Quantum transport senses community structure in networks

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Quantum time evolution exhibits rich physics, attributable to the interplay between the density and phase of a wave function. However, unlike classical heat diffusion, the wave nature of quantum mechanics has not yet been extensively explored in modern data analysis. We propose that the Laplace transform of quantum transport (QT) can be used to construct an ensemble of maps from a given complex network to a circle $S^1$, such that closely-related nodes on the network are grouped into sharply concentrated clusters on $S^1$. The resulting QT clustering (QTC) algorithm is as powerful as the state-of-the-art spectral clustering in discerning complex geometric patterns and more robust when clusters show strong density variations or heterogeneity in size. The observed phenomenon of QTC can be interpreted as a collective behavior of the microscopic nodes that evolve as macroscopic cluster “orbitals” in an effective tight-binding model recapitulating the network. Python source code implementing the algorithm and examples are available at https://github.com/jssong-lab/QTC.

Grouping similar objects into sets is a fundamental task in modern data science. Many clustering algorithms have thus been devised to automate the partitioning of samples into clusters, or communities, based on some similarity or dissimilarity measures between the samples that form nodes on a graph [1, 2]. In particular, physics-inspired approaches based on classical spin-spin interaction models [3, 4] and Schrödinger equation [5] have been previously proposed; however, the former usually requires computationally intensive Monte Carlo simulations which may get trapped in local optima, while the latter essentially amounts to Gaussian kernel density estimation. These intriguing physical ideas thus have been under the shadow of popular contemporary approaches that are simple and computationally efficient, such as the dissimilarity-based KMeans [6–8] and hierarchical clustering [9, 10], density-based DBSCAN [11], distribution-based Gaussian mixture [12], and kernel-based spectral clustering [13]. By contrast, we here use the physics of quantum transport (QT) on data similarity networks to devise a simple and efficient algorithm. The performance of QT clustering (QTC) is comparable to the state-of-the-art spectral clustering when the clusters exhibit non-spherical, geometrically complex shapes; at the same time, QTC is less sensitive to the choice of parameters in the kernel. Moreover, unlike spectral clustering, the QT representation of data on a circle does not jump in dimension when the specified number of clusters changes.

Heat diffusion has been applied to rank web page popularity [14], probe geometric features of data distribution [15], and measure similarity in classification problems [16, 17]. By contrast, despite the formal resemblance between the heat equation and the Schrödinger equation, the time evolution of a quantum wave function has been largely ignored in machine learning. Both heat and Schrödinger equations have conserved currents; however, while the heat current is proportional to the negative gradient of heat density itself, the velocity of quantum probability current is set by the phase gradient which satisfies the Navier-Stokes equation, making quantum probability density an irrotational fluid (Supplemental Material (SM) [18], I). Thus, the Schrödinger equation embodies richer physics than heat diffusion and can capture spatiotemporal oscillations and wave interference.

One promising observation has been that quantum time evolution can be faster in reaching faraway nodes compared with heat diffusion in ordered binary tree networks, suggesting the possibility of finding practical applications of quantum mechanics in network analysis [19–22]. However, there are several outstanding challenges: e.g., unlike the heat kernel, the oscillatory quantum probability density is monotonic in neither time nor spatial distance; moreover, irregularities in either edge weights or network structure can severely restrict the propagation of a wave function through destructive interference, analogous to Anderson localization in disordered media [23]. We circumvent these difficulties associated with using the probability density itself and demonstrate the utility of the phase information for clustering network nodes.

A generic undirected weighted network, e.g. a data similarity network of $m$ samples in $\mathbb{R}^d$ represented as nodes, is encoded by an $m \times m$ symmetric adjacency matrix $A$. The row or column sum vector $\text{deg}(i) = \sum_k A_{ik} = \sum_k A_{ki}$ gives rise to the diagonal degree matrix $D = \text{diag}(\text{deg})$. Replacing the continuous Laplacian with the graph Laplacian $L = D - A$ then discretizes the heat and Schrödinger equations on data similarity networks. Enforcing the conservation of discrete heat current introduces the normalized graph Laplacian $Q = LD^{-1}$. The original graph Laplacian $L$ of an undirected network is automatically Hermitian, but we adopt the symmetrized version $H = D^{-\frac{1}{2}}LD^{-\frac{1}{2}}$ of $Q$ as our Hamiltonian, since it has the same spectrum as $Q$. With this choice, $H$ has a nontrivial ground state $\psi_0(i) \propto \sqrt{\text{deg}(i)}$ [22].

For concreteness, we define the pairwise similarity or adjacency between sample $x_i$ and sample $x_j$ by the Gaussian function $A_{ij} = \exp(-r_{ij}^2/r_0^2)$, where $r_{ij} = \|x_i - x_j\|$.  

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Our clustering algorithm stems from the observation that the phase $\Theta(i|j)$ of this transformed function is essentially constant as $i$ varies within a cluster, but jumps as $i$ crosses clusters (see discussion below; [18]). The phase information thus provides a one-dimensional representation of data on $S^1$, such that distinct clusters populate separable regions on $S^1$; intuitively, the phase distribution $\Theta(:|j)$ corresponds to a specific perspective on community structure sensed by the wave packet initialized at node $j$. In general, the phase distribution $\Theta(:|j)$ changes with the initialization node $j$. Thus, if we randomly choose $m'$ initialization nodes ($m' \approx 100$ for data sets in Fig. 1 & 2), for $1 < m' \leq m$, then we obtain an ensemble of $m'$ phase distributions, in each of which the phase is almost constant within clusters; this ensemble ultimately provides a collection of perspectives on the underlying community structure, as sensed by the wave packets initialized at the chosen nodes.

In practice, we a priori specify the number $q$ of clusters, and use the phase distribution of each wave function to partition the nodes into $q$ subsets [18]. We label each of the $m''$ distinct partitions by an integer $\alpha$, where $m'' \leq m'$, and calculate the occurrence frequency $w_{\alpha} \in (0, 1)$ of each partition, such that the normalization condition $\sum_{\alpha} w_{\alpha} = 1$ holds (SM [18], I C). Typically, we find that the frequencies are dominated by a single partition; other $m''-1$ less frequent partitions may arise from wave functions initialized at nodes of a small subnetwork isolated from the rest of the network. Hence, the minority predictions provide less holistic views of the network community structure, and we choose the majority prediction from the ensemble as our final clustering decision.

We compared the performance of QTC to spectral clustering [24] using four synthetic data sets having complex geometry (Fig. 1): (1) uniform sticks, (2) non-uniform sticks, (3) concentric annuli, and (4) the Chinese character for "thunder." Both algorithms performed equally well on the simple data set of uniformly sampled sticks (Fig. 1(a,e)) or when $r_{c}$ was chosen to be sufficiently small such that the clusters became almost disjoint subnetworks; as $r_{c}$ increased, however, QTC remained robust (Fig. 1(b-d)), while spectral clustering made mistakes (Fig. 1(f-h)).

The log-prices of a portfolio of stocks form a random walk in time with occasional jumps which are often triggered by important events such as the release of fiscal reports and sales records. The jumps then separate the fractal-like trajectory of historical log-prices into several performance segments. Figure 2(a,b) shows the log-price distribution of two stocks, AAPL and GOOGL, from January 3, 2005 to November 7, 2017, where we removed the temporal information from the data set. When we...
specified five clusters, QTC cut the trajectory into five consecutive segments in the temporal space (Fig. 2(a,c)) with heterogeneous lengths, whereas spectral clustering partitioned the trajectory into clusters of similar sizes and mixed the temporal ordering near the boundary of blue and cyan clusters (Fig. 2(b,d)). The jumps identified by QTC (Q’s in Table I) coincided with major news events for the two stocks, whereas spectral clustering (S’s in Table I) failed to identify the large drop of AAPL on 1/24/2013 and instead included several less significant stock movements. These results showed that QTC was more robust than the conventional spectral embedding method on non-spherical data distributions with anisotropic density fluctuations (Fig. 1(b,f)) or complex geometric patterns exhibiting a hierarchy of cluster sizes (Fig. 1(c,g) and (d,h); Fig. 2).

