rho_t) \tag{12}$$

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We estimate the Hamiltonian $\mathcal{H}_t$ as the one that minimizes the exchange of energy through the interaction with the environment. To this end we assume that the interaction intervenes at the end of the free evolution, where ρ_t is transformed by the Schrödinger equation into

$$\hat{\rho}_{t+1} = \exp(-i\mathcal{H}_t)\rho_t \exp(i\mathcal{H}_t) \tag{13}$$

The exchange of energy in the interaction is then

$$\begin{aligned} \mathcal{H}_t &= \arg\min_H \mathrm{Tr}(H\rho_{t+1}) - \mathrm{Tr}(H\hat{\rho}_{t+1}) \\ &= \arg\min_H \mathrm{Tr}\left(H\big(\rho_{t+1} - \exp(-iH)\rho_t \exp(iH)\big)\right) \end{aligned} \tag{14}$$

Let $\rho_t = \Phi_t \Lambda_t \Phi_t^T$ be the spectral decomposition of the state of the network at time t, equation (14) can be solved by noting that the minimum energy exchange intervenes when the interaction changes the eigenvalues of the density matrices, and with them the entropy, but does not change the corresponding eigenspaces. In other words, the Hamiltonian is the cause of the eigenvector rotation and can be recovered by it:

$$\mathcal{H}_t \approx i \log(\Phi_{t+1}\Phi_t^T) \tag{15}$$

It is worth noting that we have computed a lower bound of the Hamiltonian, since we cannot observe components on the null spaces of ρs. Furthermore, we have

$$\underbrace{\Phi_{t+1}\Phi_t^T}_{\mathcal{U}} \rho_0 \underbrace{\Phi_t\Phi_{t+1}^T}_{\mathcal{U}} = \hat{\rho}_{t+1}\,, \tag{16}$$

where $\mathcal{U} = \Phi_{t+1}\Phi_t^T$ is the unitary evolution matrix. The final change in internal energy is then

$$dU = Tr(\mathcal{H}_t\rho_{t+1}) - Tr(\mathcal{H}_t\rho_t) \tag{17}$$

The thermodynamic temperature T can then be recovered through the fundamental thermodynamic relation $dU = TdS - PdV$ but where we assume that the volume is constant, *i.e.*, $dV = 0$ (isochoric process). As a result, the reciprocal of the temperature T is the rate of change of internal energy with entropy

$$T = \frac{dU}{dS} \tag{18}$$

This definition can be applied to evolving complex networks which do not change the number of nodes during their evolution.

III. Experiments and Evaluations

In this Section we assess the ability of the proposed thermodynamic characterization to identify important topological transitions from two real-world time-evolving networks: stock price correlation of the New York Stock Exchange (NYSE) and gene expression of the *Drosophila melanogaster* (fruit fly).

NYSE: The dataset is extracted from a database consisting of the daily prices of 3799 stocks traded on the New York Stock Exchange (NYSE). To construct the dynamic network, 347 stocks with historical data from May 1987 to February 2011 are selected [7]. In order to build an evolving network, a time window of 28 days is used and it is moved along time to obtain a sequence (from day 29 to day 6004); in this way, each temporal window contains a time-series of the daily return stock values over a 28 day period. Afterward, trades among the different stocks are set as a network. For each time window, we compute the cross correlation coefficients between the time-series for each pair of stocks and create connections between them if the absolute value of the correlation coefficient exceeds a threshold. The result is a stock market network which changes over the time, with a fixed number of 347 nodes and varying edge structure for each of trading days.

Drosophila: The dataset comes from the biology field and it concerns the interactions among genes of *Drosophila melanogaster* - better known as fruit fly - during its life cycle. The data is sampled at 66 sequential developmental time points. The fruit fly life cycle is divided into four stages, namely the embryonic (samples 1-30), larval (samples 31-40) and pupal (samples 41-58) periods together with the first 30 days of adulthood (samples 59- 66). Early embryos are sampled hourly and adults are sampled at multiday intervals, according to the speed of the morphological changes. To represent this data using a time evolving network, the

