Quantum Otto cycle efficiency on coupled qudits

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Abstract

Properties of the coupled particles with spin $3/2$ (quartits) in a constant magnetic field, as a working substance in the quantum Otto cycle of the heat engine, are considered. It is shown that this system as a converter of heat energy in work (i) shows the efficiency 1 at the negative absolute temperatures of heat baths, (ii) at the temperatures of the opposite sign the efficiency approaches to 1, (iii) at the positive temperatures of heat baths antiferromagnetic interaction raises efficiency threefold in comparison with uncoupled particles.

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I. INTRODUCTION

As it is known, thermodynamics has the broadest applications for description of many physical phenomena [1, 2]. The quantum thermodynamics studies dynamics of heat and work in quantum systems. They began to study quantum thermodynamic engines after appearance of works [3, 4]. Thermodynamic cycles, such as Carnot or Otto cycles, can be reformulated for quantum systems [5, 6, 7, 8, 9, 13]. One of the important quantum thermodynamic cycles is an Otto cycle. Similarly to a classical Otto cycle the quantum Otto cycle consists of two isochoric and two adiabatic stages too. A quantum isochoric process corresponds to a thermal exchange between a working body and thermal baths. During the quantum isochoric process only population of levels is reconstructed, whereas at the adiabatic process the working body produces work at the expense of power level changes. The adiabatic process can be thermodynamic adiabatic or quantum adiabatic. A process is thermodynamic adiabatic if the working substance is thermally isolated from a heat bath. However it does not exclude transitions of purely quantum nature between levels while at the quantum adiabatic process the population density of levels is fixed.

The coupled spin systems can be used as quantum thermodynamic engines. In small systems with a finite number of degrees of freedom as finite-dimensional effects and quantum effects essentially influence thermodynamic properties of the system. The aim of this work is a research of quantum systems with a finite number of levels as a working substance in a quantum Otto cycle, including viewing of the negative absolute temperatures [14, 16].

The article is organised as follows. In section II, the properties of a working substance consisting of two coupled spins 3/2 in a constant magnetic field are described. In section III, a quantum heat Otto cycle is presented. Section IV presents the results graphically at the concrete control parameters. The final section V summarises the findings. In the Appendix auxiliary analytical formulae are presented.

II. WORKING SUBSTANCE

The choice of a working substance for operation of the quantum heat engine is essential [17, 19]. The working substance in our case is featured by the Hamiltonian $H$ of two 3/2
of spins (biquartit) with permutation symmetry of particles and the isotropic exchange interaction in a constant magnetic field $h$:

$$\hat{H} = h (E_{4 \times 4} \otimes S_3 + S_3 \otimes E_{4 \times 4}) + 4J \vec{S} \otimes \vec{S},$$  \hspace{1cm} (1)$$

in which $E_{4 \times 4}$ is the identity matrix, $S_1, S_2, S_3$ is the matrix representation of components of the spin 3/2, $J$ is the interaction constant. Cases $J > 0$ and $J < 0$ correspond to antiferromagnetic and ferromagnetic interactions, respectively.

By the known partition function $Z$ it is possible to calculate the free energy $F$, the entropy $S$, the internal energy $U$ and the heat capacity $C$:

$$F = -1/\beta \ln Z, \ S = \beta^2 \partial_\beta F, \ U = \partial_\beta \beta F, \ C = -\beta^2 \partial_\beta \beta F.$$  \hspace{1cm} (2)$$

In the formulae the $\beta$ partial differentiation indicates that the other parameters are fixed.

According to the entanglement is determined by the values of decomposition of the density matrix on the basis $\rho = \sum_{i=0}^{15} \sum_{j=0}^{15} R_{ij} C_i \otimes C_j$

$$m_{SM} = \sqrt{1/(D - 1) \sum_{i=0}^{15} \sum_{j=0}^{15} (R_{i\alpha} R_{\alpha j} - R_{ij})^2},$$  \hspace{1cm} (3)$$

where $D$ is the qudit dimension of basis $C_i$ (for a quartit $D = 16$, for a qubit $D = 4$) and $R_{ij}$ are the components of the Bloch vector.

