What role does the third law of thermodynamics play in Szilard engines?

Kang-Hwan Kim\(^1\) and Sang Wook Kim\(^2\)

\(^1\)Department of Physics, Pusan National University, Busan 609-735, Korea and 
\(^2\)Department of Physics Education, Pusan National University, Busan 609-735, Korea

(Dated: December 19, 2018)

The role of the third law of thermodynamics in the Szilard engine has been addressed. If the ground state is non-degenerate, the entropy production defined as the work extractable from the engine divided by temperature vanishes as temperature approaches zero due to the third law. The degenerate ground state induced by the symmetry or by accident gives rise to non-zero entropy production at zero temperature associated with the residual entropy. Various physical situations such as the SZE consisting of bosons or fermions either with or without interaction have been investigated.

PACS numbers: 05.70.-a, 89.70.Cf, 03.67.-a, 03.65.Ta, 05.70.Ln

I. INTRODUCTION

Based upon the second law of thermodynamics Carnot proposed that every cyclic engines should consist of at least two reservoirs with two distinct temperatures, namely high and low temperature reservoirs. The former supplies entropy accompanying heat into the engine, while the latter absorbs the supplied entropy to eliminate it from the engine. It has been shown, however, that the engine proposed by Szilard [1], referred to as the Szilard engine (SZE), can be operated by using only a single reservoir, so that it was regarded as the so-called Maxwell’s demon [2] which is believed to violate the second law of thermodynamics. The thermodynamic cycle of the SZE consists of three steps as shown in Fig. 1: (A) to insert a wall so as to divide a box into two parts, (B) to perform measurement to obtain information on which side the atom is in, and (C) to attach a weight to the wall to extract work via isothermal expansion with a thermal reservoir of temperature \(T\) contacted. Now it is widely accepted that the SZE does not contradict the second law since the information entropy of the SZE is transferred to the reservoir via measurement and erasure mediated by the demon [2, 6]. The second law thus forces us to directly relate information to physical entropy, which reveals a profound role of information in nature. The SZE has been exploited to understand many physical problems in various contexts [7–9] and realized in experiment [10, 11].

The third law of thermodynamics, proposed by Nernst in 1906 [14], asserts that the entropy of a substance approaches zero as temperature approaches absolute zero. This statement is true only if the ground state of the substance is unique. Otherwise, the entropy approaches non-zero finite value called as the residual entropy. Many quantum statistical behavior in low temperature, e.g. the specific heat of solids, is governed by the third law. However, it is now found that the third law is a derived law rather than a fundamental law. Interestingly there is no study on the relation between the information and the third law. Moreover, it has never even been asked what the role of the third law is in the context of the information heat engine, especially the SZE. In the classical SZE, the entropy production defined as the work extracted from the engine divided by temperature is independent of temperature.

In this paper we show that the third law of thermodynamics manifests itself in the SZE, particularly in the low temperature. The entropy production is limited by the third law; the entropy production vanishes as temperature approaches zero. Exception occurs when the ground state exhibits degeneracies either by accident or due to symmetry. The entropy production then approaches a non-zero finite value completely determined by the number of the degeneracies. Moreover, various non-trivial temperature dependence of the entropy production of
the quantum SZE containing bosons or fermions with or without interaction can be understood by considering
the third law and such degeneracies. Through this paper
we assume that all the measurement is performed in a
perfect manner. How the imperfect measurement modi-
fies the results of the classical SZE has been investigated
in Ref. [15]. The non-equilibrium effect in the classical
SZE has also been considered in Ref. [16].

The rest of this paper is organized as follows. In Sec.
II, we introduce the work formula of the quantum SZE
and discuss one tricky point of when and how the mea-
surement has been done during the thermodynamic pro-
cess. Section III is the main part of this paper. We
show the role of the third law in the SZE and present
the simplest model, one particle SZE. In Sec. IV, we in-
vestigate various physical situations of two particle SZE,
which shows rich behaviors of a simple information heat
engine in the low temperature. Finally, we conclude this
paper.

