The quantum refrigerator: The quest for absolute zero

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received 17 November 2008; accepted in final form 18 January 2009
published online 13 February 2009

PACS 05.30.-d - Quantum statistical mechanics
PACS 05.70.-a - Thermodynamics
PACS 07.20.Pe - Heat engines; heat pumps; heat pipes

Abstract – The emergence of the laws of thermodynamics from the laws of quantum mechanics is an unresolved issue. The generation of the third law of thermodynamics from quantum dynamics is analysed. The scaling of the optimal cooling power of a reciprocating quantum refrigerator is sought as a function of the cold bath temperature as $T_c \to 0$. The working medium consists of noninteracting particles in a harmonic potential. Two closed-form solutions of the refrigeration cycle are analyzed, and compared to a numerical optimization scheme, focusing on cooling toward zero temperature. The optimal cycle is characterized by linear relations between the heat extracted from the cold bath, the energy level spacing of the working medium and the temperature. The scaling of the optimal cooling rate is found to be proportional to $T_c^{3/2}$ giving a dynamical interpretation to the third law of thermodynamics.

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Walter Nernst stated the third law of thermodynamics as follows: “it is impossible by any procedure, no matter how idealized, to reduce any system to the absolute zero of temperature in a finite number of operations” [1, 2]. This statement has been termed the unattainability principle [3–6]. In the present study the unattainability statement is viewed dynamically as the vanishing of the cooling rate $\dot{Q}_c$ when pumping heat from a cold bath whose temperature approaches absolute zero. Finding a limiting scaling law between the rate of cooling and temperature $\dot{Q}_c \propto T_c^{\delta}$ quantifies the unattainability principle.

The second law of thermodynamics already imposes a restriction on $\delta$ [7]. For a cyclic process entropy $S$ is generated only in the baths: $\sigma = -\dot{Q}_c/T_c + \dot{Q}_h/T_h > 0$. If $\dot{Q}_h$ stays bounded, $|\dot{Q}_h| < C$, as $T_c$ approaches 0, then rearranging the inequality above gives $C/T_h > \dot{Q}_h/T_h > \dot{Q}_c/T_c$, and so $\left(\frac{T_c}{T_h}\right) T_c > \dot{Q}_c$. This forces $\dot{Q}_c \to 0$ as $T_c \to 0$ and, expanding $\dot{Q}_c$ as a series near $T_c = 0$, the dominant power $\delta$ in $\dot{Q}_c \propto T^\delta$ must satisfy $\delta \geq 1$. Such an exponent has been realized in refrigerator models [7, 8] where the source of irreversibility is the heat transfer. The vanishing of $\dot{Q}_c$ is also consistent with the vanishing of the quantum unit of heat transport $\hbar \omega / \tau$ [9].

Our goal in the present study is to set more stringent limits on the exponent $\delta$ for a reciprocating four stroke cooling cycle. The cooling rate is replaced by the average refrigeration power $R_c = \dot{Q}_c/\tau$ where $\tau$ is the cycle period.

The quantum Otto heat pump. – We consider a refrigerator using a controllable quantum medium as its working fluid. Our objective is to optimize the cooling rate in the limit when the temperature $T_c$ of the cold bath approaches absolute zero. A necessary condition for operation is that upon contact with the cold bath the temperature of the working medium be lower than the bath temperature $T_{int} < T_c$ [10]. The opposite condition exists on the hot bath. To fulfill these requirements the external controls modify the internal temperature by changing the energy level spacings of the working fluid.

The control field varies between two extreme values $\omega_c$ and $\omega_h$, where $\omega$ is a working medium frequency induced by the external field. The working medium consists of an ensemble of non-interacting particles in a harmonic potential. The Hamiltonian of this system, $\hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{K}{2} \hat{Q}^2$, is controlled by changing the curvature $K = m \omega^2$ of the confining potential.