Next, we provide a physical interpretation of the agglomeration phenomena observed in QTC using an effective tight-binding model. For this purpose, we rewrite the Laplace transform as \( \mathcal{L}^\phi(i,j)|S\rangle \equiv \mathcal{L}G(i, j; is) \), where

\[
G(i, j; z) \equiv \langle i| (z - H)^{-1} |j\rangle = \sum_{n=0}^{m-1} \frac{\langle i| \psi_n \rangle \langle \psi_n | j \rangle}{z - E_n} \tag{2}
\]

is the resolvent of \( H \), and \( \psi_n \) and \( E_n \) are the eigenfunctions and eigenvalues of \( H \), respectively, for \( n = 0, 1, \ldots, m-1 \). We assume that \( E_n \) are ordered in a non-decreasing way. As a result of our choice of short-proximity adjacency measure, the largest contributions to \( G(i, j; is) \) come from the low energy collective modes in the case of well-separated \( q \) clusters indexed by \( \mu = 0, 1, \ldots, q-1 \). In this case, the ground state density \( |\psi_0(i)|^2 \propto \deg(i) \) will be accumulated around the hub nodes within each cluster. Furthermore, \( H \) is essentially \( q \)-block diagonal upon relabeling the nodes and exhibits a large energy gap separating the low energy collective modes \( \{|\psi_n\rangle\}_{0 \leq n < q} \) from the high energy eigenstates \( \{|\psi_n\rangle\}_{q \leq n < m} \), capturing microscopic fluctuations within each cluster. Notice that the major contribution to the resolvent in Eq. 2 comes from terms with \( n < q \), and that the number of low energy states equals the number of well-separated clusters (SM [18], I B and Fig. S1). These observations thus motivate a \( q \)-dimensional coarse-grained Hamiltonian describing only the low energy collective modes.

Let \( \{\phi_\mu\}_{\mu=0}^{q-1} \) be the cluster wave functions, or “atomic orbitals,” satisfying \( \phi_\mu(i) > 0 \) for \( i \) in cluster \( \mu \) and zero elsewhere, and \( \langle \phi_\mu | \phi_\nu \rangle = \delta_{\mu\nu} \). The effective tight-binding Hamiltonian is

\[
H = \sum_{\mu, \nu=0}^{q-1} h_{\mu\nu} \phi_\mu(i) \phi_\nu(i), \quad h_{\mu\nu} = \xi_\mu \delta_{\mu\nu} + v_{\mu\nu}. \tag{3}
\]

where \( \xi_\mu = \langle \phi_\mu | H | \phi_\mu \rangle \) describes the ground state energy of each \( \phi_\mu \), and the off-diagonal matrix \( v_{\mu\nu} = \langle \phi_\mu | H | \phi_\nu \rangle \) for \( \mu \neq \nu \), with \( v_{\mu\mu} = 0 \), couples the atomic orbitals \( \phi_\mu \) and \( \phi_\nu \). Through the diagonalization of the tight-binding Hamiltonian \( h_{\mu\nu} \), the \( q \) atomic orbitals are then linearly combined into \( q \) molecular orbitals.

To illustrate the effects of off-diagonal coupling, we split \( H \) into diagonal \( H_0 \) and off-diagonal \( V \), and study the Born approximation of the Lippmann-Schwinger equation

\[
\tilde{G}(z) = \tilde{G}_0(z) + \tilde{G}_0(z) \tilde{V} \tilde{G}(z), \tag{4}
\]

where \( \tilde{G}(z) = (z - H)^{-1} \) and \( \tilde{G}_0(z) = (z - H_0)^{-1} \). The effective resolvent matrix can thus be expanded as

\[
g_{\mu\nu}(z) = \frac{\delta_{\mu\nu}}{z - \xi_\mu} + \frac{v_{\mu\nu}}{(z - \xi_\mu)(z - \xi_\nu)} + O(v^2), \tag{5}
\]

which is a weighed sum over all tunneling paths from cluster \( \mu \) to \( \nu \), and converges quickly if \( |v_{\alpha\beta}| / |z - \xi_\alpha| \) for all \( \alpha, \beta = 0, 1, \ldots, q-1 \) (SM [18], I D, Eq. S3). The propagator from node \( j \) to \( i \) in the effective tight-binding theory, approximating Eq. 2, is directly related to \( g_{\mu\nu}(z) \) as

\[
g(i, j; z) = \sum_{\mu, \nu=0}^{q-1} \phi_\mu(i) g_{\mu\nu}(z) \phi_\nu(j). \tag{6}
\]

If the nodes \( i \) and \( j \) belong to two non-overlapping clusters \( \mu \) and \( \nu \), respectively, then the propagator reduces to \( g(i, j; z) = \phi_\mu(i) \phi_\nu(j) g_{\mu\nu}(z) \) and \( \arg g(i, j; z) = \arg g_{\mu\nu}(z) \), because of the disjoint support and the non-negativity of cluster wave functions. In other words, the propagator initiated at \( j \) has a constant phase at all nodes \( i \) within each cluster, and the phase associated with each cluster is completely determined by the phase of resolvent matrix \( g_{\mu\nu} \), which in turn depends on the weak coupling \( v_{\mu\nu} \) via Eq. 5.

As an example, consider two sets of \( m \) samples drawn from \( N((\pm \ell, 0)^T, \sigma^2 I_{2 \times 2}) \), respectively. The effective 2-level Hamiltonian and resolvent matrices are

\[
h = \begin{pmatrix} \xi_0 & v \\ v & \xi_1 \end{pmatrix}, \quad \text{and} \quad g(z) = \begin{pmatrix} z - \xi_0 & -v \\ -v & z - \xi_1 \end{pmatrix}^{-1}. \tag{7}
\]

As we vary \( \ell = 3\sigma, 2.7\sigma, \) and \( 2.4\sigma, \) with a fixed proximity length scale \( r_c = \sigma \), the cluster configuration ranges from (a) well-separated, (b) in proximity, and (c) overlapping (Fig. 3; Fig. S2). For each case, Fig. 3(d-f) show the phase distribution of all samples when quantum transport is initialized at one of the nodes in the left cluster; it is seen that our theoretical prediction \( \arg \{|g_{\mu\nu}(i,s)\} \) and its perturbative approximations calculated from Eq. 5 agree well. Furthermore, if the two clusters are identical, i.e. \( \xi_0 = \xi_1 \), then the effective 2-level model can be mapped to the classic double-well tunneling model (SM [18], I E); in this case, the phase distribution of the Laplace transform of exact instanton solution matches that of our simulated Gaussian clouds (Fig. S3(a)). When the weak coupling assumption is not satisfied, the low-energy theoretical predictions serve only as asymptotic limits, and some ambiguous points
Figure 3. Two Gaussian clouds from \( \mathcal{N}((\pm \ell, 0)^\top, \sigma^2 I_{2\times 2}) \) with variations in the center-to-center distance (a) \( \ell = 3\sigma \), (b) \( \ell = 2.7\sigma \), and (c) \( \ell = 2.4\sigma \). Adjacency matrices were calculated using \( r_e = \sigma \). The radius of the faint large circle around each data point indicates \( r_e/2 \). (d-f) The phase distributions (red circles) of all sample points from (a-c), respectively; exact theoretical predictions \( \arg(\xi_{\mu\nu}(is)) \) from the low-energy effective model (solid line); the first, second, and third order perturbative approximations (dashed lines). The Laplace transform parameter was set to \( s = 1.2(E_1 - E_0) \). The \( \ast \) in (a), (b), and (c) mark the initialization nodes.

in a strongly mixed region may have a phase that interpolates between the theoretical predictions (Fig. 3(c,f); Fig. S4 & S5).