II. QUANTUM SZILARD ENGINE

To correctly address the behavior of the SZE in low
temperature, we should deal with it in a quantum me-
chanical way. Recently it has been found by one of us
that the work of the quantum SZE is expressed as

$$\langle W \rangle = -k_B T \sum_{m=0}^{N} p_m \ln \left( \frac{p_m}{p_m^*} \right) \equiv k_B T \Delta S, \quad (1)$$

where $p_m$ and $p_m^*$ represent the probability to find $m$
atoms in the left side of the box among total $N$ atoms
right after a wall is inserted for the time-forward proto-
col, and that for the time-reversed protocol, respectively.
Here $k_B$, $T$ and $\Delta S$ denote the Boltzmann constant,
the temperature of a heat reservoir and the entropy pro-
duction, respectively. Recently we reported, however, that
Eq. (1) itself can be derived from fully classical consider-
ation. The partition functions, required to calculate $p_m$
and $p_m^*$, differ in whether the classical or the quantum me-
chanics are taken into account [15]. All the calculations
performed in this paper are based upon Eq. (1).

Now we would like to address one frequently asked
question on the SZE: when and how the measurement
process has been done during the thermodynamic pro-
cess. The answer is that the measurement is automati-
cally done by the reservoir when the box is completely
separated into two parts by inserting a wall. It is noted
that the process of inserting a wall should be performed in
an isothermal way in the quantum SZE, which inevitab-
ly introduces the reservoir into the problem [17]. In order
to make the engine have a well-defined temperature at ev-
every moment the reservoir has to observe the eigenenergy
of the engine so that each energy eigenstate is properly
occupied following the canonical distribution. Below we
show that such a measurement of the energy corresponds
to that of the information on which part of box the par-
ticle is located in when the wall is inserted.

The engine and the wall can be modeled as an one-
dimensional box and a potential barrier, respectively;
that is,

$$V_{\text{box}} = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases} \quad (2)$$

and

$$V_{\text{wall}}(l) = V_0 \delta(x - L/2), \quad (3)$$

where $V_0$ is the hight of the wall. For simplicity as-
sume that temperature is negligibly small so that only
the ground state is dominantly occupied. When $V_0$ is
large enough, the ground and the first excited state, de-
noted as $|0\rangle$ and $|1\rangle$, respectively, are nearly degenerate
so as to be almost equally occupied. Thus the density
operator is written as

$$\rho = (|0\rangle\langle 0| + |1\rangle\langle 1|)/2. \quad (4)$$

Now we introduce $|L\rangle \ (|R\rangle)$, which describes a localized
state in the left (right) side of the box, as follows

$$|L\rangle = (|0\rangle + |1\rangle)/\sqrt{2} \quad (5)$$

$$|R\rangle = (|0\rangle - |1\rangle)/\sqrt{2}. \quad (6)$$

Explicitly $|L\rangle$ is written as

$$|L\rangle = \begin{cases} \sqrt{4/L} \sin(2\pi x/L) & \text{if } 0 < x < L/2 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

$|R\rangle$ can be given in a similar way with the probability lo-
calized in the right side. One can then show that Eq. (4)
is mathematically equivalent to

$$\rho = (|L\rangle\langle L| + |R\rangle\langle R|)/2. \quad (8)$$

It means that the state is now represented as the proba-
bility mixture of the left and the right side. It is thus no
need to perform any additional measurement on which
side the particle is in since it has already been done by
the reservoir. When the wall is completely inserted the
state of the engine is not a coherent superposition of two
states $|L\rangle$ and $|R\rangle$ but rather their probability mixture.
The similar argument can be found in Ref. [19], where
once the wall is completely inserted the reservoir is con-
tacted with the engine in order to perform the isothermal
expansion. In our case, however, the reservoir should be
contacted during the whole process of inserting a wall.

