A Coupled Quantum Otto Cycle

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We study the 1-d isotropic Heisenberg model of two spin-1/2 systems as a quantum heat engine. The engine undergoes a four-step Otto cycle where the two adiabatic branches involve changing the external magnetic field at a fixed value of the coupling constant. We find conditions for the engine efficiency to be higher than the uncoupled model; in particular, we find an upper bound which is tighter than the Carnot bound. A new domain of parameter values is pointed out which was not feasible in the interaction-free model. Locally, each spin seems to effect the flow of heat in a direction opposite to the global temperature gradient. This seeming contradiction to the second law can be resolved in terms of local effective temperature of the spins.

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I. INTRODUCTION

Quantum generalisations of classical heat cycles have now been studied for some years. When the working medium is a few-level quantum system, new lines of enquiry open up due to additional features like discreteness of states, quantum correlations, quantum coherence and so on [1,2]. Many models have served to investigate the validity of second law of thermodynamics in the quantum regime [3,4]. The possibility of small scale devices and information processing machines [10] has generated further interest into the fundamental limits imposed on the heat generation, cooling power and thermal efficiencies achievable with these models [11-13]. Quantum analogues of Carnot cycles, Otto cycles and other brownian machines have been analysed [14,15]. Further, both infinite [2-4] and finite-time [16-22] thermodynamic cycles have attracted attention.

The quantum Otto cycle which occupies our interest here consists of a working substance with hamiltonian \( H \) and initial density matrix \( \rho \) being manipulated between two heat reservoirs (the reservoir temperatures satisfy \( T_1 > T_2 \)) under two adiabatic and two isochoric branches. On the adiabatic branches, the system is assumed to follow quantum adiabatic theorem and thermodynamic work is defined in terms of the change in energy levels at given occupation probabilities. If the hamiltonian is changed from \( H_1 \) to \( H_2 \) by controlling an external parameter then the work performed is defined as \( \text{Tr}[\rho(H_2 - H_1)] \). On the other hand, while traversing the isochoric branches, heat is exchanged with the reservoirs. Thus if the density matrix of the system changes from \( \rho_1 \) to \( \rho_2 \) for a given hamiltonian \( H \), then heat exchanged is \( \text{Tr}[(\rho_2 - \rho_1)H] \). As an example, for an effectively two-level system whose energy splitting can be varied from \( E_1 \) to \( E_2 \), the Otto efficiency has been found to be \( 1 - E_2/E_1 \), which is bounded from above by Carnot value due to the condition \( E_2/E_1 > T_2/T_1 \) [2].

Recently, some authors have studied the role of different quantum interactions using spin-1/2 particles in a Quantum Otto cycle [3,5]. In particular, the role of quantum entanglement has been conjectured using measure like concurrence and the second law has been shown to hold in such models. In this paper, we also investigate a coupled Otto engine using a 1-d Heisenberg model with isotropic exchange interactions between two spin-1/2 particles (see Eq. (1) below). In [3] the same model was analysed, where during the adiabatic steps, the exchange constant \( J \) was altered between two chosen values (\( J_1 \rightarrow J_2 \rightarrow J_1 \)), while keeping the external magnetic field at a fixed value. From an experimental point of view, it is also interesting to investigate a cycle where the exchange constant is fixed and only the magnetic field is varied during the adiabatic steps. Further, the uncoupled model cycles considered earlier in literature can be taken as a benchmark with which to compare the engine performance of the coupled model.

The paper is organised as follows. In section II, we present the quantum model of our working medium, enumerating the energy eigenstates and eigenvalues. In IIIA, the various stages of the heat cycle are described and expressions for heat exchanged with reservoirs and work delivered are calculated. It is instructive to develop the engine operation based on local description. It is shown that all the work is done locally by each spin. In subsections IIIB and IIIC we develop two cases i) \( B_1 > B_2 \) and ii) \( B_2 > B_1 \). The latter case is possible only in the presence of interactions. It is observed for this case that second law of thermodynamics can be violated at the local scale. General conditions are derived when the efficiency is higher than the noninteracting model. We also present an upper bound for efficiency which is lower than the Carnot bound. The proof is sketched in the Appendix. In IIIC, we interpret some nontrivial features of the engine operation in terms of local spin temperatures. The final section IV summarises our findings.

