A Steady State Thermodynamic Entanglement Witness

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We present a method for entanglement detection in steady state systems using a thermodynamic witness. To illustrate, we consider an example and find that for an XX spin chain, the presence of an energy current increases the region of entanglement detected by the steady state witness. Further, we find that entanglement exists even at a high steady state temperature. We also discuss concurrence in the steady state system and find that the amount of entanglement can be increased by the current.

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Entanglement is one of the most fascinating aspects of quantum physics and is an important resource in the field of quantum information. While a separable state can be written as a convex sum of pure product states, \( \sigma = \sum_i p_i \sigma_i^1 \otimes \sigma_i^2 \otimes \cdots \otimes \sigma_i^n \), an entangled state cannot. Many-body entanglement is not easy to quantify; however, attempts have been made to provide a framework for many-body entanglement [1].

During dynamical processes, no equivalent formulation for nonequilibrium thermodynamics exists at present. While thermal pairwise entanglement can be measured using concurrence, measuring multipartite entanglement is a difficult task. Entanglement witnesses are a useful alternative to these measures. An entanglement witness is an expectation value of an operator for which a bound can be found for any separable state.

The subject of quantum thermodynamics has already contributed to the success of entanglement witnesses [2, 3]. For example, magnetic susceptibility can witness entanglement [2], as can an average over the nonequilibrium work done during a process [3]. At present, thermodynamic witnesses are used to detect entanglement in equilibrium systems. Our aim is to extend the success of equilibrium entanglement witnesses to nonequilibrium steady state systems.

In this letter, we demonstrate how a steady state entanglement witness can be found. Specifically, we find a steady state thermodynamic quantity, a current, which can detect entanglement in steady state systems. We consider an XX spin chain in the thermodynamic limit to exemplify this witness and find that the introduction of an energy current increases the region of entanglement detected. In order to gain insight into whether the entanglement itself increases with the driving field, we also calculate the chain’s correlation functions and use them to determine the nearest and next nearest neighbour concurrence. We discover that the concurrence can be increased by the presence of the energy current.

Thermodynamics has been used in many areas of physics. It is limited to equilibrium systems, although some thermodynamic concepts such as work done apply during dynamical processes. No equivalent formulation for nonequilibrium thermodynamics exists at present. However, attempts have been made to provide a framework for steady state thermodynamics since these systems are time independent and simpler to investigate than the general out of equilibrium case. There are also methods by which steady state systems can be modeled.

In particular, the Hamiltonian of an equilibrium system can be modified to allow a steady state current passing through the system to be described [4, 5]. In this way, nonequilibrium steady state systems can be mapped onto equilibrium systems. For an energy current, this is achieved by defining the operator of the current using continuity equations, \( \partial h(x, t)/\partial t + \partial j(x, t)/\partial x = 0 \) where \( h(x, t) \) is the energy density operator and \( j(x, t) \) is the heat flux operator. For a chain with \( N \) sites, the discrete form of this is \( dh_l/dt = j_{l-1} - j_l \), and the left hand side can be written \( dh_l/dt = i[H, h_l] \). For one dimensional systems \( H_0 = \sum_{l=1}^N (h_l^0 + V(l, l + 1)) \), this has been shown to be [12]

\[
\begin{align*}
    j_l &= \frac{i}{2} \left( [h_l^0 - h_{l+1}^0, V(l, l + 1)] + [V(l, l + 1), \right. \\
    &\left. V(l + 1, l + 2)] + [V(l - 1, l), V(l, l + 1)) \right). \tag{1}
\end{align*}
\]

Here, \( h_l^0 \) is the non-interacting part of the Hamiltonian, and \( V(l, l + 1) \) is the interaction. The energy current operator is \( J^E = \sum_l j_l \) and can be incorporated into the Hamiltonian formalism using a Lagrange multiplier, \( \lambda \), so that we have \( H = H_0 - \lambda J^E \). In the case that \([J^E, H_0] = 0\), and \( H_0 \) can be diagonalised analytically, the total Hamiltonian \( H \) can also be diagonalised using the same method.

We note that the origin of the steady state current is not important when using this method. That is, the current is given by Eq. (1) whether it is induced by an external driving field or by a reservoir [13]. For example, the steady state could be achieved by holding opposite ends of an open spin chain at different, constant, temperatures, but the formalism above is not limited to this scenario.