When the clusters in data show strong mixing, no single partition may be clearly dominant, so using the partition corresponding to the highest occurrence frequency \( w_n \) may be unstable. In this scenario, we propose a "fuzzy" summary of the ensemble. Across \( m' \) different initializations, we count the number of times where two nodes, say \( i \) and \( k \), are assigned to the same cluster, and then divide the count by \( m' \). We thereby arrive at a symmetric consensus matrix \( C_{sk} \) with 1 along the diagonal and other entries in \([0, 1]\) (SM [18], I C). The consensus matrix provides a useful visualization of processed clustering structure and also serves as a new input similarity measure suitable for many popular statistical learning algorithms, such as spectral clustering, hierarchical clustering, and SVM.

For instance, we used the somatic copy number alteration (SCNA) data in low-grade glioma (LGG) and glioblastoma (GBM) patients from the Cancer Genome Atlas to construct an adjacency matrix of genomic locations (SM [18]), and performed QTC with the chosen number of clusters equal to 2, 3, 4, or 5. We summarized the predicted similarity between genomic coordinates by averaging the consensus matrices \( \langle C(q) \rangle_{q=2} \) for LGG and GBM separately, yielding \( \langle C_{\text{LGG}} \rangle \) and \( \langle C_{\text{GBM}} \rangle \). The block structures in SCNA captured by QTC closely resembled the 3D chromatin interaction HiC contact matrix (Fig. 4) [25]; the Pearson correlation coefficients between \( \langle C_{\text{LGG/GBM}} \rangle \) and \( \tanh((C_{\text{HiC}})_{ij}/C_{\text{HiC}}) \in [0, 1] \) was 0.87, whereas the same correlation involving the raw SCNA data was less than 0.50 (Fig. S6). Our QTC consensus matrix thus denotes the SCNA data and helps support the previously observed phenomenon linking genomic alterations in cancer with the 3D organization of chromatin [26].

In summary, a quantum mechanical wave function is dramatically different from a classical heat density; even for an initial point source, the former demonstrates an oscillatory wave behavior, while the latter is smooth and monotonic in both space and time. Overcoming the previous difficulties in measuring data similarity using wave functions, we here devised a stand-alone clustering algorithm based on quantum transport on network graphs. Realistic data usually consist of a large number of features, and the large feature dimensions can often render clustering algorithms inefficient [27]. Although we do not directly address this issue here, our QTC algorithm may be combined with known methods for ameliorating the "curse of dimensionality" [28]. Another major challenge in clustering arises when putative clusters are strongly mixed; in such a case, supervised learning is usually the most efficient solution by introducing manually labeled training samples [2].

In addition to high dimensionality and strong mixing, geometric complexity remains an outstanding challenge; e.g., the cheese-stick distribution shown in Fig. 1(b) with several visually separable pieces confuses almost all clustering algorithms. But, we have demonstrated that the coherent phase information encoded in the two-point Green’s functions, or equivalently the Laplace-transformed wave functions, are as powerful as the widely applied spectral clustering. Furthermore, the QTC shows more robustness when the data distribution contains density fluctuations or a hierarchy of cluster sizes (SM [18], III A). Using multiple initialization sites, QTC generates an ensemble of phase distributions, which in turn provide a collection of discrete cluster labels (SM [18], I C). We may either select the most popular partition from the ensemble or encode the votes from the ensemble members into a consensus matrix. If most members favor a par-
ticular partition, it is an indication that the clusters are easily separable; conversely, split votes between several partitions may indicate suboptimal model parameters or strongly mixed clusters. Thus, QTC provides a useful self-consistency criterion absent in most clustering methods. Even in the case of split votes, the consensus matrix can still be used in other clustering or supervised learning methods as an improved similarity measure. In addition to the consensus matrix, we have explored other ways of constructing a QT kernel that can be used as an input to numerous (dis)similarity-based algorithms (SM [18], III, Fig. S8 & S9). For example, we have tested the time-average of squared transition amplitude as a similarity measure in spectral clustering (Fig. S8 & S9); the performance was slightly better than spectral clustering using Gaussian affinity, although some intrinsic weaknesses of spectral embedding persisted (SM [18], III A). These results provide evidence for potential benefits that may arise from studying data science using quantum physics.

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Supplemental Material

CONTENTS

I. Quantum Transport Clustering (QTC) 5
   A. Laplace transform of time evolution 6
   B. Choosing the number of clusters 6
   C. Phase information 6
      1. Direct extraction 7
      2. Consensus matrix 8
   D. Effective tight-binding model 8
   E. Two-level toy model 8

II. Data Preparation 10
   A. Synthetic Data Sets 10
   B. Time Series Stock Price Data 10
   C. Genomic Data 11

III. Comparison with other methods 11
   A. Spectral embedding 11
   B. Time-averaged transition amplitude 13
   C. Density information of Laplace-transformed wave functions 14
   D. Jensen-Shannon divergence of density operators 14

References 15

I. QUANTUM TRANSPORT CLUSTERING (QTC)

The Schrödinger equation for a free particle is, up to the Wick rotation \( t \to \ii t \), formally similar to the heat equation with heat conductance \( \kappa \):

\[
\partial_t u = \kappa \nabla^2 u.
\]

Assuming that the heat conductance \( \kappa \) is constant in space, the heat equation can be rewritten as

\[
\partial_t u = \kappa \nabla^2 u = -\nabla \cdot (-\kappa \nabla u).
\]

Defining the heat current as

\[
j = -\kappa \nabla u,
\]

the heat equation then becomes the conservation law

\[
\partial_t u + \nabla \cdot j = 0.
\]

The Schrödinger equation also embodies a conservation law. For example, consider the Schrödinger equation with a time-independent potential \( V(x) \):

\[
i \partial_t \psi = -\frac{\nabla^2 \psi}{2m} + V(x) \psi,
\]

in units where \( \hbar = 1 \). Writing its solution as \( \psi(x,t) = \sqrt{\rho(x,t)} e^{\ii \theta(x,t)} \), where \( \rho \) is the probability density and \( \theta \)
the phase, we see that the Schrödinger equation is not one but two coupled equations for $\rho$ and $\theta$,

$$\dot{\rho} = -\nabla \cdot \left( \frac{\nabla \theta}{m} \right), \quad \dot{\theta} = \frac{1}{2} m \mathbf{v}^2 + V + Q,$$

where $\mathbf{v} = \nabla \theta / m$ is the group velocity of a quantum mechanical particle, and $\mathbf{j} = \rho \mathbf{v}$ the current density; and

$$-\frac{\nabla \theta}{m} \equiv -\nabla \cdot \left( \frac{\rho \mathbf{v}}{m} \right) = -\nabla \cdot \mathbf{j},$$

where $Q = -\frac{1}{2m} \left[ \nabla^2 \rho / \sqrt{\rho} \right]$ is the “quantum potential.”

Notice that the quantum current is proportional to $\nabla \theta$ instead of $\nabla \rho$. Thus, the phase gradient drives the propagation of the wave function, which encodes richer physics than classical heat density. This observation suggests that the phase information may be useful for devising quantum algorithms.

A. Laplace transform of time evolution

The Laplace transform of a wave function $|\psi(t)\rangle$, evolved from an initial state $|\psi(0)\rangle$ via a time-independent Hamiltonian $H$, is given by

$$|\tilde{\psi}(s)\rangle \equiv \mathcal{L}(|\psi\rangle)(s) = \int_0^\infty e^{-st} e^{-iHt} |\psi(0)\rangle \, dt.$$

Since $H$ is time-independent, we have

$$|\tilde{\psi}(s)\rangle = \frac{1}{s + iH} |\psi(0)\rangle = iG(s) |\psi(0)\rangle,$$

where $G(z) \equiv (z - H)^{-1}$ is the resolvent operator of $H$. In the main text, we interpret $G(z)$ using an effective tight-binding model. Here, we study the Laplace-transformed wave function explicitly. The inverse of the variable $s$ sets the time scale within which the Schrödinger time evolution is averaged; i.e., this scale sets the extent to which oscillation in time is smoothed out and destructive interference that can potentially localize the transport gets ameliorated. Motivated by this observation, this paper demonstrates that taking the Laplace transform can resolve the issues of wave function oscillation and localization that have hindered the application of quantum mechanics to clustering problems.