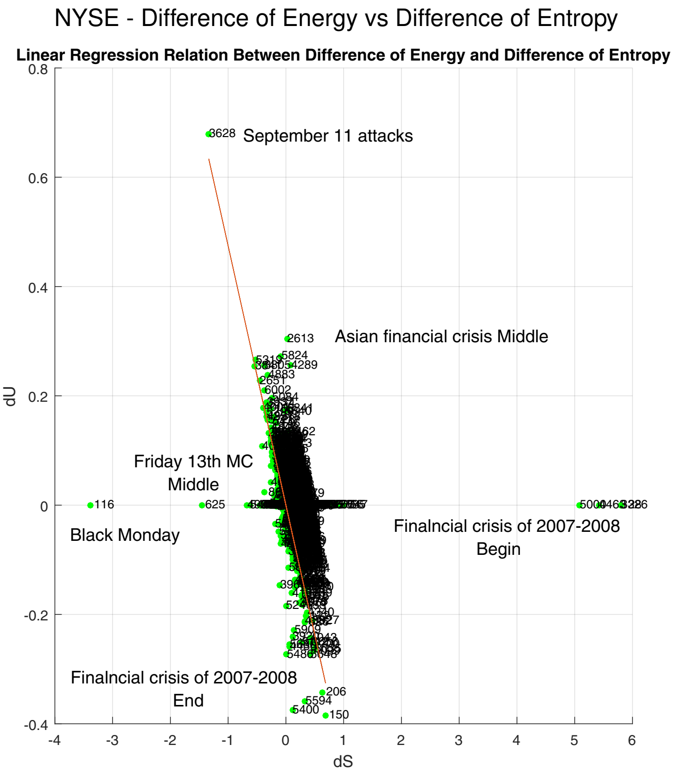

Fig. 1: Scatter plot of the difference of energy vs difference of entropy, as alternative representation of the network temperature. The red line highlights the common trend of the temperature. Significant events result as outliers (Black Monday (19th October 1987), Friday the 13th Mini-Crash Middle (October 1989), Asian Financial Crisis Middle (July 1997 – October 1997) , Financial Crisis of 2007-2008 Begin and End (March 2007 - October 2008))