III. THE ROLE OF THE THIRD LAW OF
THERMODYNAMICS

Here we prove that the entropy production, $\Delta S$, is
bounded by the entropy of a system, $S$, which guaran-
tees that $\Delta S$ vanishes as $S$ vanishes. When the wall is
inserted, the entropy of the system is expressed as

\[ S/k_B = - \sum_{m=0}^{N} \sum_{n} p_m(n) \ln p_m(n), \quad (9) \]

where \( p_m(n) \) represents the probability that the system has a discrete energy \( E_n \) when \( m \) atoms reside in the left side of the box, and \( N - m \) in the right. According to \( p_m(n) = p_m p(n|m) \), where \( p(n|m) \) is the conditional probability that the system has an energy \( E_n \), once \( m \) atoms are found in the left side, one finds

\[ S/k_B = - \sum_{m} p_m \ln p_m + \sum_{m} p_m S_m \geq \Delta S, \quad (10) \]

where \( S_m = - \sum_n p(n|m) \ln p(n|m) \). Here \( S_m \geq 0 \) and \( -\ln p_m \geq -\ln(p_m/p_m^*) \) are exploited. As temperature approaches zero, the entropy of system \( S \) and accordingly \( \Delta S \) approach zero due to the third law.

Now we consider the SZE containing a single atom with the wall inserted at \( r = x/L \), where \( x \) and \( L \) denote the distance between the wall and the left end of the box, and the size of the box, respectively. Here the box is modeled as an infinite potential well. It is shown in Fig. 2 that the entropy productions of the quantum SZE for various \( r \) vanish as \( T \to 0 \) except \( r = 0.5 \). Note that the entropy production of the classical SZE remains constant, i.e. a binary entropy \( \Delta S_{cl}(r) = -r \ln r - (1 - r) \ln(1 - r) \), independent of temperature. The deviation of the entropy production between the quantum and the classical SZE becomes prominent around \( k_B T \sim E_{sym} = |E^L_1 - E^R_1| \), where \( E^{L(R)}_n \) denotes the \( n \)th eigenenergy of the left (right) side of the box \( (n = 1, 2, \cdots) \), namely \( E^L_n = \hbar^2 n^2/8mx^2 \) and \( E^R_n = \hbar^2 n^2/8m(L-x)^2 \), where \( \hbar \) and \( m \) are the Planck constant and a mass of the atom, respectively. The reason is that if \( E^L_1 \) is larger (smaller) than \( E^R_1 \) the left (right) side of the box is predominantly occupied once \( k_B T \leq E_{sym} \) is satisfied. This is confirmed in the inset of Fig. 2, where \( \Delta S \) scaled by \( \Delta S_{cl}(r) \) as a function of \( T \) scaled by \( E_{sym} \), coalesces with each other for all \( r \), and all the curves start to bend at \( k_B T/E_{sym} \sim 1 \).

It should be noted that it was reported in Ref. [17] that the work of the quantum SZE is exactly equivalent to that of the classical one as far as a single atom is concerned. This statement is true only if the wall is inserted precisely at \( r = 0.5 \), at which the ground state exhibits the degeneracy due to the reflection symmetry. The entropy production associated with this degeneracy exactly corresponds to the classical one, namely \( \ln 2 \). In a generic case, i.e. \( r \neq 0.5 \), however, the quantum result should deviate from the classical due to the third law.

Let us discuss the meaning of the vanishing entropy production due to the third law in the context of information entropy. As temperature goes to zero, only the ground state becomes dominantly occupied. For \( 0 < r < 0.5 \), the ground state is located in the right side due to \( E^L_1 > E^R_1 \). Thus it is no doubt that the atom occupies the ground state of the right side at zero temperature so that the atom should be found in the right without any uncertainty. In the viewpoint of information entropy, the entropy is zero since there is no uncertainty for the location of the atom. It also means one cannot transfer any information or entropy to the reservoir by performing measurement and erasure. Therefore, the work cannot be extracted from the engine.

IV. TWO PARTICLE SZILARD ENGINE

If more than one atom is considered, the quantum statistical nature such as bosons and fermions comes into play. However, the third law still governs the low temperature behavior of the entropy production. When the ground state of the system is unique, the entropy production of two atoms vanishes at zero temperature no matter what they are bosons or fermions.