Of note, recall that spectral clustering uses the $j$-th entries of the first few lowest-eigenvalue eigenvectors of the graph Laplacian to represent the $j$-th node. By contrast, one distinct advantage of QTC lies in utilizing the eigenvectors $\psi_n$ twice when computing the phase of

$$\langle j | \tilde{\psi}(s) \rangle = \sum_n \frac{\langle \psi_n | \psi(0) \rangle}{s + iE_n} \psi_n(j);$$

namely, both the $j$-th entries $\psi_n(j)$, just as in spectral clustering, and the projections $\langle \psi_n | \psi(0) \rangle$ onto the initialization node are used. In this way, as the initialization node varies during the random sampling step, the phase representations of two nodes within a cluster will stay close to each other, and this information is pooled together in the QTC algorithm.

B. Choosing the number of clusters

If $q > 1$ clusters are well-separated, the Hamiltonian is approximately $q$-block diagonal. Fluctuations between the $q$ macroscopic modes have lower kinetic energy, which mainly arises from inter-cluster tunneling, than microscopic fluctuations within each cluster. In this case, there exists an energy gap separating the low-energy macroscopic modes from the high-energy microscopic oscillations. Furthermore, the low-energy states can be approximated as linear combinations of cluster wave functions; thus, the number of low-energy states equals the number of putative clusters. For illustration, we generated well-separated $q = 2, 3, 4$ Gaussian clusters in three dimensions (Fig. S1(a,b,c)); the adjacency matrix was computed using the 10%-quantile of pairwise distance distribution as the proximity scale in Gaussian kernel. The first 6 eigenvalues of the Hamiltonian are plotted in Fig. S1(d,e,f).

![Figure S1. (a,b,c) Gaussian distributions ($\sigma = 0.1$) in $\mathbb{R}^3$, with the means located at the vertices of a regular tetrahedron of length 1. The inter-cluster distance is thus 10$\sigma$. (d,e,f) The spectrum of symmetric normalized graph Laplacian $H$ corresponding to the data distributions in (a,b,c), respectively.](image)

C. Phase information

In applications, we numerically calculate the Laplace transform of a wave function initialized at a given node and then extract the phase distribution. As in the main text, we will assume that the total number of nodes is $m$.
and the a priori determined number of clusters is $q$. The phases of nodes belonging to different clusters are typically separated by gaps, allowing us to assign discrete class labels to nodes. We propose two methods for converting the phases to class labels $0, 1, \ldots, q - 1$: (Method 1) direct difference, and (Method 2) clustering. The steps in Method 1 are as follows:

**Method 1**

1. Let $\pi(i)$ denote the rank of the phase of node $i$, then form an ensemble of class labels, organized into a matrix $(\Omega_{ij})$, where $i = 0, 1, \ldots, m - 1$ runs through all nodes and $j = 0, 1, \ldots, m' - 1$ indexes the iteration of initialization. 

Notice that the class labels may get permuted across different initialization. We introduce two methods to handle this issue and summarize the $\Omega$-matrix: (1) direct extraction, and (2) consensus matrix.

1. **Direct extraction**

We want to count the multiplicity of the columns of $\Omega$, up to permutation of class labels; i.e. two columns are considered equivalent if they are equal upon permuting the class labels. We will then choose the most frequent column vector as the desired partition of nodes. For this purpose, we first devise a scheme for testing whether a subset of columns are all equivalent.

Let $\{p_l\} = \{2, 3, 5, 7, \cdots\}$ be the set of primes, then $\{\sqrt{p_l}\}$ is a set of irrational numbers serving as linearly independent vectors over the field $\mathbb{Q}$ of rational numbers. Let $A$ be an index set containing at least two columns indices of $\Omega$. For each node $i$, we then compute the quantity 

$$
\xi_i = \sum_{k \in A} \Omega_{ik} \sqrt{p_k}.
$$

For any two nodes $i$ and $j$,

$$
\xi_i - \xi_j = \sum_{k \in A} (\Omega_{ik} - \Omega_{jk}) \sqrt{p_k} = \sum_{k \in A} b_k \sqrt{p_k}.
$$

Suppose $i$ and $j$ are in the same cluster for all $k \in A$, then $b_k = 0$ for all $k$, and thus $\xi_i = \xi_j$; the converse is also true, because $\{\sqrt{p_l}\}$ is linearly independent over $\mathbb{Q}$. Thus, $\xi_i = \xi_j$ iff node $i$ and node $j$ are assigned to the same class by all columns indexed by $A$. The minimum number of distinct $\xi_i$ is $q$, since any column of $\Omega$ partitions the nodes into $q$ clusters. If the number of distinct $\xi_i$ exceeds $q$, then there exists at least two columns that disagree on the partition, so the columns indexed by $A$ are not all equivalent.

Our algorithm including this scheme is as follows:

**Ensemble Method 1**

3. Let $K' = \{0, 1, \ldots, m' - 1\}$ be the full index set indexing the columns of $\Omega$. Denote any non-empty subset of $K$ as $K'$, and let $k_0'$ denote the first column index appearing in $K'$.

2. **Define** function $\text{IsEquiv}(\{\Omega_{ik}\}_{k \in K'})$ to tell whether the columns of $\Omega$ indexed by $K'$ yield an equivalent clustering:

   **For** $i = 0, 1, \ldots, m - 1$:

   $$
   \xi_i = \sum_{k \in K'} \Omega_{ik} \sqrt{p_k}
   $$

   Count the number $q'$ of distinct $\xi_i$

   **If** $q' = q$, then **Return** True

   **Else** Return False

3. Let $H$ be a hash table with non-negative integer keys $\alpha$ indexing the equivalence classes of columns of $\Omega$ and values $H_{\alpha}$ equal to the corresponding index sets of equivalent columns. Each key $\alpha$ is chosen from $H_{\alpha}$ to represent the class.

4. **Define** function $\text{Pigeonhole}(\{\Omega_{ik}\}_{k \in K'}, H)$:

   **If** $\text{IsEquiv}(\{\Omega_{ik}\}_{k \in K'}) = \text{True}$, then:
   
   IsExisting $= \text{False}$

   **For** $\alpha$ in $H$:
If IsEquiv($\{\Omega_{ik}\}_{k=1}^{N}$) = True:
IsExisting = True
Merge $K'$ and $H_\alpha$
break for-loop
If IsExisting = False:
Create a new key $\alpha'$ and $H_{\alpha'} = K'$
Else: Split $K'$ in two halves, $K'_1$ and $K'_2$
Call $H = \text{Pigeonhole}(\{\Omega_{ik}\}_{k \in K'_1}, H)$
Call $H = \text{Pigeonhole}(\{\Omega_{ik}\}_{k \in K'_2}, H)$
Return $H$

5. Call $\text{Pigeonhole}(\{\Omega_{ik}\}_{k \in K}, H^0)$, where $H^0$ is an empty hash table

2. Consensus matrix

Even though the class labels may get randomly permitted for different initializations, whether two nodes share the same class label within each initialization is independent of the labeling convention. Therefore, we define a consensus matrix $C$ with elements

$$C_{ij} = \frac{\sum_{k=1}^{m'} \delta(\Omega_{ik} - \Omega_{jk})}{m'},$$

where $\delta$ is the Kronecker delta or indicator function, and $m' \leq m$ is the number of the chosen initialization nodes.

