No energy transport without discord

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(Dated: October 20, 2015)

Quantum systems can be correlated in ways that classical systems can not. A wide variety of non-classical forms of correlation exist [1–15]: amongst the best known are entanglement [1] and discord [2–5, 9, 10]. Quantum correlations can be used to enhance measurement accuracy [16] and energy transport [17–19]. This paper shows that quantum correlations – in the form of discord – are mandatory for any energy transport. Without discord, energy transport cannot occur. Moreover, we show that the initial rate of heat transfer between two systems prepared at different temperatures is directly proportional to the rate of increase in diagonal/energetic discord [14] between the systems. We measured the increase of energetic discord induced by nanoscale heat flow across an aluminum-sapphire interface. The rate of increase of discord is measured to be $4.28 \times 10^{24}$ bits m$^{-2}$ K$^{-1}$ s$^{-1}$.

Discord measures the difference between quantum mutual information and the classical mutual information between measurement results. Diagonal discord is discord defined by measurement made in the diagonal basis for subsystems [14]: the discord $D(A \rightarrow B)$ measures the minimum reduction in correlation between two quantum systems, $A$ and $B$, induced by measurements made on $A$ [2–5, 9, 10]. Similarly, $D(B \rightarrow A)$ measures the minimum reduction in correlation induced by measurements made on $B$. Because of the minimization, discord can be difficult to calculate. A natural and more easily calculated version of discord is diagonal discord [14] – the reduction in correlation when $A$ and $B$ are measured in the bases that diagonalize the density matrices for $A$ and $B$. In the case of thermal states, diagonal discord is the ‘energetic’ discord defined by measurement in the energy eigenbasis. As a consequence, diagonal discord has a direct interpretation in terms of flows of energy and entropy, and can be determined directly from measurement.

Our first result is that the presence of discord – ordinary or diagonal – is a prerequisite for any non-trivial interaction between systems. In particular, we prove the following

**Theorem 1.** Consider two quantum systems $A$ and $B$ evolving continuously from an initial state $\rho_{AB}(0)$ under a unitary time evolution $U_{AB}(t)$. If the discord from $A$ to $B$ and from $B$ to $A$ is zero for all times $t$, then the time evolution for $A$ and $B$ can always be written as

$$\rho_{AB}(t) = U_{A}(t) \otimes U_{B}(t) \rho_{AB}(0) U_{A}^{\dagger}(t) \otimes U_{B}^{\dagger}(t).$$

In other words, a system with zero two-way discord is effectively non-interacting.

The proof of this theorem is given in the supplementary material. The proof is by and large straightforward but possesses two subtleties. First, the theorem requires that the time evolution evolves continuously from the identity transformation, i.e., $U(0) = I$. Discontinuous transformations such as the SWAP operator that interchanges the states of $A$ and $B$ need not generate discord, but if such transformations are the end result of a continuous unitary time evolution, then discord must be generated somewhere along the way. The second subtlety arises in the case when the initial density matrix is degenerate, so that its eigenvalues are the same on some subspace. In this case, the actual physical unitary evolution can induce couplings within the degenerate subspace: but because the subspace is degenerate, the time evolution is always equivalent to non-interacting dynamics as in the theorem. This implies our second result, that energy transport cannot take place in the absence of discord. In particular, consider two systems $A$ and $B$ with joint Hamiltonian $H_{AB}$. The proof of the theorem implies that on subspaces where $\rho_{AB}$ is non-degenerate, $H_{AB} = H_{A} + H_{B}$: there is no interaction and no energy transfer. Conversely, within degenerate subspaces, we can have interaction, but the degeneracy of these subspaces precludes energy transport. There is no energy transport without discord.

Since energy transport must generate quantum correlations, we can ask how much discord is generated when energy is transported. In fact, as we now show, the rate of quantum heat transport is directly proportional to the creation of a particular kind of discord. The diagonal discord $D_{\text{diag}}(A \rightarrow B)$ is the reduction in correlation between $A$ and $B$ when $A$ is measured in its Schmidt basis – the basis in which $\rho_{A}$ is diagonal. Similarly, $D_{\text{diag}}(B \rightarrow A)$ is the reduction in correlation between $A$ and $B$ when $B$ is measured in its Schmidt basis. Diagonal discord is a natural measure of quantum correlation that measures how much quantum mutual information is
lost when \( A \) and \( B \) are measured in their diagonal bases. Because the Schmidt basis measurement is not necessarily the measurement that yields the maximum mutual information, diagonal discord is greater than or equal to the ordinary discord. By the proof of the theorem above, however, non-zero diagonal discord implies non-zero discord. Most important, because thermal states are diagonal in the energy eigenbasis, diagonal discord has a direct physical interpretation in terms of energy flow and entropy increase, and the resulting energetic discord can be measured experimentally.