II. THE COUPLED QHE

The working medium for our QHE consists of two spin-1/2 particles within the 1D isotropic Heisenberg model...
where $\sigma^{(1)} = (\sigma_x^{(1)}, \sigma_y^{(1)}, \sigma_z^{(1)})$ are the Pauli matrices, $J = J_x = J_y = J_z$ is the exchange constant and $B$ is the magnetic field along $z$-axis. Cases $J > 0$ and $J < 0$ correspond to antiferromagnetic and ferromagnetic interactions, respectively. In this paper, we consider antiferromagnetic case only. The energy eigenvalues of $H$ are $-6J, (2J - 2B), 2J$ and $(2J + 2B)$. If $|0\rangle$ and $|1\rangle$ represent the state of the spin along and opposite to the direction of the magnetic field respectively, then in the natural basis $\{|11\rangle, |10\rangle, |01\rangle, |00\rangle\}$, we can write the density matrix as

$$\rho = P_1|\psi_-\rangle\langle\psi_-| + P_2|00\rangle\langle00| + P_3|\psi_+\rangle\langle\psi_+| + P_4|11\rangle\langle11|,$$

where $|\psi_+\rangle = (|10\rangle \pm |01\rangle)/\sqrt{2}$ are the maximally entangled Bell states. The occupation probabilities of the system in the thermal state at temperature $T$ are given by

$$P_1 = \frac{e^{8J/T}}{Z}, \quad P_2 = \frac{e^{2B/T}}{Z}, \quad P_3 = \frac{1}{Z}, \quad P_4 = \frac{e^{-2B/T}}{Z},$$

where, $Z = (1 + e^{8J/T} + e^{2B/T} + e^{-2B/T})$ is the normalisation constant.

A. The heat cycle

The four stages involved in our quantum Otto cycle are described below:

Stage 1: the system with the external magnetic field at $B_1$ attains thermal equilibrium with a bath of temperature $T_1$. Let occupation probabilities be $p_1, p_2, p_3,$ and $p_4$ as tabulated above with $T = T_1$ and $B = B_1$. Stage 2: the system is isolated from the hot bath and the magnetic field is changed from $B_1$ to $B_2$ by an adiabatic process. According to quantum adiabatic theorem, the process should be slow enough to maintain the individual occupation probability of each energy level. Stage 3: the system is brought in thermal contact with a cold bath at temperature $T_2$. Upon attaining equilibrium with the bath, the occupation probabilities become $p_1', p_2', p_3', \text{ and } p_4'$ corresponding to the thermal state with $T = T_2$ and $B = B_2$. On the average, the system gives off heat to the bath. Stage 4: the system is removed from the cold bath and undergoes another quantum adiabatic process which changes the magnetic field from $B_2$ to $B_1$ but keeps the probabilities $p_1', p_2', p_3', \text{ and } p_4'$ unaffected. Finally, the system is brought back to touch the hot bath. On the average, heat is absorbed from the bath and the system returns to its initial state.

The heat transferred in Stage 1 and in Stage 3 of the cycle respectively is

$$Q_1 = \sum_i E_i(p_i - p_i')$$

and

$$Q_2 = \sum_i E_i'(p_i' - p_i)$$

where $E_i$ and $E_i'$ ($i = 1, 2, 3, 4$) are the energy eigenvalues of the system in Stage 1 and Stage 3 respectively. $Q_1 > 0$ and $Q_2 < 0$ corresponds to absorption of heat from hot bath and release of heat to cold bath respectively. Comparing the equations for heat transfer between the system and the reservoirs, Eqs. (9) and (10), the quantity of heat $8J(p_1' - p_1)$ appears in both the equations. Obviously, this term is absent in the uncoupled case for which $J = 0$. As will be shown below, the sign $(\pm)$ of this term determines whether the efficiency in the coupled case will be higher or lower than the uncoupled case.