Notice that $C_{ij} = C_{ji}$ for all nodes $i, j = 1, 2, \ldots, m$. The algorithm is sketched as follows:

**Ensemble Method 2**

1. Initialize $C$ as an $m \times m$ identity matrix
2. For $i = 0, 1, \ldots, m - 1$:
   For $j = i + 1, \ldots, m - 1$:

   $$g_{\mu\nu}(z) = \frac{\delta_{\mu\nu}}{z - \xi_\mu} + \frac{v_{\mu\nu}}{(z - \xi_\mu)(z - \xi_\nu)} + \sum_{\sigma} \frac{v_{\mu\sigma}v_{\sigma\nu}}{(z - \xi_\mu)(z - \xi_\sigma)(z - \xi_\nu)} + \sum_{\sigma, \rho} \frac{v_{\mu\sigma}v_{\sigma\rho}v_{\rho\nu}}{(z - \xi_\mu)(z - \xi_\sigma)(z - \xi_\rho)(z - \xi_\nu)} + O(4).$$

Note that the resolvent matrix is thus a weighted sum over all possible tunneling paths between the $q$ clusters.

3. $C_{ij} = C_{ij}/m'$ for $i \neq j$

The consensus matrix measures the similarity of node pairs and facilitates the visualization of network structure, e.g. chromatin interaction information between distant genomic loci, as in Fig. 4. It can also be used as a similarity measure or dissimilarity measure, e.g. $\delta_{ij} - C_{ij}$, in (dis)similarity-based algorithms such as spectral clustering and hierarchical clustering.

**D. Effective tight-binding model**

In the extreme case where the clusters are completely separated from each other, the Hamiltonian $H$ is strictly in $q$ diagonal blocks; each block governs the dynamics within a cluster and has its own ground state wave function $\phi_{\mu}(i) = \langle i|\phi_\mu \rangle$, which is positive for node $i$ belonging to the $\mu$-th cluster and zero otherwise. We have $H|\phi_\mu \rangle = \xi_\mu|\phi_\mu \rangle$ and $\langle \phi_\mu|\phi_\nu \rangle = \delta_{\mu\nu}$ for all $\mu, \nu = 0, 1, \ldots, q - 1$. As we gradually turn on off-diagonal couplings $v_{\mu\nu} = \langle \phi_\mu|H|\phi_\nu \rangle$ between clusters $\mu \neq \nu$, the wave functions $\phi_\mu$ are no longer eigenstates of $H$. The effective tight-binding model assumes that in the weak coupling limit, we can project $H$ onto the subspace spanned by $\{\phi_\mu\}_{\mu=0}^{q-1}$ and diagonalize the projected Hamiltonian $h_{\mu\nu} = \langle \phi_\mu|H|\phi_\nu \rangle$ to approximate the first $q$ lowest energy eigenstates.

The resolvent matrix $g_{\mu\nu}$ of $h_{\mu\nu}$ is defined through

$$g^{-1}(z)_{\mu\nu} = z\delta_{\mu\nu} - h_{\mu\nu}.$$  

The resolvent matrix can be expanded if $|v_{\mu\nu}| < |z - \xi_\nu|$, for all $\mu, \nu = 0, 1, \ldots, q - 1$, as

$$g_{\mu\nu}(z) = \frac{\delta_{\mu\nu}}{z - \xi_\mu} + \frac{v_{\mu\nu}}{(z - \xi_\mu)(z - \xi_\nu)} + \sum_{\sigma} \frac{v_{\mu\sigma}v_{\sigma\nu}}{(z - \xi_\mu)(z - \xi_\sigma)(z - \xi_\nu)} + O(4).$$

clusters have the same ground state energy, the ground state $|\psi_0\rangle$ and the first excited state $|\psi_1\rangle$ of the tight-binding Hamiltonian are

$$|\psi_0\rangle = \frac{|\phi_0\rangle + |\phi_1\rangle}{\sqrt{2}}, \quad |\psi_1\rangle = \frac{|\phi_0\rangle - |\phi_1\rangle}{\sqrt{2}}.$$  

Setting the ground state energy $E_0 = 0$, and defining the first energy gap $E \equiv E_1 - E_0$, we have

$$|\psi(s)\rangle = \frac{1}{s + iE}|\psi(0)\rangle \approx \frac{c_0|\psi_0\rangle}{s} + \frac{c_1|\psi_1\rangle}{s + iE}.$$  

**E. Two-level toy model**

Consider the case of two Gaussian clusters in $\mathbb{R}^2$ with mean at $(\pm \ell, 0)^T$, as shown in Fig. 3(a-c) and Fig. S2(a-c). We expect two low energy states, i.e. the ground state and the first excited state (Fig. S3(b)). Let $\phi_0$ and $\phi_1$ denote the cluster wave functions for the left and right Gaussian clouds, respectively. Assuming that the two
where \(c_j = \langle \psi_j | \psi(0) \rangle\). Thus,

\[
|\psi(s)\rangle = \left( \frac{c_0}{s} + \frac{c_1}{s + iE} \right)|\phi_0\rangle + \left( \frac{c_0}{s} - \frac{c_1}{s + iE} \right)|\phi_1\rangle
\]

from which we easily extract the phase in the left and right clusters to be

\[
\Theta_0 = \arctan \frac{E c_0}{(c_0 + c_1)s} - \arctan \frac{E}{s}, \quad \text{and}
\]

\[
\Theta_1 = \arctan \frac{E c_0}{(c_0 - c_1)s} - \arctan \frac{E}{s}.
\]

If the initial state \(\psi(0)\) is a delta function located deep in the (1) left or (2) right cluster, then (1) \(c_0 = c_1\) or (2) \(c_0 = -c_1\), respectively. The phases of the left and right clusters in case (1) are

\[
\Theta_{00} = \arctan \frac{E}{2s} - \arctan \frac{E}{s},
\]

\[
\Theta_{01} = \frac{\pi}{2} - \arctan \frac{E}{s}; \quad \text{(S5)}
\]

while in case (2), the phases are

\[
\Theta_{10} = \frac{\pi}{2} - \arctan \frac{E}{s},
\]

\[
\Theta_{11} = \arctan \frac{E}{2s} - \arctan \frac{E}{s}. \quad \text{(S6)}
\]

Notice that \(\Theta_{\mu \nu}\) is a constant diagonal symmetric matrix that preserves the left-right symmetry.

The two-cluster model can be mapped to the classic double-well instanton tunneling model which will be briefly summarized below; detailed derivations can be found in [30]. The model Hamiltonian is

\[
H = -\frac{1}{2} \partial_x^2 + \lambda (x^2 - \ell^2)^2,
\]

where \(\lambda > 0\). The potential \(V(x) = \lambda (x^2 - \ell^2)^2\) has two minima at \(x = \pm \ell\) for \(\ell > 0\) and one minimum at \(x = 0\) for \(\ell = 0\). The barrier height is \(V(0) = \lambda \ell^4\) which grows rapidly with the separation distance \(\ell\). In the vicinity of minima, \(V(\pm \ell + \varepsilon) = \lambda (\pm 2 \varepsilon \pm \ell^2)^2 = 4 \lambda \ell^2 \varepsilon^2 + \mathcal{O}(\varepsilon^3)\); the local harmonic frequency is thus \(\omega = 2\ell \sqrt{2\lambda}\) and \(V(0) = \omega^4 / 64\lambda\).

In the limit \(\lambda \to 0\) while keeping \(\omega\) constant, the barrier is infinite, and the ground state is two-fold degenerate with harmonic ground state energy \(E_0 = \frac{\omega}{2}\) and expected position \(x = \pm \ell\). For any finite barrier, however, we should have \(x = 0\), which is enforced by symmetry; the symmetric solution cannot be obtained via perturbation around either of the local minima.