Suppose that the initial states of \( A \) and \( B \) are thermal states at temperatures \( T_A, T_B, T_A > T_B \). In the supplementary material we show that the flow of heat from \( A \) to \( B \) over a sufficiently short time \( \Delta t \) is

\[
\Delta E_B = k \frac{T_A T_B}{T_A - T_B} \Delta D_{\text{diag}}(B \to A),
\]

where \( k \) is Boltzmann’s constant, and \( \Delta D_{\text{diag}}(B \to A) \) is the change in the diagonal discord. Writing \( \beta_A = 1/kT_A = \Delta S_A/k\Delta E_A, \beta_B = 1/kT_B = \Delta S_B/\Delta E_B \), we see that \( \Delta D_{\text{diag}}(B \to A) = \Delta E_B(\beta_B - \beta_A) \) is just the increase in entropy induced by the heat transfer. (When system \( B \) is at zero temperature the rate of increase of entropy initially diverges.) Indeed, this interpretation of the increase in diagonal discord follows directly from its definition: in the weak coupling limit the density matrices for \( A \) and \( B \) remain diagonal in the energy eigenbasis, and diagonal discord is the increase in the entropy of \( AB \) when a measurement of energy is made on \( A \) or \( B \). We conjecture that in this particular case – short time interaction between initially uncorrelated thermal states – diagonal discord is in fact equal to discord. However, the maximization over all possible measurements inherent in the definition of discord makes this conjecture, if true, nontrivial to prove.

As a simple example, consider two two-level systems (qubits) such as spins or two-level atoms, each with the same energy spacing, and with an exchange coupling. This model can be solved analytically (see supplementary material): it is a simple tunneling model in which the state of \( A \) is continuously swapped with the state of \( B \). If the two systems are initially in thermal states at different temperatures, \( T_A > T_B \), the initial heat flow from \( A \) to \( B \) and the rate of creation of diagonal discord can be easily calculated and obey Eq. (2). Interestingly, the maximum rate of energy transport occurs halfway through the tunneling process, which coincides with the point of maximum diagonal discord between \( A \) and \( B \). In fact, the coincidence of the point of maximum energy transport with maximum generation of discord suggests a relationship between the creation of quantum correlations and environmentally assisted quantum transport [17–19]: transport is maximized when the time over which coherent correlations can build up (the localization time) is matched with the time over which the environment effectively measures the state of the system (the decoherence time).

**Experimental quantification of increase in discord.**—Equation (2) shows that we can directly determine the rate of increase in diagonal discord by measuring ultrafast transient heat flow in nanoscale transport experiments [20, 21]. We measured the rate of creation of diagonal discord induced by nanoscale heat transfer across an aluminum-sapphire interface. The measurement directly determines the rate of increase in diagonal discord \( \Delta E_B(1/kT_B - 1/kT_A) = \Delta D_{\text{diag}}(B \to A) \) per square meter per second. The technical details of the experiment are given in the supplementary material. A femtosecond laser pulse deposits energy in a thin film of aluminium on a sapphire substrate. In the vicinity of the laser spot, the electrons in the aluminium rapidly thermalize over a time scale \( t_{\text{tr}} \approx 100 \) fs that is much shorter than the time scale \( t_s \approx 50 - 100 \) ps of initial energy transfer to the sapphire (see Fig. 1). The temperature of the aluminium at the center of the spot is monitored by reflectivity as shown in Fig. 1. Combining the change in temperature with the known specific heat of aluminium allows a determination of the rate of heat transfer from the aluminium to the sapphire substrate.

Because the film is thin (\( \sim 70 \) nm), the primary mode of heat loss from the spot is from propagation from the aluminium to the sapphire. The change in energy per unit area per unit time of the hot spot on the aluminium is given by \( \Delta E/\Delta x^2 \Delta t = \theta C \Delta T_A/\Delta t \), where \( C \) is the specific heat of aluminium per unit volume, \( \theta \) is the film
thickness, and $\Delta T_A$ is the change in the temperature of the aluminum over time $\Delta t$. The change in diagonal discord per unit area per unit time is then

$$\frac{\Delta D}{\Delta x^2 \Delta t} = \theta C \frac{\Delta T_A}{\Delta t} \left( \frac{1}{kT_B} - \frac{1}{kT_A} \right)$$

$$= \theta C \left( \frac{T_A}{T_B} - 1 \right) \frac{1}{\Delta T_A} \frac{\Delta T_A}{\Delta t},$$

(3)

where $T_B$ is the temperature of the sapphire. Using the data as shown in figure 1, we obtain a value for $\Delta D/\Delta x^2 \Delta t$ of $4.28 \times 10^{24}$ bits m$^{-2}$ K$^{-1}$ s$^{-1}$.