Using Eq. (1) the ground state correlation functions of an Ising spin chain have been investigated [13, 14]. Also at zero temperature, a steady state XX spin chain with an energy current increases the entanglement present [10]...
compared to the equilibrium case, and quantum state transfer can be improved [17]. In this letter, we take this formulation of steady state systems into the thermal regime using the method outlined below.

It is possible to construct a steady state thermal density matrix [18, 19] which is similar in form to the equilibrium case: $\rho = e^{-\beta H_0 - \gamma J^E}/Z$, where $Z = \text{tr}(e^{-\beta H_0 - \gamma J^E})$ is the steady state partition function. $J^E$ is the steady state energy current operator discussed above, and $\beta$ and $\gamma$ are Lagrange multipliers. $\beta = 1/T$ can be thought of as a generalised inverse temperature which is valid in steady state systems, while $\gamma = -\lambda \beta$ is the driving term of the energy current and has no analogue in equilibrium thermodynamics.

This definition of the steady state density matrix allows a nonequilibrium steady state entanglement witness of the form

$$W_{ss} = \zeta \frac{\partial}{\partial \gamma} \ln Z = \eta Q,$$

where $\zeta$ and $\eta$ are constants and $Q = \langle J^E \rangle = \text{tr}(J^E \rho)$ is the expectation value of the energy current, to be calculated. Thus we can detect entanglement in the steady state system using the energy current, a steady state quantity. We note that other currents, such as a magnetisation current, can be calculated in a similar way to that described above. Therefore other currents can be used to witness entanglement similarly to $Q$ in Eq. (2).

To illustrate how the witness works, we consider an XX spin chain in the thermodynamic limit,

$$H_{XX} = -\frac{J}{2} \sum_l (\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y) - B \sum_l \sigma_l^z,$$

where $J$ is the coupling strength between nearest neighbour sites and $B$ is an external magnetic field. Using Eq. (4) the energy current for $H_{XX}$ is

$$J^E = -BJ \sum_l (\sigma_l^y \sigma_{l+1}^x - \sigma_l^x \sigma_{l+1}^y)$$

+ $\frac{J^2}{2} \sum_l (\sigma_l^y \sigma_{l+1}^x \sigma_{l+2}^y - \sigma_l^x \sigma_{l+1}^y \sigma_{l+2}^x).$

We consider $J$ and $B$ to be positive throughout the letter. The total Hamiltonian, $H = H_{XX} + \frac{2}{\beta} J^E$ can be diagonalised [20] using a Jordan-Wigner transformation, $a_l = \prod_{m=-1}^{-l} a_m^z \otimes (\sigma_m^x - i a_m^y) / 2$ and a Fourier transform, $a_l = \sum_k e^{i \pi k l} \text{tr} \to H = \sum_k (2 \Lambda_k a_k^z a_k - 1B)$ where $\Lambda_k \to \Lambda(q) = (B - J \cos q) (2\gamma J \sin q + 1)$ as $N \to \infty$. Although we consider the thermodynamic limit, our method for calculating a steady state witness can be applied to a system of any size.

To aid in our later calculations for the witness, we introduce an extra term, $b_0$, into the Hamiltonian such that Eq. (3) becomes $H_{XX} = -\frac{J}{2} \sum_l (\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y) - b B \sum_l \sigma_l^z$. The total Hamiltonian, $H$, can again be diagonalised using the transformations described above. The partition function is thus $\ln Z = \frac{2\gamma}{\beta} \int_0^{2\pi} dq \ln[2 \cosh(\beta \xi(q))]$ where $\xi(q) = Bb - J \cos q + 2\gamma J \sin q$. Once the calculations are performed, we set $b = 1$ in order to recover the original system.

We now introduce two entanglement witnesses. The first is similar to existing witnesses, [3, 4] and is found by calculating the expectation value of the Hamiltonian and rearranging the resulting equation. The second is found using Eq. (4) and is a genuine steady state witness. We consider both to demonstrate why the steady state witness is important.

The first witness is

$$W_1 = 2 \left| \frac{U + BM - JQ}{JN} \right|$$

where $U = \langle H \rangle$ is the steady state equivalent of internal energy, $U = -\frac{\partial}{\partial \beta} \ln Z - \frac{\partial}{\partial \gamma} \ln Z$. The second term, $-\frac{\partial}{\partial \gamma} \ln Z$ is equivalent to $\frac{\partial}{\partial \beta} \ln Z$ and is contained in the final term in Eq. (5). We also have $-\frac{\partial}{\partial \beta} \ln Z = \frac{\partial}{\partial \beta} \ln Z \bigg|_{b=1}$ rather than by $\frac{\partial}{\partial \beta} \ln Z$, though each definition gives the same witness on appropriate consideration of the remainder of the expectation value of the Hamiltonian. Thus $M/N = \int_0^{2\pi} dq \tanh(\beta \Lambda(q))$.