A. Local temperatures

For the Hamiltonian the biquartit density matrix and a local Hamiltonian are diagonal. The local entropy $s$ and the internal energy $u$ are defined by formulae

$$s = -\sum_{k=1}^{4} \pi_k \ln \pi_k, \ u = \sum_{k=1}^{4} \varepsilon_k \pi_k,$$  \hspace{1cm} (4)$$

where the diagonal elements of the reduced density matrix look like

$$\pi_1 = 1/20(5 - 5p_1 + p_2 - 5p_3 - 5p_4 - 5p_5 + 5p_6 + 5p_7 + 4p_9 - 4p_{11} + 15p_{12} - 5p_{13} - 5p_{14} - p_{15} + 5p_{16}),$$  \hspace{1cm} (4)$$

$$\pi_2 = 1/20(5 + p_1 + 3p_2 - 5p_3 + 5p_4 - 5p_5 - 5p_6 + 5p_7 - 4p_9 + 4p_{11} - 5p_{12} - 5p_{13} - 14p_{14} + 7p_{15} + 5p_{16}),$$  \hspace{1cm} (4)$$

$$\pi_3 = 1/20(5 + 3p_1 + p_2 + 5p_3 - 5p_4 - 5p_5 + 5p_6 - 5p_7 - 4p_9 + 4p_{11} - 5p_{12} + 5p_{13} + 7p_{14} - p_{15} - 5p_{16}),$$  \hspace{1cm} (4)$$
\[\pi_4 = \frac{1}{20}(5 + p_1 - 5p_2 + 5p_3 + 5p_4 + 15p_5 - 5p_6 - 5p_7 + 4p_9 - 4p_{11} - 5p_{12} + 5p_{13} - p_{14} - 5p_{15} - 5p_{16}),\]

and the eigenvalues \(\varepsilon_k\) of a local Hamiltonian quartit are equal \(h/2(3, 1, -1, -3)\). Formulae of level populations \(p_i\) are given in the Appendix. The local qudit temperature is equal

\[
\beta_{\text{loc}} = \frac{1}{T_{\text{loc}}} = \frac{\partial s}{\partial u} = \frac{\partial s/\partial \beta}{\partial u/\partial \beta}.
\]

(5)

The local temperature is not equal to the system temperature of two coupled quartits \(\beta = 1/T\) [18]. We define the inverse spectroscopic temperature as [22] :

\[
\beta_{M\text{loc}} = -\left(1 - \frac{\pi_1 + \pi_M}{2}\right)^{-1} \sum_{i=2}^{M} \left(\frac{\pi_i + \pi_{i-1}}{2}\right) \left(\frac{\ln \pi_i - \ln \pi_{i-1}}{e_i - e_{i-1}}\right).
\]

(6)

where \(\pi_i\) is the probability to find the quantum system at the energy \(e_i\), \(M\) is the number of the highest energy level \(e_M\), while the lowest one is labelled \(e_1\). Actually it is a definition of the ensemble average of a random quantity \(-\frac{\ln \pi_i - \ln \pi_{i-1}}{e_i - e_{i-1}}\) with the distribution function density \((1 - \frac{\pi_1 + \pi_M}{2})^{-1} (\frac{\pi_i + \pi_{i-1}}{2})\).

We shall compare this expression for the local temperature with the temperature definition \(\beta\) in section IV.

### III. HEAT OTTO CYCLE

Let’s feature 4 stages of a quantum quasi-static Otto cycle [17].