A. Particles without interaction

In the case of bosons, the degeneracy of the ground state occurs when the reflection symmetry takes place, that is, \( E_{sym} = 0 \). The vanishing entropy production then becomes prominent for \( T \lesssim E_{sym} \), which is clearly shown in the inset of Fig. 3 presenting the entropy production of two non-interacting spin-0 bosons. Note here that there exists another energy scale \( \Delta E = \min \{ E^L_1 - E^L_1, E^R_1 - E^R_1 \} \), at which the entropy production starts to increases as \( T \) decreases although it is not so dramatic in the inset of Fig. 3. This rather peculiar behavior is associated with the residual entropy \((2/3) \ln 3\) appearing at \( r = 0.5 \) at \( T = 0 \) [17], which is larger than the entropy production in the high temperature limit, namely \( \ln 2 \). As temperature decreases \( \Delta S \) first increases
around \( \Delta E \) and then decreases around \( E_{\text{sys}} \) (See the dashed curve in the inset of Fig. 3). Such behavior becomes obscure when \( \Delta E \lesssim E_{\text{sym}} \) (See the dashed dotted curve in the inset of Fig. 3).

Two fermions exhibit completely different behavior. It is shown in Fig. 3 that the entropy production of two non-interacting spinless fermions approaches zero even for \( r = 1/2 \). The reason is that the ground state of two fermions is non-degenerate due to the Pauli’s exclusion principle \[17]. However, at \( r = 1/3 \) as temperature decreases the entropy production first decreases but finally approaches \( \ln 2 \) (See the dashed curve in Fig. 3). This unexpected behavior is ascribed to the accidental degeneracy between the ground state of the left side and the first excited state of the right as shown in Fig. 3(a). One fermion then occupies the ground state of the right while the second fermion is allowed to occupy either the left or the right, which contributes to entropy by \( \ln 2 \).

**B. Particles with interaction**

Let us now consider more realistic situations, namely two spin-zero bosons with either attractive or repulsive interaction and two spin-1/2 fermions with either ferromagnetic or anti-ferromagnetic interaction. It is not surprising that the results will become more complicated. However, the basic principle is the same as before: how the entropy production behaves in the low temperature limit is completely determined by the third law. Now we have one more energy scale, i.e. the interaction energy. Make sure that the work can still be expressed as Eq. (1) even if the interaction between atoms takes place.

1. **Spin-0 bosons with attractive or repulsive interaction**

Here two interacting bosons are taken into account. For simplicity the interaction potential \( V \) for two bosons is modeled as follows: \( V = V_0 \), where \( V_0 \) is negative (positive) for the attractive (repulsive) interaction, if two bosons are at the same side, otherwise \( V = 0 \). For the attractive interaction there exist two degenerate ground states for \( r = 1/2 \) at zero temperature giving rise to \( \Delta S = \ln 2 \) since two atoms behave like a molecular pair by residing in the same side. This is indeed equivalent to the single atom case studied above, and becomes pronounced when \( k_B T \lesssim |V_0| \). The slight increase of \( \Delta S \) larger than \( \ln 2 \) (The dotted curve of Fig. 4) is a classical effect (See the solid curve of Fig. 4). Even in the classical case it is more likely for two atoms to reside at the same side when the attractive interaction exists, from which configuration one can extract more entropy production than a non-interacting case. For the repulsive interaction, the residual entropy at zero temperature is zero since for \( k_B T \lesssim V_0 \) two bosons considerably repel each other like two spinless fermions discussed above (See the dashed-dotted curve of Fig. 4). The similar behavior can also be observed in classical case (The dashed curve of Fig. 4). Note that these correspondences between the quantum and the classical SZE are available only at \( r = 1/2 \). As \( r \) decreases from 1/2, the entropy...
production at $k_B T/E_1 = 0.05$ rapidly vanishes for the attractive potential as shown in the inset of Fig. 4. For the repulsive potential, however, the maximum occurs at $r \sim 0.47$ since the accidental degeneracy between two configurations shown schematically in the inset of Fig. 4 can occur at $V_0 = E_{\text{sym}}$.