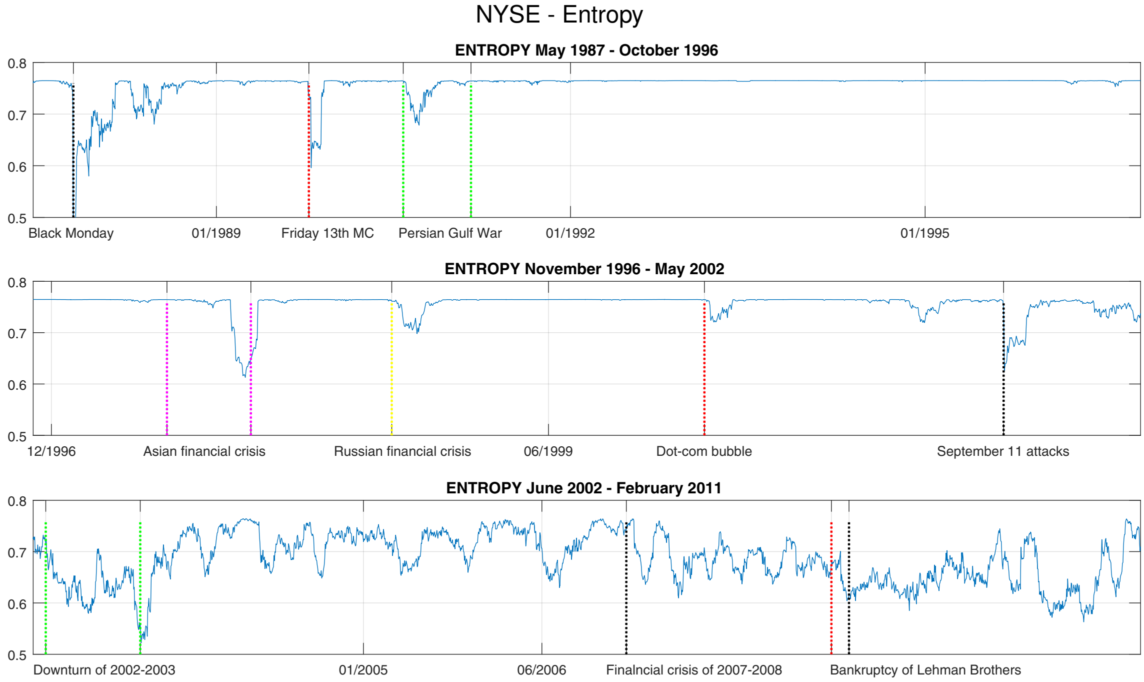

Fig. 2: The von Neumann Entropy (log_{10}) versus time (May 1987 - February 2011), for the dynamic stock correlation network. The vertical colored lines signal important events. Up-bottom: Black Monday (19th October 1987), Friday the 13th Mini-Crash (13rd October 1989), Persian Gulf War (2nd August 1990 - 17th January 1991), Asian Financial Crisis (July 1997 – October 1997), Russian Financial Crisis – Ruble devaluation (17th August 1998), Dot-com bubble - climax (10th March 2003), September 11 attacks, Downturn of 2002-2003, Financial Crisis of 2007-2008 (February 2007 - October 2008), Bankruptcy of Lehman Brothers (15th September 2008)

following steps are followed [9]. At each developmental point the 588 genes that are known to play an important role in the development of the *Drosophila* are selected. These genes are the nodes of the network, and edges are established based on the microarray gene expression measurements reported in [8]. In addition, any self-loop in the obtained undirect graph - at each time - has been removed to make more tractable the normalized Laplacian. This dataset yields a time-evolving network with a fixed number of 588 nodes, sampled at 66 developmental time points.

We aim at investigating how the thermodynamic variables characterize the evolution of the networks and whether it can be used to detect the critical events in the network evolution (*e.g.*financial crises or crashes in the stock market and transcription changes in the fruit fly life cycle).

We commenced by computing the normalized Laplacian of the network at each time step and the three main thermodynamic variables: that is entropy, energy, and temperature, as shown in equations (6), (17), (18) respectively.

Fig. 2 shows the variation of the entropy of the network throughout the time series. We can see that the entropy drops down rapidly in proximity of some major events in the early time period characterized by low volatility. However, as the network becomes more volatile, the signal gets drown rapidly in the overall noise. Indeed, we can see in the bottom chart (June 2002 – February 2011), that the trend appears rather confused.

In Fig. 1 we show a scatter plot of the variation in energy dU over the variation in entropy dS. Here an interesting feature of the networks emerges: there emerges an underlying operating temperature of the structure (depicted by the slope of the red line). However, there are outliers exhibiting substantial changes from the underlying modes of operation. These outliers correspond to major events in the stock market, like the Black Monday or September 11.

To identify this deviation from the fundamental operating slope, in Fig. 3 we plot the ratio of the exponentiated thermodynamical quantities $\frac{\exp(dU)}{\exp(dS)}$. This quantity enhances the variations, allowing us to mark the phase changes on the time series.

For instance, during the last period (bottom chart – from June 2002 to February 2011) pinpointing the two crises is easier, thanks to the peaks of the variations (always within the boundaries of each crisis). Consequently, the remaining important events, which really perturb the system, e.g. September 11 attacks or the Black Monday, are identified clearly.

Fig.4 shows the L_1 distance between ρ_t and $\hat{\rho}_t$, (see equation 13). We can see that key events have a large difference between the two densities, indicating that there is a huge interaction with the environment, resulting in consistent energy exchange and large variations in entropy.

We now turn our attention to the *Drosophila melanogaster* dataset. Fig.6 displays the scatter plot of energy over entropy (dU Vs. dS). Again, an underlying operating temperature of the network emerges from the plot and some events strike