The system is entangled when $W_1 > 1$. This bound is calculated using the expectation value, $|\langle \sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y |$), which is equal to Eq. (3). The bound is found for pure product states [2, 4] using the Cauchy-Schwarz inequality, $\sum_{l=1}^N (x_l y_l)^2 \leq \sum_{l=1}^N x_l^2 \sum_{l=1}^N y_l^2$ and the definition of a single site density matrix which leads to the inequality $\langle \sigma_l^x \rangle^2 + \langle \sigma_l^y \rangle^2 \leq 1$. Since the set of separable states is convex, this bound is also true for all separable states.

Fig. (1) shows the region of entanglement detected by witness $W_1$. It shows that increasing the driving quantity $\gamma$ increases the region of entanglement detected by the witness. This is an interesting result since it indicates that introducing an energy current increases the entangled region in this thermal system. That is, $\gamma$ increases which values of $B$, $T$ etc. the system is entangled for. In addition, we see that entanglement can exist even at high steady state temperatures with a large enough $\gamma$. However, witness $W_1$ is not easily experimentally measured since $U$ and $M$ are now steady state thermodynamic quantities and thus no longer correspond to clear
measurable quantities. Therefore, we use Eq. 2 to calculate a genuine steady state entanglement witness,

\[ W_{ss} = \frac{2|Q|}{JN(2B + J)}. \]  

Here we use the average energy current, \( Q \), itself to detect entanglement. Since \( Q \) is the expectation value of Eq. 5, we can again use the Cauchy-Schwarz inequality and the definition of the density matrix to find a bound for separable states. This leaves \( |Q| \leq BJN + \frac{D}{2} \sum_{|l\rangle} |\langle l| \rangle| \) for pure product states. For any pure product state, \( |\langle l| \rangle| \leq 1 \), hence we can rearrange the inequality and find that entanglement can be detected when \( W_{ss} > 1 \). The expectation value of the energy current is \( Q = \sum_{l} f_{l} dq(J \cos q - B) \sin q \tan h(\beta \Lambda(q)) \). The steady state witness is shown in Fig. 2. Again increasing \( y \) increases the region of entanglement detected, and entanglement is detected even at high steady state temperatures. For this witness, no region is detected at low values of \( B \) and \( T \), but an extra region exists when \( B \) is close to zero and higher \( T \). An interesting way to view this witness is to consider \( W_{ss} \) itself. It shows a large, absolute, expectation value of the energy current will detect entanglement (after scaling by the constant \( \eta = 2/|JN(2B + J)| \)).

How the expectation value of the energy current would be measured experimentally is dependent on the cause of the steady state. For example, for a spin chain in a constant temperature gradient, the heat conduction and hence \( Q \) can be experimentally determined [21].

By considering the concurrence, we can confirm that it is the amount of entanglement which increases with \( \gamma \).

Concurrence quantifies entanglement between two mixed qubits, and is given by \( C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4) \) where \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \). The \( \lambda_8 \)'s are the square roots of the eigenvalues of the matrix \( \rho \tilde{\sigma} \) where \( \tilde{\sigma} = (\sigma^y \otimes \sigma^y)(\sigma^y \otimes \sigma^y) \). Since \([H, \sum_{l} \sigma^z]\) = 0, the concurrence is given by \( C(\rho_{i+R}) = 2 \max\{|z| - \sqrt{vy}, 0\} \) [22] where \( z = (\langle \sigma_i^z \sigma_i^z \rangle + \langle \sigma_i^x \sigma_i^x \rangle - i(\langle \sigma_i^y \sigma_i^y \rangle - \langle \sigma_i^z \sigma_i^z \rangle))/4 \), \( vy = ((1 + \langle \sigma_i^z \sigma_i^z \rangle)^2 - 4 \langle \sigma_i^y \rangle^2)/16 \), and we have used that \( \langle \sigma_i^z \rangle = \langle \sigma_i^z \rangle_{i+1} \) due to the chain’s translational invariance.