The work done by the QHE is

$$W = Q_1 + Q_2 = 2(B_1 - B_2)(p_2' - p_2 + p_4' - p_4).$$

Note that $W > 0$ corresponds to work performed by the system.

III. THE LOCAL DESCRIPTION

In this section, we discuss how the individual spins in the system undergo the cycle. Again, let $\varphi_{12}$ and $\varphi_{12}'$ represent the thermal states in the natural basis when the
system is in equilibrium in Stage 1 and Stage 3 respectively. Explicitly, the density matrices are

\[ \rho_{12} = \begin{pmatrix} p_4 & 0 & 0 & 0 \\ 0 & \frac{p_4+p_3}{2} & \frac{p_4-p_3}{2} & 0 \\ 0 & \frac{p_4-p_3}{2} & \frac{p_4+p_3}{2} & 0 \\ 0 & 0 & 0 & p_2 \end{pmatrix}, \tag{12} \]

\[ \rho'_{12} = \begin{pmatrix} p'_4 & 0 & 0 & 0 \\ 0 & \frac{p'_4+p'_3}{2} & \frac{p'_4-p'_3}{2} & 0 \\ 0 & \frac{p'_4-p'_3}{2} & \frac{p'_4+p'_3}{2} & 0 \\ 0 & 0 & 0 & p'_2 \end{pmatrix}. \tag{13} \]

Let \( \rho_1 \) and \( \rho_2 \) be the reduced density matrices in Stage 1 for the first and the second spin, respectively. Then from the normalization constraints, \( \Sigma_i p_i = \Sigma_i p'_i = 1 \), we get

\[ \rho_1 = \rho_2 = \left( \frac{1}{2} - \frac{(p_2 - p_4)}{2} \right) \begin{pmatrix} 0 & 1 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & p_2 & p_4 \\ \frac{1}{2} & p_4 & 0 & p_2 \\ \frac{1}{2} & p_2 & p_4 & 0 \end{pmatrix}. \tag{14} \]

Similarly in Stage 3, the reduced density matrices for the first and second spin are

\[ \rho'_1 = \rho'_2 = \left( \frac{1}{2} - \frac{(p'_2 - p'_4)}{2} \right) \begin{pmatrix} 0 & 1 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & p'_2 & p'_4 \\ \frac{1}{2} & p'_4 & 0 & p'_2 \\ \frac{1}{2} & p'_2 & p'_4 & 0 \end{pmatrix}. \tag{15} \]

Since the applied magnetic field is the same for each spin, their local Hamiltonian is also same. Let \( H_1 \) and \( H'_1 \) be the local Hamiltonians for individual spins with eigenvalues \( (B_1, -B_1) \) and \( (B'_2, -B'_2) \) in Stage 1 and Stage 3 respectively. The heat transferred locally between one spin and a reservoir is given by

\[ q_1 = B_1(p'_2 - p_2 + p_4 - p'_4), \tag{16} \]
\[ q_2 = -B_2(p'_2 - p_2 + p_4 - p'_4). \tag{17} \]

for the hot and the cold reservoir, respectively. So we get the net work done by an individual spin as

\[ w = q_1 + q_2 = (B_1 - B_2)(p'_2 - p_2 + p_4 - p'_4). \tag{18} \]

From Eqs. (15) and (11)

\[ W = 2w. \tag{19} \]

Thus the total work performed is the sum of work obtained from the two spins locally.

Further, the total heat absorbed by the system can be written as

\[ Q_1 = 8J(p'_1 - p_1) + 2q_1, \tag{20} \]

and similarly for the heat released to the cold bath is

\[ Q_2 = -8J(p'_1 - p_1) + 2q_2. \tag{21} \]

Now it can be seen that because the work is done only due to change in local hamiltonians, so only the part of the heat which is absorbed locally by a spin can be converted into heat. The part \( 8J(p'_1 - p_1) \) cannot potentially be converted into work due to the nature of the adiabatic process involved and is transferred directly between the reservoirs. But it may not be transferred only from the hot to the cold bath, in which case it may be regarded like a heat leakage term. In fact, the flow of this heat can be in the opposite direction which is directly related to the enhancement of efficiency due to coupling, as shown below.