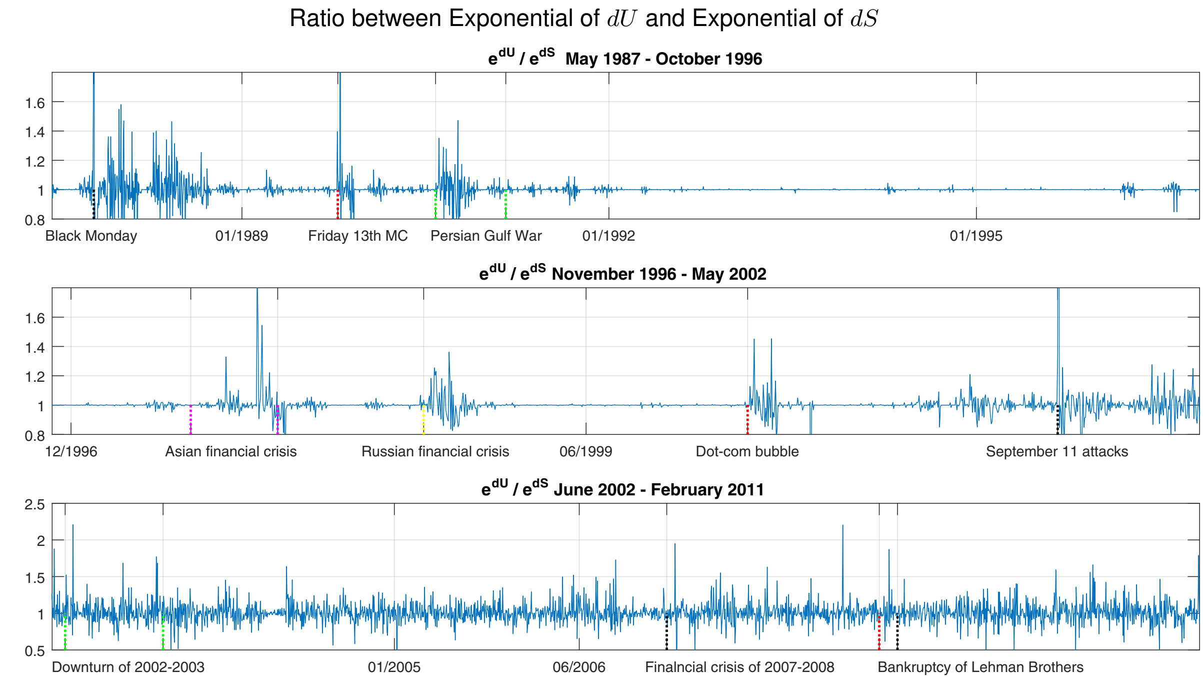

Fig. 3: The ratio between e^{dU} and e^{dS} versus time. The vertical colored lines refer to the most important and devasting events for the trade market. Up-bottom: Black Monday (19th October 1987), Friday the 13th Mini-Crash (13rd October 1989), Persian Gulf War (2nd August 1990 - 17th January 1991), Asian Financial Crisis (July 1997 – October 1997), Russian Financial Crisis – Ruble devaluation (17th August 1998), Dot-com bubble - climax (10th March 2003), September 11 attacks, Downturn of 2002-2003, Financial Crisis of 2007-2008 (February 2007 - October 2008), Bankruptcy of Lehman Brothers (15th September 2008)

