Figure S1: Bar chart representing contributions of each of the N=90 AAL brain areas to the fronto-parietal FC state of interest ($V_c(n)>0$ in red, blue otherwise) across clustering solutions k = 6 through k = 10. In each clustering solution, the probability of occurrence of this state was significantly reduced following the psilocybin injection. The Bonferroni-corrected p-values (i.e. p-val * k) were: 0.022 (k = 6); 0.002 (k = 7); 0.008 (k = 8); 0.026 (k = 9) and 0.019 (k = 10). Regional contributions to the cluster centroid of interest show a high level of consistency across the clustering solutions.
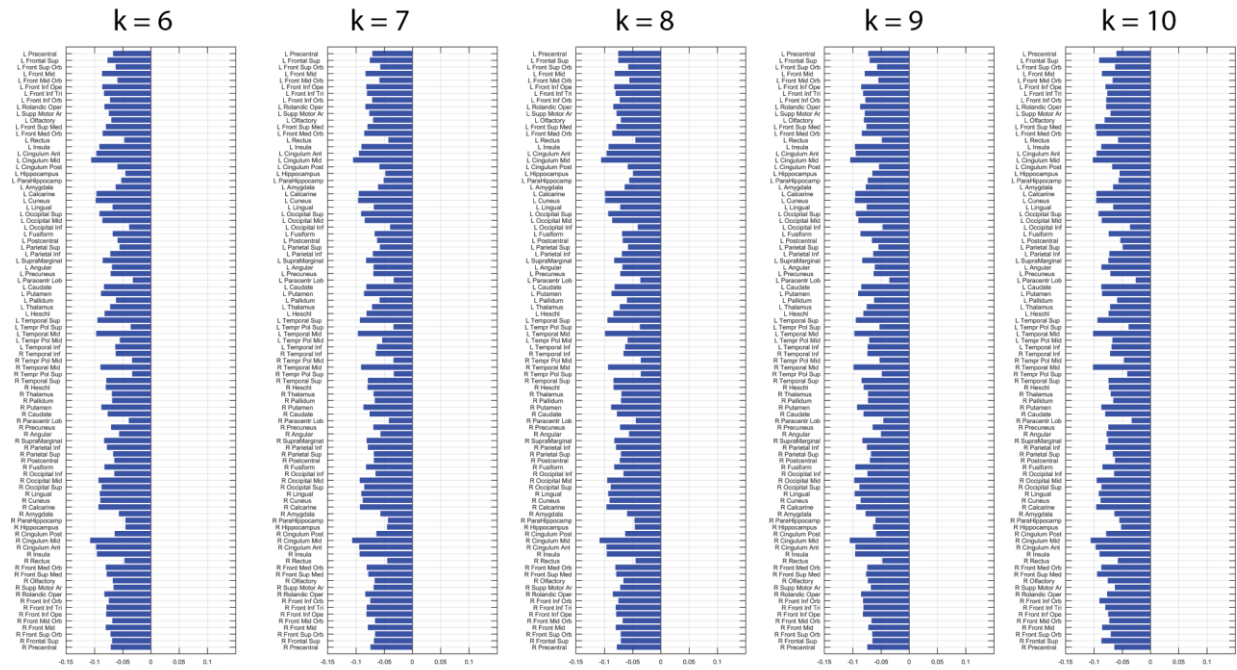
Figure S2: Bar chart representing contributions of each of the N=90 AAL brain areas to the globally coherent state of interest ($V_c(n)>0$ in red, blue otherwise) across clustering solutions k = 6 through k = 10. In each clustering solution, the probability of occurrence of this state was higher following the psilocybin injection, surviving the Bonferroni correction for k = 7 and k = 10. We note that prior to the Bonferroni correction, all the p-values were significant ($\alpha = 0.05$). The Bonferroni-corrected p-values (i.e. p-val * k) were: 0.13 (k = 6); 0.047 (k = 7); 0.14 (k = 8); 0.10 (k = 9); 0.032 (k = 10). Regional contributions to the cluster centroid of interest show a high level of consistency across the clustering solutions.
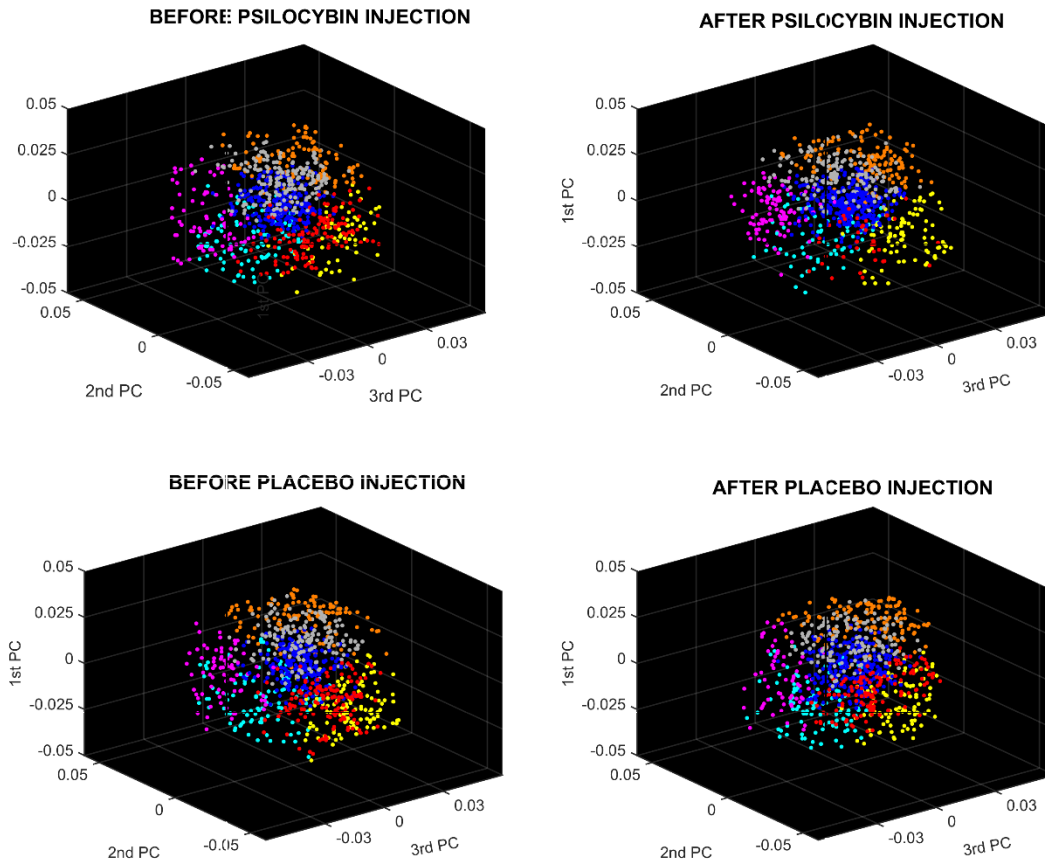
Figure S3 - 3D embedding of FC patterns (different projection angle). Identical results as in Fig. 3 in the main text, displayed using a different perspective of the same 3D scatter plots.