**Discussion.**—At bottom, all systems are quantum mechanical. But some systems behave in a more quantum mechanical way than others. This letter addressed the role played by quantum coherence in interaction and energy transport. We showed that quantum correlations are mandatory for energy transport: without quantum discord, energy transport cannot occur. In addition, we provided a simple criterion for quantifying the amount of discord, energy transport cannot occur. We showed that quantum correlations play a role in interaction and energy transport. We showed that quantum mutual information measures the total amount of correlation between energy transport and quantum correlation opens the way to direct experimental measurement of quantum correlations during heat transfer. We measured the rate of creation of discord due to nanoscale heat transfer across an aluminum–sapphire interface and determined it to be $4.28 \times 10^{24}$ m$^{-2}$ K$^{-1}$ s$^{-1}$.

**Acknowledgements.**—This work was supported by DARPA, ARO under a MURI program, the MIT Energy Initiative, and Jeffrey Epstein.

[1] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, 2000).

**SUPPLEMENTARY MATERIAL**

Here we review the definition of quantum discord, provide a proof of the main theorem, and show that energy flow is proportional to the rate of increase of discord. The details of the experiment are presented.

**Definition of discord**

To define discord consider a joint quantum system $AB$ described by a density matrix $\rho_{AB}$. The systems $A$ and $B$ considered individually are described by reduced density matrices $\rho_A = \tr_B \rho_{AB}$, $\rho_B = \tr_A \rho_{AB}$ respectively, where $\tr_{A,B}$ represents the partial trace over $A,B$. The quantum mutual information $I(A : B) = I(A) - I(AB)$ is defined to be the difference between the information of $A$: $I(A) = -\tr A \ln \rho_A$ and the quantum conditional information $I(A|B) = -\tr_{A|B} \ln \rho_{AB} + \tr_B \ln \rho_B$. The quantum mutual information measures the total amount of correlation.
between A and B. Discord compares the quantum mutual information with the mutual information obtained when a measurement is made on B. Consider a measurement made on B alone. The measurement has outcomes b with probabilities p(b), and the state of A given the outcome B is \( \rho(A|b) \). The mutual information between A and the results of this measurement on B is equal to \( I(A:B) = I(A) - \sum_b p(b) I(A|b) \), where \( I(A|b) = -\text{tr} \rho(A|b) \ln \rho(A|b) \).

The quantum discord is defined to be the minimum difference between the quantum mutual information and the mutual information given a measurement on B:

\[
D(B \rightarrow A) = I(A:B) - \max I(A: \hat{B}),
\]

where the maximum is taken over all possible measurements on B. The symmetric discord is the minimum difference between the quantum mutual information and the maximum classical mutual information of the results of measurements made on both A and B [22].

Define the diagonal discord \( D_{\text{diag}}(B \rightarrow A) \) to be the difference between the quantum mutual information and the mutual information given a measurement of B consisting of rank one projectors onto the states of the Schmidt basis: that is, we measure B in the basis with respect to which \( \rho_B \) is diagonal. (If \( \rho_B \) has degenerate eigenvalues we use the basis for the degenerate subspace that minimizes the entropy increase.) Clearly, \( D_{\text{diag}}(B \rightarrow A) \geq D(B \rightarrow A) \).

Like ordinary discord, diagonal discord is a natural measure of quantum correlation, that quantifies the reduction in mutual information induced by measurement. But because we let the state \( \rho_B \) define the measurement to be made, diagonal discord is (much) easier to calculate than ordinary discord. In addition, as will be seen below, diagonal discord has a natural physical interpretation and can be measured directly by experiment.

**Proof of the main theorem**

Zero discord from A to B, \( D(A \rightarrow B) = 0 \), implies that

\[
\rho_{AB}(t) = \sum_j p_j |j(t)\rangle_A \langle j(t)| \otimes \rho_B^j(t),
\]

where \( |j(t)\rangle_A \) is the Schmidt basis for A at time t, i.e., the basis with respect to which \( \rho_A(t) \) is diagonal, and \( \rho_B^j(t) \) is a density matrix for B [10]. Similarly, zero discord from B to A implies that

\[
\rho_{AB}(t) = \sum_k p_k \rho_A^k \otimes |k(t)\rangle_B \langle k(t)|,
\]

where \( |k(t)\rangle_B \) is the Schmidt basis for B. The simple intuitive criterion for zero discord from A to B is that measuring/decohering A in the Schmidt basis leaves the density matrix for \( \rho_{AB} \) unchanged. As a consequence, the set of states with zero diagonal discord and the set of states with zero discord are the same.