We calculate each of the correlation functions following the method in [22], and calculate the nearest neighbour, \( R = 1 \), and next nearest neighbour, \( R = 2 \), concurrence. Generally,

\[
\langle \sigma_i^z \sigma_i^z \rangle + \langle \sigma_i^y \sigma_i^y \rangle = -2(\langle A_i \prod_{m=1}^{R-1} (A_{i+m} B_{i+m}) B_{i+R} \rangle + \langle B_i \prod_{m=1}^{R-1} (A_{i+m} B_{i+m}) A_{i+R} \rangle) - \langle \sigma_i^z \sigma_i^z \rangle_{i+R} = -ie^{i\pi R} \langle A_i \prod_{m=1}^{R-1} (A_{i+m} B_{i+m}) A_{i+R} \rangle + ie^{i\pi R} \langle B_i \prod_{m=1}^{R-1} (A_{i+m} B_{i+m}) B_{i+R} \rangle) = \langle A_i B_i A_i B_i \rangle + \langle \sigma_i^z \rangle = \langle A_i B_i \rangle \text{ where } A_i = (a_i^+ + a_i) \text{ and } B_i = (a_i^+ - a_i). \]

Using Wick’s theorem, we can rewrite each of these in terms of two point correlation functions. For example, the \( zz \) correlation function is \( \langle A_i B_i A_i B_i \rangle = G_{0} - G_{R} + S_{R} \) where we have defined \( G_{R} = \langle A_i B_i \rangle \) with \( G_{R} = -\langle B_i A_i \rangle \) and \( S_{R} = \langle B_i B_i \rangle = -\langle A_i A_i \rangle \).

Using the same method of diagonalisation as for the Hamiltonian, we can write \( \langle \sigma_i^z \rangle = \frac{1}{N} \sum_{k} (1 - 2d_i^k d_k) \). In addition, \( G_{R} = \frac{1}{N} \sum_{k} \cos \left( \frac{2\pi R}{N} \right) (1 - 2d_i^k d_k) \) and \( S_{R} = \frac{1}{N} \sum_{k} \sin \left( \frac{2\pi R}{N} \right) (1 - 2d_i^k d_k) \). Therefore, the thermodynamic expressions for \( G_{R} \) and \( S_{R} \) are found directly from the magnetisation, \( M/N = \langle \sigma_i^z \rangle \) calculated previously.
and c) and f) when $\gamma = 0$, b) and e) when $\gamma = 1$, and c) and d) when $\gamma = 2$. We have set $J = 1$ throughout.

\[
G_R = \int_0^{2\pi} \frac{dq}{2\pi} \cos(qR) \tanh(\beta \Lambda) \tag{7}
\]
\[
S_R = i \int_0^{2\pi} \frac{dq}{2\pi} \sin(qR) \tanh(\beta \Lambda). \tag{8}
\]

We plot the concurrence against the magnetic field and steady state temperature in Fig. 3. We find for nearest neighbour concurrence, Figs. 3 a), b) and c), that the amount and region of entanglement decreases with increasing $\gamma$, and also that the region of entanglement decreases. The amount and region of entanglement increases with $\gamma$ when $T$ and $B$ are higher. The plot coincides with both witnesses which detect entanglement at high $B$ and $T$. Fig. 4 shows that the witness also detects a region of entanglement at low $B$ and $T$ that decreases with increasing $\gamma$ which is reflected in Fig. 5. However, also detects a region of entanglement at low magnetic field, and higher $T$ and $\gamma$, which indicates this witness detects entanglement which cannot be categorised as nearest neighbour. Therefore we consider next nearest neighbour concurrence plotted in Fig. 6(d), e) and f). Both the amount and region of entanglement are reduced compared to nearest neighbour concurrence. The peak at low temperature remains constant for each value of $\gamma$, while as $\gamma$ is increased, new regions of entanglement appear at low temperature and higher magnetic field. Thus for next nearest neighbour entanglement, the introduction of an energy current again increases the amount of entanglement. However, this does not explain the region of entanglement at low $B$ and higher $T$ and $\gamma$ detected in Fig. 2. It would be interesting to determine the type of entanglement here.

We have introduced a nonequilibrium steady state entanglement witness and using an XX spin chain, have demonstrated how such a witness works. We have shown that introducing an energy current increases the entanglement detected in this system at high steady state temperature, and increases entanglement itself on consideration of the concurrence.

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