**Stage 1:** the system of two coupled quartits in a magnetic field \(h\) attains thermodynamic equilibrium with a heat bath of temperature \(T\). The occupation probabilities are determined by temperature \(T\) and a magnetic field \(h\). Thus the occupations change, and the energy levels do not change. The work is not produced during this isochoric process, and the working substance absorbs heat \(Q_1\) from the bath:

\[
Q_1 = \sum_{i=1}^{16} e_i (p_i - p_i').
\]

(7)

**Stage 2:** the system is isolated from the heat bath and the magnetic field is changed from \(h\) to \(h'\) by an adiabatic process, and the energy levels slowly change. According to the adiabatic theorem the occupation probabilities of each energy level maintain. The work is produced:

\[
W_2 = \sum_{i=1}^{16} p_i (e_i' - e_i).
\]

(8)
Stage 3: the system is brought in contact with a heat bath at temperature $T'$. Upon attaining thermodynamic equilibrium with the bath the occupation probabilities are determined by temperature $T' < T$ and a magnetic field $h'$. The system gives off heat energy $Q_3$ to the bath:

$$Q_3 = \sum_{i=1}^{16} e'_i(p'_i - p_i).$$  \hspace{1cm} \text{(9)}$$

Stage 4: the system is removed from a cold bath and undergoes another adiabatic process which changes the magnetic field from $h'$ to $h$ but keeps the occupation probabilities unaffected. The energy levels slowly change and the work $W_4$ is produced:

$$W_4 = \sum_{i=1}^{16} p'_i(e_i - e'_i).$$  \hspace{1cm} \text{(10)}$$

The system is brought in contact with a heat bath at temperature $T$. Heat is absorbed from the bath and the system returns to its initial state. All the cycle is presented on the diagramme (11).

1 \xrightarrow{Q_1} 2 \\
\uparrow W_4 \\
\downarrow W_2 \\
4 \xleftrightarrow{Q_3} 3 \\
\text{(11)}$$

The energy change during the cycle is equal to zero:

$$Q_1 + W_2 + Q_3 + W_4 = 0.$$  \hspace{1cm} \text{(12)}$$

The heat transferred in Stage 1 and in Stage 3 respectively is

$$Q_1 = \sum_{i=1}^{16} e_i(p_i - p'_i) = Jm + hn, \quad Q_3 = \sum_{i=1}^{16} e'_i(p'_i - p_i) = -Jm - h'n,$$  \hspace{1cm} \text{(13)}$$

where

$$m = -11(p_1 - p'_1 + p_2 - p'_2 + p_9 - p'_9) + 9(p_5 - p'_5 + p_{11} - p'_{11} + p_{12} - p'_{12} + p_{13} - p'_{13} + p_{14} - p'_{14} + p_{15} - p'_{15} + p_{16} - p'_{16}) - 3(p_3 - p'_3 + p_4 - p'_4 + p_6 - p'_6 + p_7 - p'_7 + p_{10} - p'_{10}) - 15(p_8 - p'_8),$$

$$n = -p_1 + p'_1 + p_2 - p'_2 + p_4 + p'_4 + p_6 - p'_6 - p_{14} + p'_14 + p_{15} - p'_{15} + 2(-p_3 + p'_3 + p_7 - p'_7 - p_{13} + p'_13 + p_{16} - p'_{16}) + 3(-p_5 + p'_5 + p_{12} - p'_{12}).$$
The work is done in Stage 2 and Stage 4 when the energy levels change at the fixed occupation probabilities. Due to energy level changes the work done by the quantum heat engine is

\[ W_{out} = W_2 + W_4 = (h - h')n, \quad (15) \]

where

\[ W_2 = (h - h') (p_1 - p_2 + 2p_3 + p_4 + 3p_5 - p_6 - 2p_7 - 3p_{12} + 2p_{13} + p_{14} - p_{15} - 2p_{16}), \quad (16) \]

\[ W_4 = (h' - h) (p'_1 - p'_2 + 2p'_3 + p'_4 + 3p'_5 - p'_6 - 2p'_7 - 3p'_{12} + 2p'_{13} + p'_{14} - p'_{15} - 2p'_{16}). \quad (17) \]

The efficiency of transformation of heat into work at \( Q_1 > 0, Q_3 < 0 \) is

\[ \eta = \frac{W_{out}}{Q_{in}} = \frac{- (W_2 + W_4)}{Q_1} = \frac{\eta_0}{1 - \frac{Jm}{n}}. \quad (18) \]

It is obviously that the interaction between particles can give both the enhancement and the reduction of the efficiency concerning noninteracting particles. For uncoupled particles that is \( J = 0 \) the efficiency is \( \eta_0 = 1 - \frac{h'}{h} \)[23].