Zero symmetric discord implies that measurement of both A and B in their Schmidt bases leaves \( \rho_{AB} \) unchanged. Equations (S2,S3) then immediately imply that \( \rho_B^j(t) \) is diagonal in the Schmidt basis for B, for all j, and \( \rho_A^k(t) \) is diagonal in the Schmidt basis for A. In other words, at all times t the density matrix

\[
\rho_{AB}(t) = \sum_{jk} p_{jk} |j(t)\rangle_A \langle j(t)| \otimes |k(t)\rangle_B \langle k(t)| = U_A(t) \otimes U_B(t) \rho_{AB}(0) U_A^\dagger(t) \otimes U_B^\dagger(t),
\]

where \( U_A(t), U_B(t) \) transform the Schmidt bases of A,B at time 0 to time t: \( |j(t)\rangle_A = U_A(t) |j(0)\rangle_A, |k(t)\rangle_B = U_B(t) |k(0)\rangle_B \). This proves the theorem: zero symmetric discord implies that A and B are effectively uncoupled.

Equation (S4) implies that, to preserve zero symmetric discord, the effective Hamiltonian for A and B must be of the form \( H = \hat{H}_A \otimes I_B + I_A \otimes \hat{H}_B \). Indeed, for short times \( \Delta t \), write \( U_A(\Delta t) = e^{-i\hat{H}_A \Delta t}, \) and \( U_B(\Delta t) = e^{-i\hat{H}_B \Delta t} \).

Expanding to first order in \( \Delta t \), we have

\[
(H_A \otimes I_B + I_A \otimes H_B + H_{AB}) |i\rangle_A |j\rangle_B = (\hat{H}_A \otimes I_B + \hat{I}_A \otimes \hat{H}_B) |i\rangle_A |j\rangle_B,
\]

for all \( |i\rangle_A |j\rangle_B \). In other words, \( H_{AB} = (\hat{H}_A - H_A) \otimes I_B + I_A \otimes (\hat{H}_B - H_B) \), and the two systems are effectively non-interacting.
Heat flow is proportional to diagonal discord

Now we prove that when \(A\) and \(B\) are initially prepared in thermal states at different temperatures, the rate of energy flow from \(A\) to \(B\) is directly proportional to the rate of generation of diagonal discord. The initial density matrix for \(AB\) is \(\rho_{AB} = Z_A^{-1} e^{-H_A/kT_A} \otimes Z_B^{-1} e^{-H_B/kT_B}\). The two systems are uncorrelated; the Schmidt bases for \(A\) and \(B\) are their energy eigenbases; and the discord and diagonal discord are zero. Over a brief period of time \(\Delta t\), \(\rho_{AB}\) evolves to \(\rho_{AB} + \Delta \rho_{AB} = U(\Delta t)\rho_{AB} U(\Delta t)\). For example, we can take \(U(\Delta t) = e^{-iH\Delta t}\), where \(H = H_A + H_B + H_{AB}\), and expand the time evolution to second order in \(\Delta t\) (to first order in \(\Delta t\) there is no energy transfer). Conservation of energy and weak coupling imply that \(A\) and \(B\) are still diagonal in their energy eigenbases. The increase in the diagonal discord over time \(\Delta t\) is the difference between the quantum mutual information between \(A\) and \(B\) at time \(\Delta t\) and the mutual information when \(B\)'s energy is measured:

\[
\Delta D_{\text{diag}}(B \rightarrow A) = I_{\Delta t}(A : B) - I_{\Delta t}(A : \tilde{B}).
\]  

This expression for the change in energetic discord can be simplified. Because the time evolution is unitary, we have \(\Delta I(AB) = 0\). The infinitesimal change in entropy \(I = -\text{tr} \rho \log \rho\) when \(\rho \rightarrow \rho + \Delta \rho\) is \(\Delta I = -\text{tr} \Delta \rho \log \rho\). Using this relationship and noting that \(\rho_B\) is already diagonal in the energy eigenbasis, we have \(\Delta I(B) = \Delta I(\tilde{B})\). Substituting these relations into Eq. \(S7\) yields

\[
\Delta D_{\text{diag}}(B \rightarrow A) = \Delta I(\tilde{A}B) = -\text{tr} \Delta \rho_{A\tilde{B}} \log \rho_{AB}.
\]  