In the following, we consider two cases whereby magnetic field may be decreased or alternately, increased in Stage 2. It will be seen that the second case is feasible only in the presence of interactions, \( J \neq 0 \). In the first case when \( J = 0 \), the above equations go back to those for Kieu’s model with two uncoupled spins where an engine operation is obtained given \( T_1 > T_2 \) and \( B_1 > B_2 \) with the additional condition \( B_2/T_2 > B_1/T_1 \).

**A. The case \( B_1 > B_2 \)**

From Eq. (11), the condition that the work performed be positive (\( W > 0 \)) is given by

\[ (p'_2 - p'_4) > (p_2 - p_4). \tag{22} \]

Secondly, for the heat to be absorbed from the hot bath (\( Q_1 > 0 \)), from Eq. (6) we have one of the following two possibilities: (i) \( p'_1 > p_1 \) or (ii) \( p'_1 < p_1 \). Alongwith the possibility (ii), we must also have \( (p'_2 - p_2 + p_4 - p'_4) > (4J/B_1)(p_1 - p'_1) \). Now we rewrite Eq. (8) as

\[ Q_1 = 8J(p'_1 - p_1) + \frac{WB_1}{(B_1 - B_2)}, \tag{23} \]

or \( 8J(p'_1 - p_1) = Q_1(1 - \eta/\eta_0) \), where \( \eta = W/Q_1 \) is the efficiency of the coupled engine and \( \eta_0 = (B_1 - B_2)/B_1 \) is the efficiency of the uncoupled i.e. \( J = 0 \) case. Thus for \( J > 0 \), if \( p'_1 > p_1 \), then \( \eta < \eta_0 \), or the presence of coupling between the spins decreases the efficiency from its value \( \eta_0 \). The global efficiency is equal to the local efficiency in two situations, when \( J = 0 \) or \( p_1 = p'_1 \).

On the other hand, if \( p'_1 < p_1 \), then it is possible that the efficiency of the coupled engine can be higher than the uncoupled case. Using the latter condition with Eq. (22), we have

\[ \frac{(p'_2 - p'_4)}{p'_1} > \frac{(p_2 - p_4)}{p_1}. \tag{24} \]

From the explicit expressions for the probabilities, the above inequality can be simplified to give

\[ \frac{B_2}{T_2} > \frac{B_1}{T_1}. \tag{25} \]

Thus we see that the above condition which is necessary to extract work in the \( J = 0 \) model is also the condition for the coupled case to obtain an efficiency higher than \( \eta_0 \). But additionally, for a set of given values of \( T_1, T_2, \)}
B1 and B2, there is a maximum value of J beyond which the efficiency drops below the η0 value. See Fig. 2

The reason for the lowering of efficiency when p1 < p′1, is that the term 8J(p′1 − p1) is positive and it acts like heat leakage term which reduces the efficiency. On the other hand, when p1 > p′1, this term is negative which means that although each spin locally absorbs heat equal to q1 from the hot bath, due to interaction the effective total heat absorbed by the two-spin system is less than 2q1, which raises the efficiency for a given quantity of the work performed. It is interesting to know how much maximum gain in efficiency is possible for a given set of parameters. We have proved an upper bound for the global efficiency, given by

\[ η ≤ \frac{1 - B2/B1}{1 - 4J/B1} < ηc, \] (26)

where ηc = 1 − T2/T1 is the Carnot bound. Also for η > η0, we have the condition B1 > 4J. This implies that the ordering of energy levels which gives an enhancement of efficiency (over the uncoupled model) is:

\[ (2J - 2B1) < -6J < 2J < (2J + 2B1), \] (27)

and which after the first quantum adiabatic process, becomes

\[ (2J - 2B2) < -6J < 2J < (2J + 2B2). \] (28)

The proof of Eq. (26) is given in the Appendix.