Non-perturbative instanton solution splits the degeneracy:

\[
E_0 = \frac{\omega}{2} \left( 1 - 2 \sqrt{\frac{\omega^3 e^{-\omega^3 / 12\lambda}}{2\pi \lambda}} \right),
\]

\[
E_1 = \frac{\omega}{2} \left( 1 + 2 \sqrt{\frac{\omega^3 e^{-\omega^3 / 12\lambda}}{2\pi \lambda}} \right).
\]

The transition amplitudes are

\[
\langle \pm \ell | e^{-iHt} | - \ell \rangle = i \sqrt{\frac{\omega}{2\pi \lambda}} e^{-i\omega \ell t / 2} \sin(\omega \rho_{\text{inst}} t) \quad \text{and}
\]

\[
\langle -\ell | e^{-iHt} | - \ell \rangle = \sqrt{\frac{\omega}{2\pi \lambda}} e^{-i\omega \ell t / 2} \cos(\omega \rho_{\text{inst}} t),
\]

where the instanton density \(\rho_{\text{inst}} = \sqrt{\omega^3 / 2\pi \lambda} e^{-\omega^3 / 12\lambda}\). Notice that the energy gap is \(E = 2\omega \rho_{\text{inst}}\); thus,

\[
\langle \pm \ell | e^{-iHt} | - \ell \rangle = \sqrt{\frac{\omega}{2\pi \lambda}} e^{-i\omega \ell t / 2} \sqrt{e^{iE \ell t / 2} + e^{-iE \ell t}} / 2
\]

\[
= \sqrt{\frac{\omega}{2\pi \lambda}} e^{-i\omega \ell t / 2} \sqrt{e^{iE \ell t} + e^{-iE \ell t}} / 2
\]

\[
= \sqrt{\frac{\omega}{2\pi \lambda}} e^{-iE \ell t} \left( 1 \mp e^{-iE \ell t} / 2 \right). \quad \text{(S7)}
\]

If we reset the ground state energy to zero, the Laplace transform of Eq. S7 yields the resolvent matrix elements

\[
g_{00}(is) = \frac{1}{2} \sqrt{\frac{\omega}{2\pi \lambda}} \left( \frac{1}{s + 12\lambda} + \frac{1}{s + 12\lambda} \right)
\]

\[
g_{01}(is) = \frac{1}{2} \sqrt{\frac{\omega}{2\pi \lambda}} \left( \frac{1}{s + 12\lambda} - \frac{1}{s + 12\lambda} \right), \quad \text{(S8)}
\]

where 0 and 1 denote the states localized at \(x = -\ell\) and \(x = +\ell\), respectively. The phases are thus

\[
\Theta_{00}(s) = \arctan \frac{E}{2s} - \arctan \frac{E}{s},
\]

\[
\Theta_{01}(s) = \frac{\pi}{2} - \arctan \frac{E}{s}. \quad \text{(S9)}
\]
Note that the above phase distribution is exactly the same as that from the low-energy two-cluster model (Eq. S5) upon identifying the energy gaps.

The phase separation between the diagonal and off-diagonal elements of the resolvent is \( \pi/2 - \arctan \frac{\ell}{E} \), and this difference is thus controlled by the ratio \( s/E \). In other words, the Laplace transform parameter \( s \) controls the separability between clusters in the QTC algorithm. For \( s \ll E \), \( s = E/2 \), or \( s \gg E \), the phase differences are 0, \( \pi/4 \), or \( \pi/2 \), respectively. Fig. S3(a) shows the phases \( \Theta_{00} \) and \( \Theta_{01} \) for different values of \( s/E \) in the range \([10^{-2}, 10^2]\), suggesting that \( s \) should be chosen to be at least as large as the energy gap \( E \).

In practice, for an ambiguous point located between two clusters, its phase interpolates smoothly between the cluster phases. Figure S4(b) shows the phases of the outlier for QTC initialized from a point deep in the left cluster. Moreover, Figure S5(b) shows the mean phases of the left and right clusters for QTC initialized at an outlier located at \((-\ell(1-\alpha_{out}) + \ell \alpha_{out}), 0\)^\top\), and it demonstrates that a wave function initialized from an ambiguous point loses contrast between the two clusters.

Similarly, for cases involving more than two clusters, the full \( \Theta \)-matrix for all nodes essentially amounts to the effective tight-binding matrix \( \arg(\psi_{ij}(is)) \). Our experience shows that choosing \( s \) based on the average gap, \( E = (E_q - E_0)/(q - 1) \), still provides a helpful guideline and yields good multiclass clustering results.

II. DATA PREPARATION

A. Synthetic Data Sets

For a sufficiently small proximity measure \( r_z \) in the synthetic data in Fig. 1 (b-d & f-h), both QTC and spectral clustering were able to produce the correct clustering results. But, as \( r_z \) increased, spectral clustering made mistakes, while QTC remained robust. For sufficiently large proximity values, both spectral clustering and QTC failed to recognize the clusters. Thus, there was a finite interval of \( \varepsilon \) for each data set in which QTC outperformed spectral clustering. For the data sets in Fig. 1 (b-d & f-h), the intervals were approximately \([3.1\%, 3.9\%],[0.61\%, 0.85\%],[0.39\%, 0.46\%]\), respectively.

B. Time Series Stock Price Data

The stock price data consisted of the “adjusted close” prices of the AAPL and GOOGL stocks between January 3, 2005 and November 7, 2017, downloaded from Yahoo Finance. We log transformed the data and subtracted the two time series by the respective log-prices on the first day (1-3-2005). We computed the pairwise Euclidean distance in \( \mathbb{R}^2 \) and took 1%-quantile of the distance distribution as the proximity length \( r_{1\%} = 0.05 \). Next, we assembled the Gaussian similarity measure \( A_{ij} = \exp[-(r_{ij}/r_{1\%})^2] \) and performed QTC and spectral clustering; the number of clusters was chosen to be five. Spectral clustering was able to produce the clus-
tering obtained by QTC at 1%-quantile only for shorter proximity lengths \(\varepsilon \in [0.2\%, 0.5\%]\); for \(\varepsilon \lesssim 0.1\%\), the clusters started to become disjoint subnetworks.

C. Genomic Data

Figure S6. Pearson correlation coefficients between the tanh-normalized HiC matrix and various similarity measures. For (a) LGG and (b) GBM samples, respectively, correlations were computed using the “unweighted” raw counts \(N_{ij}\) of SCNA labeled by genomic location pair \((i, j)\), the weighted adjacency \((A_{\text{LGG/GBM}})_{ij} = N_{ij}w_{ij}\) with Gaussian weight \(w_{ij} = \exp(-(r_{ij}/r_c)^2)\), and the QTC consensus matrix \(C_{\text{LGG/GBM}}\) calculated assuming a different number of clusters. Both weighted and unweighted similarity matrices were tanh-normalized.

The TCGA somatic copy number alteration (SCNA) data in low-grade glioma (LGG) and glioblastoma (GBM) patient samples were downloaded from the GDC Data Portal under the name “LGG/GBM somatic copy number alterations.” To link these data to chromatin contact information, we followed the analysis described in [26]. We partitioned the genome into 1Mb bins and defined \(N\) to be a null square matrix of dimension equal to the total number of bins. For each amplified or deleted genomic segment starting at the \(i\)-th bin and ending at the \(j\)-th bin, we then incremented the \((i, j)\)-th entry of \(N\) by 1. The main idea behind this analysis is that genomic amplification and deletion events are mediated by the physical co-location of the segment junctions. The raw count matrix \(N\) was thus to be compared with the HiC chromatin contact matrix. In cancer samples, however, an entire arm of a chromosome or even a whole chromosome can be duplicated or deleted, potentially leading to fictitious long-range off-diagonal elements in \(N\). Therefore, we weighted the counts \(N_{ij}\) by \(w_{ij} = \exp(-(r_{ij}/r_c)^2)\) where \(r_{ij}\) is the genomic distance between the bins and \(r_c = 10\)Mb. Using this weighted matrix as an adjacency matrix, we performed QTC with \(s = 5(E_4 - E_2)\), assuming the number of clusters to be \(q = 2, 3, 4, 5\), and computed the respective consensus matrices \(C(q)\). Finally, we took the arithmetic mean \(\langle C \rangle = \sum_{q=2}^{5} C(q)/4\).