**A. Local description**

In this subsection, following the article[17], we feature how the individual quartits undergo the cycle. Heat, transfered locally between one quartit and a heat bath, is

\[ q_1 = \frac{h}{2} n, \quad q_2 = -\frac{h'}{2} n, \quad (19) \]

for hot and cold baths accordingly. The work done by one particle is

\[ w = q_1 + q_2 = \frac{h - h'}{2} n. \quad (20) \]

\[ W = 2w = (h - h')n. \quad (21) \]

Thus the total performed work is the sum of local work obtained from each qudit. It is a consequence of permutation symmetry of the hamiltonian.

The total heat, absorbed (produced) by the system in Stage 1 (Stage 3) can be written as

\[ Q_1 = Jm + 2q_1, \quad Q_2 = -Jm - 2q_2. \quad (22) \]
IV. RESULTS

We illustrate analytical results graphically at the specific parameters.

**Working substance.** Fig. 1 shows the entropy dependence on the internal energy. Dependences of the internal energy, the entropy and the heat capacity on inverse temperature are shown in Fig. 2. Coupling of spins breaks the symmetry which is at the equidistant disposition of energy levels in the system [14]. Dependence of the entanglement on the heat capacity is presented in Fig. 3. The dependence singularity is based on the fact that at a small constant $J$ is multivalued, and at a big one it is two-valued. Numerical comparison of dependence of local inverse temperature definitions from the inverse system temperature is given in Fig. 4. Both definitions give the same results at a small interaction constant. At $J = 0.0, 0.1, 0.15$ there is the full coincidence of definitions of local temperatures both at negative and positive $\beta$ (bold lines). At $J > 0.17$ there is an appreciable discrepancy at positive $\beta$.

We describe the efficiency of a quantum Otto cycle on coupled quartits for some possible sets of positive and negative signs of the quantities $Q_1, W_2, Q_3, W_4$. Reduced letters in plots show the characteristics of two coupled qubits (biquut) for comparison. It is possible due to control parameters $h, h', J$. It is obvious that at $h = h', J \neq 0, Q_1 > 0, W_2 = 0, Q_3 < 0, W_4 = 0$, that is heat is just transfered from a hot bath into a cold one.

**The quantum heat engine between baths with negative absolute temperatures.** At negative temperatures of heat baths $T < 0, T' < 0, |T| < |T'|$ the situation, when $Q_1 > 0, Q_3 > 0, W_2 < 0, W_4 < 0$ (see Fig. 5) is possible. In this case, the efficiency of conversion of heat in work is equal to 1 [14], according to (12) and the efficiency definition

$$\eta = \frac{W_{\text{out}}}{Q_{\text{in}}} = \frac{-(W_2 + W_4)}{Q_1 + Q_3} = 1.$$ 

**The quantum heat engine between baths with absolute temperatures of the opposite sign.** At temperatures of baths $T < 0, T' > 0$ the situation, when $Q_1 > 0, Q_3 < 0, W_2 < 0, W_4 < 0$ (see Fig. 6) is possible. In this case the efficiency of conversion of heat in work is equal

$$\eta = \frac{-(W_3 + W_4)}{Q_1} \quad (18)$$

and because of a small leakage it approaches unity, as shown in Fig. 7. A shift of the maximum efficiency in the biquartit in regard to the biquubit is observed. At a modification of driving parametres the efficiency can exceed more than three times the efficiency of uncoupled 3/2-spins, as seen from Fig. 8. For the biquubit the maximum efficiency is moved towards the increase of the interaction constant [17].
The quantum heat engine of conversion of work in heat between baths with the positive temperatures. At the positive temperatures of baths \( T > 0 \), \( T' > 0 \), \( T > T' \) the situation, when \( Q_1 < 0 \), \( Q_3 < 0 \), \( W_2 > 0 \), \( W_4 > 0 \) (see Fig. 9) is possible. In this case the efficiency of conversion of work in heat equals \( \eta = \frac{-Q_1 + Q_3}{W_2 + W_4} = 1 \). At some set of parameters \( Q_1 \) changes its sign, then the total work \( W_2 + W_4 \) changes its sign, that is in a neighbourhood \( Q_1 = 0 \) the work done over the system, is entirely converted in heat [24].