	I	II	III	IV	V	VI	VII
I		0.399	0.408	0.000	0.285	0.095	0.146
II	0.082		0.216	0.261	0.499	0.114	0.095
III	0.184	0.006		0.355	0.069	0.079	0.069
IV	0.217	0.426	0.002		0.247	0.077	0.041
V	0.006	0.171	0.038	0.145		0.366	0.380
VI	0.173	0.285	0.250	0.055	0.116		0.198
VII	0.042	0.494	0.040	0.176	0.397	0.388	

Table ST1 - The *p*-values for each entry of the switching matrix shown in Figure 5 of the main text.

Bipartition based on the leading eigenvector of the coherence matrix

In this section, we will show that a bipartition based on the signs of the entries of the leading eigenvector of the coherence matrix is optimal to produce two communities C_1 and C_2 where coherence is maximised within and minimised between. We will follow very closely the prior works of Newman and colleagues (1, 2).

Let us first define the coherence matrix B^1 at time t:

$$B_{ij}(t) = \cos\left(\theta_i(t) - \theta_j(t)\right).$$

As it is a symmetric, real valued matrix, the spectral theorem applies and thus, for each time t, there exists an eigenbasis $\{v_i\}_{i=1}^N$, with associated eigenvalues $\{\lambda_i\}_{i=1}^N$, where N is the number of ROIs. We also define a community indicator variable s_i such that :

$$s_i = \begin{cases} 1, & if \ i \in C_1 \\ -1, & if \ i \in C_2 \end{cases}.$$

The aim is to make the within community coherence higher than the between communities coherence, i.e. group nodes that have similar phases and maximise the difference between the two communities average phases. To formalise this, we define the following quantity:

$$P = \sum_{i,j} \left(\cos(\theta_i(t) - \theta_j(t))\right) \left(s_i s_j + 1\right)/2$$

that we will aim to maximise.

The only difference with Newman's derivation is presence of the constant term $A = \sum_{i,j}\left(\cos(\theta_i(t) - \theta_j(t))\right)/2$, and we can rewrite P as:

$$P = \frac{1}{2}\sum_{i,j}\left(\cos(\theta_i(t) - \theta_j(t))\right)s_i s_j + A,$$

---

[1] We use B instead of dFC, as in the main text, for the readability of the equations.

and rewriting the first term in matrix notation reads :

$$P = s'Bs + A,$$

with $'$ denoting the transposition operation. We now express B and s in the eigenbasis of B :

$$B = \sum_i \lambda_i v_i v_i', \qquad s = \sum_i a_i v_i,$$

and can now rewrite P as :

$$P = \sum_{i,j,k} a_i v_i' \lambda_i v_j v_j' a_k v_k$$
$$= \sum_i a_i^2 \lambda_i$$
$$= \sum_i (s'v_i)^2 \lambda_i,$$

where we used the orthonormality of the eigenvectors and $a_i = s'v_i$.