The HiC data in normal human astrocytes of the cerebellum (glial cells) were downloaded from ENCODE under the name “ENCSR011GNI” [25]. We extracted the 3D interaction maps on chromosome 2 at 1Mb resolution. The distribution of HiC contact matrix entries was highly heavy-tailed. In order to compare \(C_{\text{HiC}}\) with \(\langle C_{ij} \rangle\) in \([0, 1]\), we transformed \(C_{\text{HiC}}\) using \(\text{tanh}(C_{\text{HiC}}/\bar{C}_{\text{HiC}})\) \(\in [0, 1]\), where \(\bar{C}_{\text{HiC}}\) was the mean of all \(C_{\text{HiC}}\) entries. Next, we computed the Pearson correlation coefficients between the transformed \(C_{\text{HiC}}\) and averaged \(\langle C(q)_{ij} \rangle\).

III. COMPARISON WITH OTHER METHODS

In this section, we first discuss spectral embedding and then derive three additional (dis)similarity measures using quantum mechanics. These measures can be combined with spectral clustering as well as other (dis)similarity-based learning algorithms.

A. Spectral embedding

The state-of-the-art spectral clustering can be decomposed into three major steps: (1) assemble an affinity matrix \(A\) based on some similarity measure of sample points, (2) compute the symmetric normalized graph Laplacian \(H\), and (3) map each sample point indexed by \(i = 0, 1, \ldots, m - 1\) to a Euclidean feature space using the corresponding elements of eigenvectors of the graph Laplacian; this mapping is called the spectral embedding. The first two steps are essentially the same as those of QTC; the key difference lies in the final usage of “spectral properties” of the data set. A single iteration of QTC succinctly represents the data on \(S^{d}\), which we have shown is sufficient to separate distinct clusters.

By contrast, spectral embedding maps data samples to \(\mathbb{R}^q\), where \(q\) is the number of putative clusters, or the number of low energy states if all putative clusters are clearly separable; then, the algorithm performs clustering, e.g. using \(k\)-means in the feature space \(\mathbb{R}^q\). The feature vector \(v_i\) associated with the \(i\)-th sample has elements

\[
(v_i)_n = \psi_n(i), \quad n = 0, 1, \ldots, q - 1,
\]

where the \(\psi_n\)’s are the first \(q\) lowest-eigenvalue eigenvectors of \(H\). The \(L^2\) Euclidean distance between nodes \((i, j)\) is then

\[
D_{ij} = \sqrt{\|v_i - v_j\|^2} = \sqrt{\sum_{n=0}^{q-1} |\psi_n(i) - \psi_n(j)|^2} = \sqrt{\sum_{n=0}^{q-1} \langle |i\rangle - \langle j|n\rangle \langle n|(|i\rangle - |j\rangle)\rangle}.
\]

Note that if we actually used all eigenvectors of \(H\), then \(D_{ij} = \sqrt{2(1 - \delta_{ij})}\), i.e. each point is equally far away
from any other node. Thus, the useful clustering information originates from the projection to low energy states,

$$D_{ij} = \sqrt{\langle |i\rangle - \langle |j\rangle |P_{n<q} |i\rangle - |j\rangle \rangle}$$  \hspace{1cm} (S11)

$$\equiv \sqrt{\chi_{ij} + \chi_{ji} - \chi_{ij} - \chi_{ji}},$$  \hspace{1cm} (S12)

where \(\chi_{ij} = \langle |i\rangle P_{n<q} |j\rangle \rangle = \sum_{n<q} \psi_n(i)\psi_n^*(j)\).

In real data, the number of nodes as well as the distribution of node density could vary from one cluster to another. If a network is embedded in \(\mathbb{R}^d\), then high density regions contain hub nodes, provided the adjacency \(A_{ij}\) is measured with a non-negative function that decreases with increasing distance \(r_{ij}\), e.g. Gaussian function \(A_{ij} = \exp(-r_{ij}^2/r_0^2)\). For networks not embedded in \(\mathbb{R}^d\), the “density” distribution should be interpreted as the degree distribution. We next illustrate how the spectral embedding distance \(D_{ij}\) responds to outliers in the presence of density variations using the simple two-cluster model.

Using the same notation as in the main text, the ground state and first excited state, shown in Fig. S7(a,b), are \(\psi_0 = \alpha \phi_0 + \beta \phi_1\) and \(\psi_1 = \beta \phi_0 - \alpha \phi_1\), where \(\alpha, \beta > 0\), and \(\alpha^2 + \beta^2 = 1\). If we assume \(\phi_0\) and \(\phi_1\) are orthonormal, i.e. \(\langle \phi_\mu | \phi_\nu \rangle = \delta_{\mu \nu}\), for \(\mu, \nu = 0, 1\), then \(\langle \psi_n | \psi_{n'} \rangle = \delta_{n n'}\) for \(n, n' = 0, 1\). To simplify calculations, we further assume that \(\phi_0\) and \(\phi_1\) have identical shapes with the maximum value \(\hbar\) located at node \(i\) and \(j\), respectively; i.e. \(\phi_0(i) = \hbar = \phi_1(j)\). Then, \(\psi_0(i) = \alpha \hbar = -\psi_1(j)\) and \(\psi_1(i) = \beta \hbar = \psi_0(j)\).

Let \(\gamma \in (0, 1]\) such that \(\phi_0(k) = \gamma \phi_0(i) = \gamma \hbar\). Then, \(\psi_0(k) = \gamma \alpha \hbar\), and \(\psi_1(k) = \gamma \beta \hbar\) (Fig. S7(a,b))). Recall that \(\psi_0(i) = \sqrt{\text{deg}(i)}\) for a normalized symmetric Laplacian; hence, the differences in \(\psi_0\) across nodes can be viewed as capturing the density variations in a network.

Simple calculations show that

\[
\chi_{ii} = \chi_{jj} = h^2 (\alpha^2 + \beta^2) = h^2
\]

\[
\chi_{ij} = \chi_{ji} = h^2 (\alpha \beta - \beta \alpha) = 0
\]

\[
\chi_{kk} = (\gamma \hbar)^2 (\alpha^2 + \beta^2) = \gamma^2 h^2
\]

\[
\chi_{ik} = \chi_{ki} = \gamma \hbar^2 (\alpha^2 + \beta^2) = \gamma h^2
\]

and

\[
\chi_{jk} = \chi_{kj} = \gamma \hbar^2 (\alpha \beta - \beta \alpha) = 0.
\]

Hence, we find

\[
D_{ij} = \sqrt{2} h
\]  \hspace{1cm} (S13)

\[
D_{ik} = (1 - \gamma) h
\]  \hspace{1cm} (S14)

\[
D_{jk} = \sqrt{1 + \gamma^2} h
\]  \hspace{1cm} (S15)

with

\[D_{ij} \geq D_{jk} > D_{ik}\] for \(\gamma \in (0, 1]\).

In the limit \(k\) becomes an outlier of the left cluster \(\phi_1\), \(\gamma \downarrow 0\) and \(D_{ik} \approx D_{jk}\). Furthermore, although the inequalities \(D_{ij} > D_{ik}\) and \(D_{jk} > D_{ik}\) facilitate the task of grouping similar points, the inequality \(D_{jk} \leq D_{ij}\) could potentially undermine the clustering accuracy. Notice that node \(k\) can be either close or far from the right cluster (Fig. S7(a,b), respectively), but yield the same \(D_{jk}\), as long as \(\phi_{\mu}(k) = \gamma \phi_{\mu}(i)\). In other words, an outlier from the left cluster could be closer to the right cluster in spectral distance, even when the outlier has a negligible connection to the right cluster (Fig. S7(b)). By sharp contrast, in QTC, the phase at a node lying between two clusters interpolates monotonically between the phases of the two clusters (Fig. S5).