B. THE CASE B2 > B1

In this case, during the first quantum adiabatic process, the magnetic field is increased from its value B1 to B2. If there is no interaction between the spins, the system cannot work as an engine in this case because the condition W > 0 will not be satisfied [2]. The conditions T1 > T2 and B2 > B1 directly lead to

\[ p4 > p′4, \] (29)
\[ p3 > p′3. \] (30)

Further, the positive work condition implies (p′2 − p′4) < (p2 − p4), which along with (29) gives

\[ p2 > p′2. \] (31)

The normalization of probabilities and the above three conditions Eqs. (29), (30) and (31) together give

\[ p′1 > p1. \] (32)

These are the necessary conditions for the system to work as an engine given that T1 > T2 and B2 > B1. According to Eq. (15), the local work should be positive. This yields q1 < 0 and q2 > 0. This means locally the heat is absorbed from the cold bath and given to the hot bath. Also the local efficiency is

\[ \frac{w}{q2} = 1 - \frac{B1}{B2}. \] (33)

Thus locally, the spins operate counter to the global temperature gradient present due to T1 > T2. But globally we do have Q1 > 0 and Q2 < 0. Thus the function of the two-spin engine is consistent with the second law of thermodynamics, although locally we seem to have a violation of the same. This apparent contradiction is resolved below using the concept of local effective temperatures.

C. Local temperatures

Now each spin in the 2-spin system can be assigned a local effective temperature, corresponding to its local thermal state or the reduced density matrix [21, 26]. This is true regardless of the state of the total system. Particularly, in stages 1 and 3 of the cycle, from Eqs. (14), (15) along with local Hamiltonian, we get the local temperatures as

\[ T'_1 = 2B1 \left( \log \left[ \frac{2}{(1 + p4 - p2)} - 1 \right] \right)^{-1}, \] (34)
\[ T'_2 = 2B2 \left( \log \left[ \frac{2}{(1 + p4' - p2')} - 1 \right] \right)^{-1}. \] (35)

The important fact is that in the presence of interactions, the local temperatures are different from the corresponding bath temperatures. Thus T′1 ≠ T1 and T′2 ≠ T2 if J ≠ 0. Further, since the work in our heat cycle is done only locally, the total work by the system can be regarded as equal to the work by two independent spins operating between their effective temperatures.
(i) Engine working in $B_1 > B_2$: the positive work condition for a single spin is given by

$$\frac{B_2}{T_2} > \frac{B_1}{T_1}.$$  

(36)

Since $B_1 > B_2$, we get

$$T'_1 > T'_2.$$  

(37)

At $J = 0$, $T'_1 = T_1$ and $T'_2 = T_2$ and we have the result of Kieu’s model [2].

(ii) Engine working in $B_2 > B_1$: in this model, the positive work condition is satisfied only when

$$\frac{B_1}{T'_1} > \frac{B_2}{T'_2}.$$  

(38)

Thus in this case $T'_2 > T'_1$. Moreover, it can be shown from the definitions (34) and (35) that for both the cases, $T'_1 > T_1$ and $T'_2 > T_2$. Finally, based on local temperatures, the counter-intuitive mechanism which leads in case (ii) to $q_1 < 0$ and $q_2 > 0$ can be justified as follows. For $B_2 > B_1$, due to the first adiabatic process, the local temperature increases from $T'_1$ to $T'_1(B_2/B_1)$. After contact with the cold bath, the local temperature becomes $T'_2$, which due to condition (38) is more than $T'_1(B_2/B_1)$. Thus heat should flow from the cold bath to the spin or $q_2 > 0$. Similar considerations lead to rejection of heat by the spin at the hot bath or $q_1 < 0$.