The quantum heat pump of conversion of work in heat between baths with the positive temperatures. The working body of biquartit/biqubit at parameters \( T = 2 \), \( T' = 1 \), \( h = -5 \), \( h' = -1 \), works as a heat pump, as \( Q_1 < 0 \), \( W_2 > 0 \), \( Q_3 > 0 \), \( W_4 < 0 \), with the efficiency \( \eta_p = \frac{-Q_1 + Q_3}{W_2} \) (see Fig. 10).

V. CONCLUSION

The quasi-stationary quantum Otto cycle, when the working body is the coupled system of two 3/2-spins, being in a magnetic field, is explored. Some performances of the quantum Otto cycle on the coupled spins, generated by various sets of driving parameters, are considered. The analysis of possible quantities of the cycle efficiency depending on driving parameters is carried out. There are the restrictions on driving parameters \( T > T' \), \( h'/T' > h/T \) for the conversion of heat in work (see Fig. 5, 6, 7, 8). It is shown that the efficiency of conversion of heat in work at negative temperatures of heat baths equals 1, at temperatures of the opposite sign it approaches 1. At positive temperatures of heat baths the antiferromagnetic interaction of spins [17] raises the efficiency more than threefold in comparison with uncoupled spins [17]. The dependence on a system size is revealed in a displacement of the maximum efficiency in regard to the enhancement of the interaction constant (see Fig. 7, 8).
Appendix A

The matrix representation of a vector of a spin 3/2 looks like

\[
S_1 = \begin{pmatrix}
\sqrt{\frac{3}{2}} & 0 & 0 \\
\sqrt{\frac{3}{2}} & 0 & \frac{\sqrt{3}}{2} \\
0 & \frac{\sqrt{3}}{2} & 0 \\
0 & 0 & 0
\end{pmatrix},
S_2 = \begin{pmatrix}
0 & -i\sqrt{\frac{3}{2}} & 0 \\
i\sqrt{\frac{3}{2}} & 0 & -i \\
0 & i & 0 \\
0 & 0 & i\sqrt{\frac{3}{2}}
\end{pmatrix},
S_3 = \begin{pmatrix}
\frac{3}{2} & 0 & 0 \\
0 & \frac{1}{2} & 0 \\
0 & 0 & -\frac{3}{2}
\end{pmatrix}.
\]  
(A1)

The density matrix on the basis of eigenfunctions of the Hamiltonian (energy representation) looks like

\[
\rho = e^{-\beta \hat{H}}/Z = \sum_{i=1}^{16} p_i P_i,
\]  
(A2)

where \( \beta = 1/T \) is the inverse temperature, \( Z = \text{Tr} e^{-\beta \hat{H}} = \sum_{i=1}^{16} e^{-\beta e_i} \) is the partition function, \( p_i = e^{-\beta e_i}/Z \) are the occupation densities, \( P_i = |e_i><e_i| \), \( P_i P_k = \delta_{i,k} P_i \) are the projectors constructed of eigenvectors of the Hamiltonian \( |e_i> \), corresponding to the eigenvalues \( e_i(h, J) \equiv e_i \): \( e_1 = -h - 11J, e_2 = h - 11J, e_3 = -2h - 3J, e_4 = -h - 3J, e_5 = -3h + 9J, e_6 = h - 3J, e_7 = 2h - 3J, e_8 = -15J, e_9 = -11J, e_{10} = -3J, e_{11} = 9J, e_{12} = 3h + 9J, e_{13} = -2h + 9J, e_{14} = -h + 9J, e_{15} = h + 9J, e_{16} = 2h + 9J, \sum_{i=1}^{16} e_i = 0 \), \( e'_i(h', J) \equiv e'_i \).