2. Spin-1/2 fermions with anti-ferromagnetic or ferromagnetic interaction

Now let us consider two spin-1/2 fermions with spin-spin interaction modeled as

$$ V = V_0 \hat{s}_1 \cdot \hat{s}_2 / \hbar^2, $$

where $\hat{s}_1$ and $\hat{s}_2$ represent the spin of each fermion, and $V_0$ is a positive (negative) constant for anti-ferromagnetic (ferromagnetic) interaction. The interaction potential can be rewritten as

$$ V = V_0 (S^2/2\hbar^2 - 3/4) $$

with $\vec{S} = \hat{s}_1 + \hat{s}_2$. If no interaction is considered, there exist six degenerate ground states for $r = 1/2$ at zero temperature; namely $\psi_L(1)\psi_L(2) |0, 0\rangle$, $\psi_R(1)\psi_R(2) |0, 0\rangle$, $\psi_+ |1, 1\rangle$, $\psi_- |1, 0\rangle$ and $\psi_0 |1, -1\rangle$, where $\psi_L(R)$ and $|S, M\rangle$ denote the wavefunctions of the coordinate space in the left (right) side and those of the total spin states, respectively, and $\psi_{\pm}$ represents $(1/\sqrt{2})[\psi_L(1)\psi_R(2) \pm \psi_L(2)\psi_R(1)]$. It is noted that the work can be extracted only from two of them, that is, $\psi_L(1)\psi_L(2) |0, 0\rangle$ and $\psi_R(1)\psi_R(2) |0, 0\rangle$, since the others have one fermion per each side giving rise to no pressure difference between two sides. This explains the entropy production approaches $(1/3) \ln 6$ rather than $\ln 6$ at zero temperature as shown in Fig. 5.

As far as the anti-ferromagnetic interaction is concerned, six degenerate levels are split into two groups so that the energy of the spin singlets ($S = 0$), namely $-3V_0/4$, becomes smaller than that of the triplets ($S = 1$), namely $V_0/4$, as shown in Fig. 5(a). For $k_B T \lesssim V_0$, there exist three degenerate ground states instead of six. It gives rise to $\Delta S = (2/3) \ln 3$, where $2/3$ reflects that the work is extractable from two cases among three [See the lower row of Fig. 5(a)]. For the ferromagnetic interaction, on the other hand, the opposite occurs; that is, the energy of the singlets become larger than that of the triplets. Although again the degeneracy of the ground states at zero temperature is still three, the extractable work vanishes since there exists one fermion per one side in every configuration [See the upper row of Fig. 5(a)]. When the reflection symmetry is broken, i.e. $r \neq 1/2$, the entropy production $k_B T/E_1 = 0.05$ rapidly vanishes for both the non-interacting and the anti-ferromagnetic cases as shown in the inset of Fig. 5.

For the ferromagnetic case, however, the maximum occurs at $r \sim 0.47$. This might be associated with the accidental degeneracy similar to that shown in the inset of Fig. 5. However, the story is not that simple. The accidental degeneracy between two configurations, namely $S = 0$ and $S = 1$, presented schematically in the inset of Fig. 5 indeed occurs at $r \sim 0.47$. Since $S = 1$ is triple-degenerate while $S = 0$ non-degenerate, the entropy production of such configuration is given as

$$ \Delta S = - (1/4) \ln(1/4) - (3/4) \ln(3/4). $$

However, this is smaller than $\ln 2$, the maximum value of $\Delta S(r)$.

Figure 5 schematically shows the configurations of energy levels with $r$ varied. The degeneracy between $S = 0$ and $S = 1$ takes place at $r = r_{\text{deg}}$ which satisfies $\delta E(r_{\text{deg}}) = E_{\text{sym}}(r_{\text{deg}}) - V_0 = 0$. By using Eq. (1) the entropy production can be written as

$$ \Delta S = - p_0 \ln p_0 - p_1 \ln p_1, $$

where $p_0^* = 1$ and $p_1^* \approx 1$ in zero temperature limit are exploited. Here we can safely assume $p_2 \approx 0$, implying $p_0 + p_1 \approx 1$ due to $p_2/p_m \sim e^{-\Delta E_{m}/k_B T} \ll 1$ as $T \to 0$, in which $\Delta E_{m} > 0$ denotes the energy difference between the configurations of two fermions and $m$ fermions in the left side ($m = 0, 1$). Thus $p_0$ and $p_1$ are given as

$$ p_0 = \frac{1}{3e^{-\delta E/k_B T} + 1} $$

and

$$ p_1 = \frac{3e^{-\delta E/k_B T}}{3e^{-\delta E/k_B T} + 1}, $$

where $3$ represents triple-degeneracy of $S = 1$ state. Once we have $\delta E(r_{\text{deg}}) = 0$, Eq. (13) is recovered.
FIG. 6: Schematic diagram of the energy levels depending on r. $V_0/E_1(L) = -1$ is taken leading to $r_{\text{deg}} \sim 0.47$.