IV. SUMMARY

A model of coupled spins is used as working medium to realise a quantum Otto engine. The conditions for the efficiency to be higher than the non-interacting case are found. The antiferromagnetic interaction between the spins allows a fraction of the total heat to flow from cold bath to hot bath provided the total heat should flow in in a direction suggested by global temperature gradient. This mechanism increases the efficiency of the system compared to non-interacting spins case. A tighter upper bound for the efficiency is found which is lower than the Carnot value. The system can also work as a heat engine even if it undergoes an adiabatic compression ($B_2 > B_1$) in the second stage of the cycle. Here we have observed an interesting mode of operation using the reduced density matrix whereby each spin absorbs heat from the cold bath and rejects some heat to the hot bath while performing a network. This feature is also confirmed from the analysis of local effective temperatures of the spins.

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APPENDIX

Upper bound for global efficiency

We consider the case of the engine working in the range $B_1 > B_2$. The condition to get a higher efficiency as compared to uncoupled model is the case (ii) discussed in Section IIIA and is given by

$$p_1 > p'_1.$$  

(39)

From the condition $B_2/T_2 > B_1/T_1$ (Eq. (25)), we get

$$p_3 > p'_3,$$  

(40)

$$p_4 > p'_4.$$  

(41)

Then normalisation of the probabilities gives

$$p'_2 > p_2.$$  

(42)

From Eqs. (39) and (42), we have

$$\frac{p'_1}{p'_1} > \frac{p_2}{p_1},$$  

(43)

which simplifies to

$$e^{(B_2-4J)/T_2} > e^{(B_1-4J)/T_1}.$$  

(44)

Fig. 3 shows three possible ways of arranging the energy levels ($2J - 2B_1$) and $-6J$ relative to the level ($2J - 2B_2$) resulting from the first quantum adiabatic process. Equivalently, Eq. (44) is of the form $e^x > e^y$, which may be satisfied in one of the following three ways:

![Fig. 3. Three possible configurations of energy levels with eigenvalues $-6J$, $(2J - 2B_1)$ and $(2J - 2B_2)$ resulting from the first quantum adiabatic process whereby $B_1$ is changed to a lower value $B_2$. Only case (a) is possible as discussed in the Appendix.](image)

Case (a) represents $y > 0$, $x > 0$ and so $x > y$. This implies, $B_1 > 4J$ and $B_2 > 4J$.

Case (b) represents $x < 0$, $y < 0$ and $|x| < |y|$. This implies $B_1 < 4J$, $B_2 < 4J$, but due to the fact $T_2/T_1 < 1$, we obtain $B_1 < B_2$ which leads to a contradiction.

Case (c) represents $y < 0$ and $x > 0$. This possibility is also similarly ruled out.
So the only possibility is case (a) representing the fact that the energy levels \((2J - 2B_1)\) and \((2J - 2B_2)\) lie below the level \(-6J\) when the coupled engine gives a higher efficiency than the uncoupled case.

When the inequality (44) holds, we can write

\[
\frac{B_2 - 4J}{T_2} > \frac{B_1 - 4J}{T_1}.
\]

(45)

Since \(B_1 > 4J\), \(B_2 > 4J\) and \(T_1 > T_2\), we get

\[
\frac{\eta_0}{1 - 4J/B_1} < \eta_c = 1 - \frac{T_2}{T_1},
\]

(46)

where \(\eta_0 = 1 - B_2/B_1\). Now the global efficiency defined as \(\eta = W/Q_1\), can be written as

\[
\eta = \frac{\eta_0}{1 - \frac{4J(p_1 - p'_1)}{B_1(p_4 - p'_4 + p'_2 - p_2)}}.
\]

(47)

From the inequalities between the probabilities (Eqs. (39), (41) and (42)), it follows that \((p_1 - p'_1) < (p_4 - p'_4 + p'_2 - p_2)\). Therefore, we finally obtain that when the efficiency is higher than the uncoupled case (or the lower bound is \(\eta_0\)), then an upper bound for efficiency is given by

\[
\eta < \frac{\eta_0}{1 - 4J/B_1} < \eta_c.
\]

(48)

When \(J = 0\), we have \(\eta = \eta_0\). A similar kind of proof can be constructed for the case \(B_2 > B_1\). Interestingly, the same bound as Eq. (48) is obtained.