The normalized eigenvectors equal:

\[
|e_1> = \sqrt{\frac{10}{3}}(0, 1, 0_2, -\frac{2}{\sqrt{3}}, 0_2, 1, 0_2), |e_2> = \sqrt{\frac{10}{3}}(0, 1, 0_2, -\frac{2}{\sqrt{3}}, 0_2, 1, 0_2),
\]

\[
|e_3> = 1/\sqrt{2}(0_{11}, -1, 0_2, 1, 0), |e_4> = 1/\sqrt{2}(0_7, -1, 0_5, 1, 0_2), |e_5> = (0_15, 0, 0_{14}),
\]

\[
|e_6> = 1/\sqrt{2}(0_2, -1, 0_5, 1, 0_7), |e_7> = 1/\sqrt{2}(0, -1, 0_2, 1, 0_4),
\]

\[
|e_8> = 1/2(0_3, -1, 0_2, 1, 0_2, -1, 0_2, 1, 0_3), |e_9> = \sqrt{20}/3(0_3, 1, 0_2, -1/3, 0_2, -1/3, 0_2, 1, 0_6),
\]

\[
|e_{10}> = 1/2(0_3, -1, 0_2, -1, 0_2, 1, 0_2, 1, 0_3), |e_{11}> = 1/\sqrt{20}(0_3, 1, 0_2, 3, 0_2, 3, 0_2, 1, 0_6),
\]

\[
|e_{12}> = (1, 0_{15}), |e_{13}> = 1/\sqrt{2}(0_{11}, 1, 0_2, 1, 0), |e_{14}> = 1/\sqrt{5}(0_7, 1, 0_2, \sqrt{3}, 0_2, 1, 0_4),
\]

\[
|e_{15}> = 1/\sqrt{5}(0_2, 1, 0_2, \sqrt{3}, 0_2, 1, 0_7), |e_{16}> = 1/\sqrt{2}(0, 1, 0_2, 1, 0_4),
\]

where \( 0_k \equiv 0, 0, ..., 0 \).

The biqubit Hamiltonian is the same as in the equation (11) with the eigenvalues \(-3J, J, -h + J, h + J\).
Fig. 1. Entropy $S$ is plotted as a function of the internal energy $U$ for a biquartit at the fixed magnetic field $h = 1$.

Fig. 2. The internal energy $U$, the entropy $S$ and the heat capacity $C$ are plotted as functions on the inverse temperature $\beta$ for $h = 1, J = 0.1$. At $J = 0$ the entropy and the heat capacity are the even functions, the internal energy is the odd function [14].
Fig. 3. Parametric dependence of the entanglement $E_{SM}$ and the heat capacity $C$ on the inverse temperature at $h = 1$ for different coupling constants. The closed parts of graphs correspond to the negative temperature, and unclosed ones to the positive temperature.

Fig. 4. Inverse local temperature of the quartit $\beta_{loc}$ versus the inverse temperature of the biquartit $\beta$ for $h = 2$, $J = 0.0$, 0.1, 0.2.
Fig. 5. Dependence of heat and work on a coupling constant at all stages of the Otto cycle at $T = -1, T' = -3, h = 1, h' = -1$. The dashed line is the efficiency of the heat energy conversion in work. Hereinafter the bold lines are for the biquartit; the pointwise lines are for the biqubit.

Fig. 6. Heat and work versus the coupling constant for $T = -1, T' = 2, h = 4, h' = 0.155$. 

Fig. 7. Efficiency of the conversion of heat in work with parameters as in Fig. 6. The heat leakage in the biqubit equals $0.0028$; the leakage in the biquartit is $Q_3 = -0.0021$. The maximum efficiency equals 0.999 in the biqubit for $J = -0.26$, and in the biquartit for $J = -0.11$.

Fig. 8. Efficiencies $\eta$ of the biqubit and the biquartit transformations of heat in work depending on the coupling constant $J$ at $T = 2.5$, $T' = 0.25$, $h = 16$, $h' = 12$. 
Fig. 9. Heat and work versus the coupling constant for $T = 2, T' = 1, h = 4, h' = -1$. The dashed line is the efficiency of conversion of work in the heat energy.

Fig. 10. Efficiency of a heat pump $\eta_p$ as a function of the coupling constant $J$ at $T = 2, T' = 1, h = -5, h' = -1$. 

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