As a matter of fact, Eq. (14) is maximized by $\ln 2$ when $p_0 = p_1 = 1/2$ or equivalently $\delta E/k_B T = \ln 3$ is satisfied. It looks strange that the entropy production of the non-degenerate ground state is not equal to zero, and moreover exhibits the maximum possible value. This is ascribed to finite temperature effect. For a non-zero temperature, no matter how small it is, there exist $r^*$ maximizing $\Delta S$ by $\ln 2$ once $\delta E/k_B T = \ln 3$ is fulfilled. As $T \to 0$, $r^*$ approaches $r_{\text{deg}}$ as shown in Fig. 6. Therefore, the maximum value of $\Delta S$, $\ln 2$, in the inset of Fig. 5 is correct, and it occurs not at $r = r_{\text{deg}}$ but at $r = r^*$.

V. CONCLUSION

In summary, we have shown that the third law of thermodynamics plays an important role in understanding the low temperature behavior of the SZE. When there is no degeneracy in the ground state the entropy production vanishes in the zero temperature limit. Various degeneracies generated from quantum statistical nature, symmetries, interaction, and accident determine the entropy production in the low temperature, which limits the work extractable from the SZE.

We would like to thank Takahiro Sagawa, Simone De Liberato, and Masahito Ueda for useful discussions. This was supported by the NRF grant funded by the Korea government (MEST) (No.2009-0084606, No.2009-0087261 and No.2010-0024644).

[1] L. Szilard, Z. Phys. 53, 840 (1929).
[2] H. S. Leff and A. F. Rex, Maxwell’s Demons 2 (IOP Publishing, Bristol, 2003).
[3] L. Brillouin, J. Appl. Phys. 22, 334 (1951).
[4] R. Landauer, IBM J. Res. Dev. 5, 183 (1961).
[5] C. H. Bennett, Int. J. Theor. Phys. 21, 905 (1982).
[6] K. Maruyama, F. Nori, and V. Vedral, Rev. Mod. Phys. 81, 1 (2009).
[7] M. O. Scully, M. S. Zubairy, G. S. Agarwal, and H. Walther, Science 299, 862 (2003).
[8] S. W. Kim and M.-S. Choi, Phys. Rev. Lett. 95, 226802 (2005); S. W. Kim and M.-S. Choi, J. Kor. Phys. Soc. 50, 337 (2007).
[9] M. G. Raizen, A. M. Dudaev, Q. Niu, and N. J. Fisch, Phys. Rev. Lett. 94, 053003 (2005).
[10] V. Serreli, C.-F. Lee, E. R. Kay, and D. A. Leigh, Nature 445, 523 (2007).
[11] J. J. Thorn, E. A. Schoene, T. Li, and D. A. Steck, Phys.
[12] G. N. Price, S. T. Bannerman, K. Viering, E. Narevicius, and M. G. Raizen, Phys. Rev. Lett. 100, 093004 (2008).
[13] S. Toyabe, T. Sagawa, M. Ueda, E. Muneyuki, and M. Sano, Nature Phys. 6, 988 (2010).
[14] W. Nernst, Nachr. Kgl. Ges. Wiss. Gott., 1 (1906).
[15] T. Sagawa and M. Ueda, Phys. Rev. Lett. 102, 250602 (2009).
[16] T. Sagawa and M. Ueda, Phys. Rev. Lett. 104, 090602 (2010).
[17] S. W. Kim, T. Sagawa, S. De Liberato, and M. Ueda, Phys. Rev. Lett. 106, 070401 (2011).
[18] K.-H. Kim and S. W. Kim, Phys. Rev. E 84, 012101 (2011).
[19] W. H. Zurek, arXiv:quant-ph/0301076.