The cooling cycle consists of two heat exchange branches alternating with two adiabatic branches (see fig. 1). The heat exchange branches (the isochores) take place with $\omega =$ constant, while the adiabatic branches take place with

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the working medium decoupled from the baths. This is reminiscent of the Otto cycle in which heat is transferred to the working medium from the hot and cold baths under constant volume conditions.

The heat carrying capacity of the working medium limits the amount of heat $Q_c$ which can be extracted from the cold bath:

$$Q_c = E_C - E_D = h\omega_c (n_C - n_D),$$

where $E_C$ is the working medium internal energy at point C (fig. 1), $E_D$ is the energy at point D and $n = \langle N \rangle$ is the expectation value of the number operator. Examining fig. 1 $n_C \leq n_C^q$ and $n_D \geq n_A$, where equality is obtained under the quantum adiabatic condition [11]. Note that the two uses of adiabatic in thermodynamics and in quantum mechanics collide here. We use adiabatic in the thermodynamic sense to mean no heat exchange. Quantum adiabatic or quasi-static means that $\omega$ is changed sufficiently slowly that a system which starts in an eigenstate of the Hamiltonian maintains this eigenstate during the evolution [11].

The resulting condition means also $n_D \geq n_D^q$, leading to $Q_c \leq h\omega_c (n_C^q - n_B^q)$. Maximum $Q_c$ is obtained for high frequency $h\omega_c \gg k_BT_h$, leading to $n_B^q = 0$ and $E_A = \frac{1}{2} h\omega_c$ being the ground state energy. Then for $T_c \to 0$

$$Q_c^* = h\omega_c n_C^q = h\omega_c e^{-\frac{h\omega_c}{k_BT_c}} \leq k_BT_c,$$

where we have substituted the value of $n_C^q$ obtained from the partition function and the last inequality is obtained by optimizing with respect to $\omega_c$ leading to $h\omega_c = k_BT_c$. The general result is that as $T_c \to 0$, $Q_c^*$ and $\omega_c^*$ become linear in $T_c$.

Only a finite cycle period $\tau$ leads to a non-vanishing cooling power $R_c = Q_c/\tau$ [12]. This cycle time $\tau = \tau_C + \tau_H + \tau_E$ is the sum of the times allocated to each branch, cf. fig. 1. An upper bound on the cooling rate $R_c$ is required to limit the exponent as $T_c \to 0$. The optimal cooling rate $R_c^{opt}$ depends on the time allocated to the different branches.

The dynamics on the adiabatic segments is generated by an externally driven time dependent Hamiltonian $\hat{H}(\omega(t))$. The equation of motion for an operator $\hat{O}$ of the working medium is

$$\frac{d\hat{O}(t)}{dt} = i\hbar [\hat{H}(t), \hat{O}(t)] + \frac{\partial \hat{O}(t)}{\partial t}.$$  (3)

Typically $[\hat{H}(t), \hat{H}(t')] \neq 0$ which leads to friction like phenomena [13,14]: too fast adiabatic segments will generate parasitic internal energy which will have to be dissipated to the heat baths, thus limiting the performance. The dynamics on the adiabatic segments is unitary, therefore the von Neumann entropy $S_{\text{ent}} = -k_B \text{tr}(\hat{\rho} \ln \hat{\rho})$ is constant. In contrast the energy entropy $S_E$ changes, where $S_E = -k_B \sum_j P_j \ln P_j$ and $P_j = \text{tr}(|j\rangle\langle j| \hat{\rho})$ is the probability of occupying the energy level $j$. Constant $S_E$ is obtained only under quasistatic conditions. Faster operation can be shown to result in an increase in the energy entropy and consequent entropy production on the following isochore branch [14]. One can therefore use the energy entropy as a gauge to determine heat production due to the finite speed of the adiabatic branch.