Note that the thermal form of the initial state implies that \(\rho_{AB} = \rho_{A\tilde{B}}\). Substituting the thermal state into Eq. \(S8\) yields

\[
\Delta D_{\text{diag}}(B \rightarrow A) = (\text{tr} H_A \Delta \rho_A)/kT_A + (\text{tr} H_B \Delta \rho_B)/kT_B = \Delta E_A/kT_A + \Delta E_B/kT_B,
\]  

where \(\Delta E_A\) is the change in energy of \(A\) and \(\Delta E_B\) is the change in energy of \(B\). In the weak coupling limit, we have \(\Delta E_A = -\Delta E_B\), and so the change in diagonal discord is

\[
\Delta D_{\text{diag}}(B \rightarrow A) = (1/kT_B - 1/kT_A)\Delta E_B,
\]  

and the energy flow from \(A\) to \(B\) is

\[
\Delta E_B = k\frac{T_A T_B}{T_A - T_B} \Delta D_E(B \rightarrow A).
\]

The flow of energy between two systems at different temperatures is proportional to the instantaneous increase of discord.

**A simple example**

Consider two two-level systems such as spins with Hamiltonian \(H = (\hbar/2) (-\omega \sigma_z^A - \omega \sigma_z^B + \gamma (\sigma_+^A \otimes \sigma_-^B + \sigma_+^A \otimes \sigma_+^B))\). This is a simple swapping Hamiltonian that induces the continuous time tunneling evolution

\[
\begin{align*}
|0\rangle_A |0\rangle_B & \rightarrow e^{i\omega t}|0\rangle_A |0\rangle_B \\
|1\rangle_A |1\rangle_B & \rightarrow e^{-i\omega t}|1\rangle_A |1\rangle_B \\
|0\rangle_A |1\rangle_B & \rightarrow \cos \gamma t/2 |0\rangle_A |1\rangle_B - i \sin \gamma t/2 |1\rangle_A |0\rangle_B \\
|1\rangle_A |0\rangle_B & \rightarrow \cos \gamma t/2 |1\rangle_A |0\rangle_B - i \sin \gamma t/2 |0\rangle_A |1\rangle_B
\end{align*}
\]  

(S12)
The spins are prepared in thermal states at different temperatures, so that \( \rho_{AB}(0) = Z_A^{-1} e^{i \omega_1^A z \sigma^z_A / kT_A} \otimes Z_B^{-1} e^{i \omega_1^B z \sigma^z_B / kT_B} \). The energy transfer from \( A \) to \( B \) is due to the continuous swapping within the 01, 10 subspace. It is straightforward to verify that the initial energy transfer over time \( \Delta t \) obeys Eq. (2) of the text and Eq. (S11) of the supplementary material.

The continuous tunneling dynamics implies that the amount of energy transfer is proportional to \( \sin^2 \gamma t / 2 \), which reaches its maximum rate at \( \gamma t = \pi / 2 \), halfway through the tunneling process. Because of the sinusoidal nature of the tunneling dynamics, the energetic discord also rises to its maximum value at this point. The energetic discord then decreases, reaching zero when \( \gamma t = \pi \), the point at which the states of \( A \) and \( B \) have been swapped, so that \( B \) is in a thermal state at temperature \( T_A \) and \( A \) is in a thermal state at temperature \( T_B \).

**Experimental details**

We performed a thermal transport experiment between a bilayer structure of aluminum film and sapphire substrate is performed (Fig. 1). A laser pulse was used to heat the aluminum within ultrafast time period (\( \sim 200 \) fs), and the surface temperature change of aluminum was monitored by reflectivity. The experiment is in the weak coupling limit, where external heat dissipations can be ignored due to small temperature excitation (\( \sim 0.2 \) K) and ultrafast time-domain measurement (\( \sim 6 \) ns).

The normalized surface temperature of aluminum versus time is plotted in Fig. 1. The curve can be divided into two regimes. In the first \( \sim 60 \) ps, the thermal excitation is localized inside the aluminum film, resulting in an equilibration process between electron and lattice of aluminum. After \( \sim 60 \) ps, heat flows from aluminum to sapphire and the thermal transport can be described by Fourier Law. At the crossing point between the regimes, the thermal state of the sample is shown in the schematic inset: at this point, the aluminum temperature is increased to \( T_A = 300.2 \) K, while the sapphire remains at \( T_B = 300.0 \) K. For the Fourier fitting, the energy flow rate can be calculated to be \( (\Delta E_B) = 1.92 \times 10^8 \) W m\(^{-1}\) K\(^{-1}\). From Eq. (S10), the change in diagonal discord is \( 4.28 \times 10^{24} \) bits m\(^{-2}\) K\(^{-1}\) s\(^{-1}\).