It is easy to see that $s'v_i$ will be maximised if :

$$s_j = \begin{cases} 1, & if\ v_i^j \geq 0 \\ -1, & if\ v_i^j < 0 \end{cases}.$$

Finally, we order the eigenvalues such that $\lambda_1 \geq \cdots \geq \lambda_N$, thus P is maximised if the signs of s are set based on the eigenvector corresponding to v_1, the leading eigenvector.

Proportion of coherence explained by the leading eigenvector

Let us first define the coherence matrix B^2 at time t:

---

[2] We use B instead of dFC, as in the main text, for the readability of the equations.

$$B_{ij}(t) = \cos\left(\theta_i(t) - \theta_j(t)\right).$$

As it is a symmetric, real valued matrix, the spectral theorem applies and thus, for each time t, there exists an eigenbasis $\{v_i\}_{i=1}^N$, with associated eigenvalues $\{\lambda_i\}_{i=1}^N$

$$B(t) = \sum_i \lambda_i v_i v_i' = \sum_i \lambda_i P_i = V\Lambda V',$$

where N is the number of ROIs ,the columns of V are the eigenvectors of B, Λ is the diagonal matrix of eigenvalues and P_i is the projector onto the subspace spanned by v_i. We order the eigenvalues in decreasing order : $\lambda_1 \geq \cdots \geq \lambda_N$.

Using Principal Component Analysis (PCA), we can quantify the variance explained by each eigenspace of B, and thus the proportion of the signal explained by the leading eigenvector.

The entries of the ith column of B are the similarities between the phase of the ROI i and the others ROIs. We center the phases of B by removing the mean, and refer to quantities related to the centered similiarities with a subscript c :

$$B_c = B - \mathbf{1}B_{mc}',$$

where B_{mc} is the vector of the mean of the columns of B. Thus $B_c'B_c$ is the covariance matrix of the centered similarities between each pair of phases. Using standard PCA, we have :

$$B_c'B_c(i) = V_c\Lambda_c V_c'V_c\Lambda_c V_c' = V_c\Lambda_c^2 V_c' \Leftrightarrow V_c'B_c'B_c V_c = \Lambda_c^2.$$

The ratio $\lambda_{c,i}^2 / \sum_j \lambda_{c,i}^2$ is then the proportion of the total variance in the similarities of the phases captured by the ith eigenspace. As the eigenvalues are ordered in decreasing order, the space associated with $\lambda_{c,1}$ will explain the most variance, and if $\lambda_{c,1}^2 > \sum_{i>1} \lambda_{c,i}^2$, it explains most of the variance in the similarities between phases.
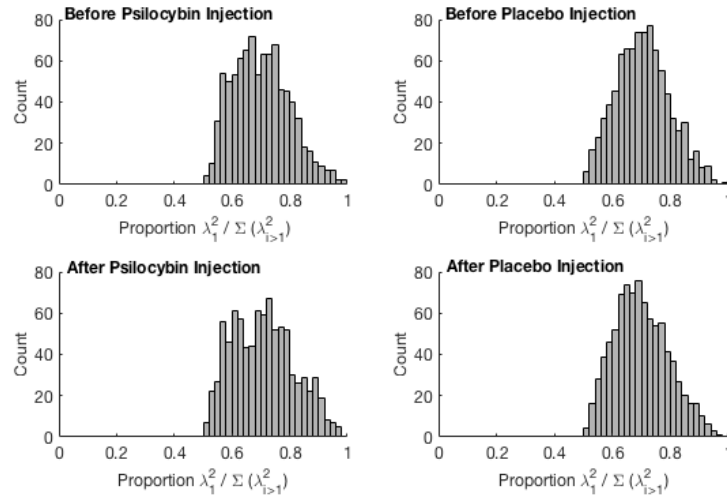
SI Figure 1. The leading eigenvector captures most of the variance in the similarities between phases at all time points. Histograms of the ratio of the leading eigenvalue with respect to the sum of all eigenvalues at each time point, for all subjects in each of the 4 experimental conditions. We find consistently that the leading eigenvalue represents more than 50% of all eigenvalues, thus confirming that $\lambda_1^2 > \sum_{i>1} \lambda_i^2$.

References

1.   Newman ME. Finding community structure in networks using the eigenvectors of matrices. Physical review E. 2006;74(3):036104.
2.   Newman ME. Modularity and community structure in networks. Proceedings of the national academy of sciences. 2006;103(23):8577-82.