![Figure S7](image_url)

**Figure S7.** (a,b) Schematic illustrations of the ground state and the first excited state involving two clusters; \(i\), \(j\), and \(k\) are node indices. Node \(k\) is an outlier (a) lying between the two clusters or (b) far from both clusters. (c,d) The normalized ground state and first excited state eigenfunctions using Approach 1. (e,f) The modified ground state and first excited state eigenfunctions using Approach 2.

This undesirable behavior of spectral clustering may be avoided by renormalizing the eigenvectors. Two common approaches are (Fig. S7(c,d) and (e,f), respectively):

**Approach 1**

1. Compute \(N(i) \equiv (\sum_{n=0}^{q-1} |\psi_n(i)|^2)^{1/2}\).

2. Divide each \(\psi_n(i)\) by \(N(i)\), i.e. \(\psi_n \rightarrow \psi_n/N\).

**Approach 2**

1. Divide each \(\psi_n(i)\) by \(\psi_0(i)\), i.e. \(\psi_n \rightarrow \psi_n/\psi_0\).
Similar to the phase plateaus in QTC, $\psi_n/N$ and $\psi_n/\psi_0$ are essentially flat within a cluster (Fig. S7(c,d) and (e,f), respectively).

In the first approach (Fig. S7(c,d)), the spectral embedding distances become

$$D_{ij}^{(1)} = \sqrt{(\alpha - \beta)^2 + (\alpha + \beta)^2} = \sqrt{2} \quad (S16)$$
$$D_{ik}^{(1)} = 0 \quad (S17)$$
$$D_{jk}^{(1)} = \sqrt{(\alpha - \beta)^2 + (\alpha + \beta)^2} = \sqrt{2}. \quad (S18)$$

In the second approach (Fig. S7(e,f)), the spectral embedding distances become

$$D_{ij}^{(2)} = \sqrt{(3/\alpha + \alpha/\beta)^2} = 1/\alpha\beta \quad (S19)$$
$$D_{ik}^{(2)} = 0 \quad (S20)$$
$$D_{jk}^{(2)} = \sqrt{(3/\alpha + \alpha/\beta)^2} = 1/\alpha\beta. \quad (S21)$$

In both cases, we have $D_{j,k}^{(1,2)} = D_{i,k}^{(1,2)}$; thus, the outlier node $k$ is much more likely to be clustered with the left cluster. (Scikit-Learn, a very popular machine learning software package in Python, implements the second approach incorrectly as $\psi_n \rightarrow \psi_n \times \psi_0$ and sometimes yields counter-intuitive clustering results. In this paper, we use our own implementation of Approach 1.)

Finally, we note that spectral embedding has an intrinsic weakness stemming from ignoring potentially useful information from high-energy states. More precisely, recall that spectral embedding assumes that the most relevant information for clustering is encoded in the first $q$ low-energy eigenstates of $H$. However, this assumption could be invalid in some cases, e.g. our synthetic data sets in Fig. 1, and time series data in Fig. 2, where the information needed to separate some small clusters are stored in higher energy modes. In such a case, spectral clustering may not have the required information to separate the small clusters, but instead chop the large clusters into fragments at their weak edges in low density regions. By contrast, QTC does not require a manual cut-off in the spectrum and incorporates all eigenstates by naturally weighing the contribution from each eigenfunction $\psi_n$ by $|s + iE_n|^{-1}$. This difference may explain why QTC is more robust than spectral embedding when there exists a hierarchy of cluster sizes.

**B. Time-averaged transition amplitude**

The time-dependent transition amplitude $G_{ij}(t)$ from node $j$ to $i$ is complex-valued and oscillatory in time, i.e.

$$G_{ij}(t) = \langle i|e^{-iHt}|j \rangle = \sum_{m,n} \langle i|\psi_m|\psi_m e^{-iHt}|\psi_n|\psi_n|j \rangle = \sum_n \psi_n(i)\psi_n^*(j)e^{-iE_n t}.$$ 

To obtain a real-valued matrix, we take the squared amplitude,

$$|G_{ij}(t)|^2 = G_{ii}(-t)G_{ij}(t) = \sum_{m,n} \psi_m(j)\psi_m^*(i)\psi_n(i)\psi_n^*(j)e^{i(E_m-E_n)t} = \sum_{m,n} \rho_{mn}(i)\rho_{nm}(j)e^{i(E_m-E_n)t}$$

where $\rho_{mn}(i) = \langle \psi_m|i\rangle\langle i|\psi_n \rangle$. The oscillation in time can be averaged as

$$P_{ij} = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \ |G_{ij}(t)|^2 = \sum_{m,n} \rho_{mn}(i)\rho_{nm}(j) \left[ \lim_{T \to \infty} \frac{1}{T} \int_0^T dt e^{i(E_m-E_n)t} \right] = \sum_{m,n} \delta_{E_m,E_n} \rho_{mn}(i)\rho_{nm}(j).$$

If there is no degeneracy in the spectrum of $H$, then the time-averaged squared transition amplitude simplifies to

$$P_{ij} = \sum_n \rho_{nn}(i)\rho_{nn}(j) = \sum_n |\psi_n(i)|^2 |\psi_n(j)|^2,$$

which is a symmetric, non-negative matrix that can be used as a similarity measure.

The performance of $P_{ij}$ as a spectral clustering affinity matrix was tested in four synthetic data sets (Fig. S8(a-d)) as well as the stock price time series data (Fig. S9(b)). The performance was similar to spectral clustering using Gaussian affinity.
Next, we define a similarity measure using the inner product of the proposed QTC method. Using small synthetic data nodes, and the computation is very slow compared with matrix scales as \( \mathcal{O}(m^2) \), where \( m \) is the total number of nodes, and the computation is very slow compared with the proposed QTC method. Using small synthetic data sets, we nevertheless implemented the JSD method and passed the JSD matrix to hierarchical clustering as a dissimilarity measure. The JSD measure did not show a significant performance improvement compared with the simple Euclidean distance.

### D. Jensen-Shannon divergence of density operators

The time evolution of the density operator \( \rho(j) = |j\rangle\langle j| \) describing a pure state localized at node \( j \) at time \( t = 0 \) is

\[
\rho(j; t) = e^{-iHt}|j\rangle\langle j| e^{iHt} = \sum_{m,n} e^{-iHt} |\psi_m\rangle \langle \psi_n| e^{iHt} = \sum_{m,n} e^{-i(E_m - E_n)t} \rho_{mn}(j) |\psi_m\rangle \langle \psi_n|,
\]

where \( \rho_{mn}(i) = \langle \psi_m|i\rangle\langle i|\psi_n\rangle \). If we again take the time average, then

\[
\bar{\rho}(j) = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \rho(j; t) = \sum_{m,n} \delta_{E_m,E_n} \rho_{mn}(j) |m\rangle\langle n|,
\]

and, in the absence of energy degeneracy, the time-averaged density operator initiated at node \( j \) simplifies to

\[
\bar{\rho}(j) = \sum_n \rho_{nn}(j) |\psi_n\rangle\langle \psi_n| = \sum_n \langle \psi_n| \rho_{nn}(j) |\psi_n\rangle |\psi_n\rangle\langle \psi_n|.
\]

For two time-averaged density operators corresponding to pure states initialized at node \( i \) and \( j \), respectively, we may measure the information-theoretic divergence between \( \bar{\rho}(i) \) and \( \bar{\rho}(j) \) using the Jensen-Shannon divergence (JSD),

\[
\mathcal{D}_{\text{JS}}(\bar{\rho}(i), \bar{\rho}(j)) = S\left[\frac{\bar{\rho}(i) + \bar{\rho}(j)}{2}\right] - \frac{1}{2} S[\bar{\rho}(i)] - \frac{1}{2} S[\bar{\rho}(j)]
\]

where \( S[\rho] = -\text{Tr}(\rho \log \rho) \) is the von Neumann entropy of \( \rho \).
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