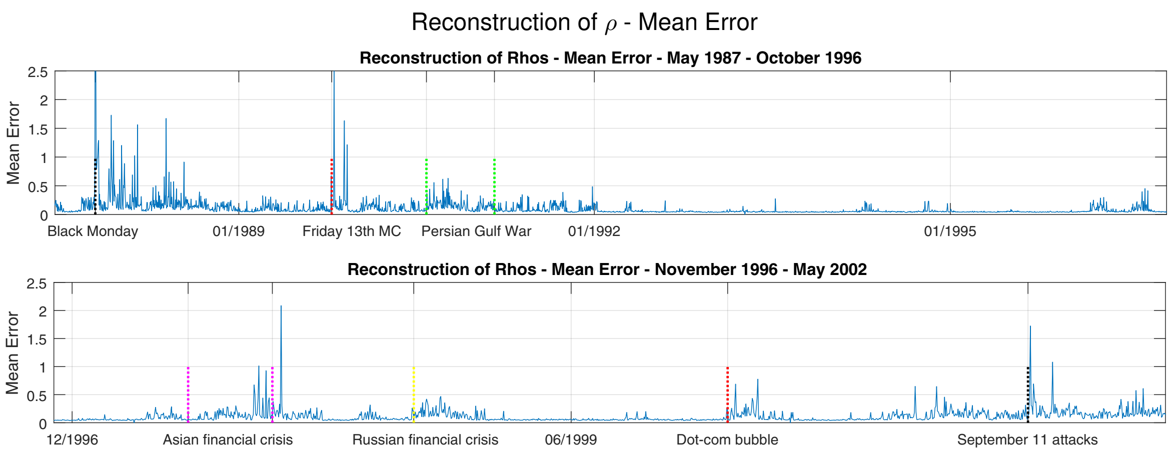

Fig. 4: The mean error deriving from the comparison of the actual ρ and the recostructed one, versus time. The vertical lines state principal incidents which may corrupt the network structure.

out as outliers. Indeed those events represent fundamental landmarks in the evolution of the Drosophila: they belong to the early moments of the embryonic stage, the middle time of the larval transaction and the final days of the pupal step. According to [8] they are three out four of the major morphological changes in terms of transcript levels of genes (actually they are the beginning and end of embryogenesis, the larval-pupal transition and the end of the pupal period).
In order to verify the magnitude of such moments, we computed the temperature, the ratio between exponential of dU and exponential of dS and finally the entropy (Fig.5). In this case the entropy does not provide clear information about this increasing/decreasing transcript level, whereas both the temperature and the exponential transformation exhibit peaks in correspondence of major evolution events.

IV. Conclusions

In this paper, we adopt a thermodynamic representation of network structure in order to visualize and understand the evolution of time-varying networks. We provide expressions

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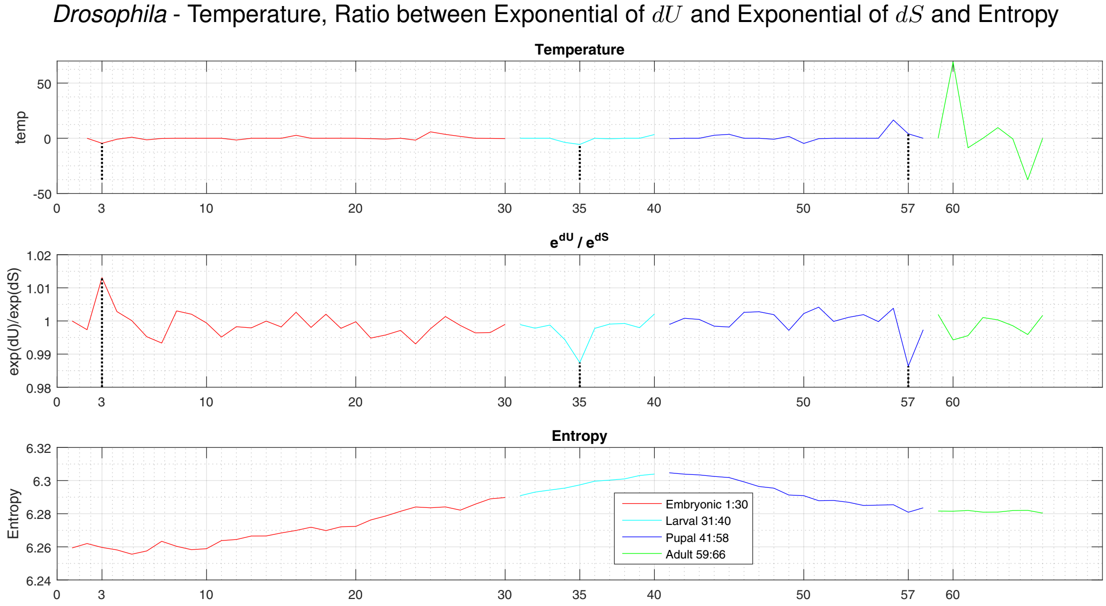

Fig. 5: Up-Bottom: Temperature, Ratio between e^{dU} and e^{dS} and Entropy - versus time. The developmental periods of the fruit fly are colored differently and the significant moments are hightlighted.

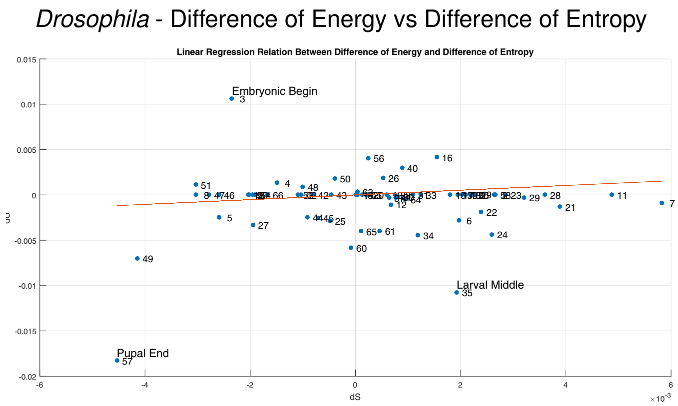

Fig. 6: Scatter plot of the difference of energy vs difference of entropy, as alternative representation of the network temperature. The red line fits the trend of the temperature. Outliers are moments where the transcript levels of genes changed.

for thermodynamic variables on networks, including the entropy, internal energy and temperature. This analysis is based on quantum thermodynamics and connects to recent work on the von Neumann entropy of networks. The internal energy and the temperature are derived by estimating an unknown Hamiltonian operator governing the free evolution through the Schrödinger equation. We have evaluated the method experimentally using data representing real world complex systems taken from the financial and biological domains. The experimental results demonstrate that the thermodynamic variables are efficient in analyzing the evolutionary properties of dynamic networks, including the detection of abrupt changes and phase transitions in structure or other distinctive periods in the evolution of time-varying complex networks.

References

[1] M. E. Newman, "The structure and function of complex networks," *SIAM review*, vol. 45, no. 2, pp. 167–256, 2003.

[2] E. Estrada, *The structure of complex networks: theory and applications*. OUP Oxford, 2011.

[3] D. C. Mikulecky, "Network thermodynamics and complexity: a transition to relational systems theory," *Computers & chemistry*, vol. 25, no. 4, pp. 369–391, 2001.

[4] K. Huang, "Statistical mechanics," 1987.

[5] M. A. Javarone and G. Armano, "Quantum–classical transitions in complex networks," *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2013, no. 04, p. P04019, 2013.

[6] F. Escolano, E. R. Hancock, and M. A. Lozano, "Heat diffusion: Thermodynamic depth complexity of networks," *Physical Review E*, vol. 85, no. 3, p. 036206, 2012.

[7] T. D. Peron and F. A. Rodrigues, "Collective behavior in financial markets," *EPL (Europhysics Letters)*, vol. 96, no. 4, p. 48004, 2011.

[8] M. N. Arbeitman, E. E. Furlong, F. Imam, E. Johnson, B. H. Null, B. S. Baker, M. A. Krasnow, M. P. Scott, R. W. Davis, and K. P. White, "Gene expression during the life cycle of drosophila melanogaster," *Science*, vol. 297, no. 5590, pp. 2270–2275, 2002.

[9] L. Song, M. Kolar, and E. P. Xing, "Keller: estimating time-varying interactions between genes," *Bioinformatics*, vol. 25, no. 12, pp. i128–i136, 2009.

[10] F. Passerini and S. Severini, "Quantifying complexity in networks: the von neumann entropy," *International Journal of Agent Technologies and Systems (IJATS)*, vol. 1, no. 4, pp. 58–67, 2009.

[11] E. Farhi and S. Gutmann, "Quantum computation and decision trees," *Physical Review A*, vol. 58, no. 2, p. 915, 1998.

[12] M. Nielsen and I. Chuang, *Quantum computation and quantum information*. Cambridge university press, 2010.

[13] C. Ye, A. Torsello, R. C. Wilson, and E. R. Hancock, "Thermodynamics of time evolving networks," in *Graph-Based Representations in Pattern Recognition*. Springer, 2015, pp. 315–324.

[14] C. Ye, C. H. Comin, T. K. D. Peron, F. N. Silva, F. A. Rodrigues, L. d. F. Costa, A. Torsello, and E. R. Hancock, "Thermodynamic characterization of networks using graph polynomials," *Physical Review E*, vol. 92, no. 3, p. 032810, 2015.

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