The external power of the compression/expansion segments is the rate of change of the internal energy of the working medium [15]. Therefore inserting $\hat{H}$ for $\hat{O}$ in equation (3) leads to the power $\frac{dE}{dt} = \mathcal{P} = \langle \frac{\partial \hat{H}}{\partial t} \rangle$. Using the Heisenberg picture, the dynamics on the heat exchange branches, termed isochores, are generated by $\mathcal{L}(\hat{O}) = \frac{1}{\hbar}[\hat{H}, \hat{O}] + \mathcal{L}_D(\hat{O})$ [16] with the dissipative Lindblad term $\mathcal{L}_D$ leading the system toward thermal equilibrium of an harmonic oscillator defined by $\omega^2 = \frac{k_B}{\hbar^2 T}$ [14]. For the dissipative dynamics, the heat flow from the cold/hot bath is $\dot{Q} = \mathcal{Q}_P = \mathcal{Q}_H$ [13,14].

At thermal equilibrium the energy expectation value is sufficient to fully characterize the state of a system. For the working medium not in equilibrium, there is a family of generalized Gibbs states [14] that completely characterize the system during the cycle. This is because starting from an arbitrary initial state, the system will relax to a unique limit cycle [17]. The states along this limit cycle are generalized Gibbs states. Note that thermal states are also included among the Gibbs states, which are defined by three operators: the time-dependent Hamiltonian $\hat{H} = \frac{1}{2m} \hat{P}^2 + \frac{K_0}{2} \hat{Q}^2$, the Lagrangian $\mathcal{L} = \frac{1}{2m} \hat{P}^2 - \frac{K_0}{2} \hat{Q}^2$ and the correlation $C = \omega(t) (\hat{Q}\hat{P} + \hat{P}\hat{Q})$. As a result $\hat{\rho} = \hat{\rho}(\hat{H}, \mathcal{L}, C)$. The invariance of the set $\hat{H}, \mathcal{L}, C$ under the equation of motion, due to this set forming a closed Lie algebra, which leads to closed equations of motion on the adiabats as well as on the isochores [14,18].

The dynamics of the operators on the adiabats is obtained from eq. (3):

$$\frac{d}{dt} \begin{pmatrix} \hat{H} \\ \mathcal{L} \\ C \end{pmatrix}(t) = \omega(t) \begin{pmatrix} 0 & \mu & -\mu \\ -\mu & 0 & -\mu \\ \mu & -\mu & 0 \end{pmatrix} \begin{pmatrix} \hat{H} \\ \mathcal{L} \\ C \end{pmatrix}(t),$$

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where $\mu = \frac{\omega}{\sqrt{\pi}}$ is the dimensionless adiabatic parameter. The power becomes: $P = \mu \omega (\mathbf{H} - \mathbf{L})$ [14,18]. The solution of eq. (4) depends on the functional form of $\omega(t)$. When $\mu \ll 1$, the number $n(t)$ will remain constant on the adiabats; these are the quasistatic conditions. For most other functions $\omega(t)$, the time evolution will involve some quantum friction [14] and $n(t) \gg n_f$ due to the resultant parasitic increase in the internal energy $\Delta E = h \omega_r (n(t) - n_f)$.

The dissipation of this energy in particular into the cold bath counters the cooling: $Q_c = h \omega_r (n(t) - n_c)$, therefore when $n_c > n_e$ the refrigerator can no longer cool.

On the isochores the energy displays an exponential approach to equilibrium:

$$\frac{d \mathbf{H}}{dt} = -\Gamma (\mathbf{H} - \langle \mathbf{H} \rangle_{eq}), \quad (5)$$

where $\Gamma = k_1 - k_1$ is the heat conductance. $\langle \mathbf{H} \rangle_{eq}$ is the equilibrium expectation of the energy. The heat transfer becomes $Q = -\Gamma (\mathbf{H} - \langle \mathbf{H} \rangle_{eq})$.

The operators $\mathbf{L}$ and $\mathbf{C}$ display an oscillatory decay to an expectation value of zero at equilibrium:

$$\frac{d}{dt} \left( \mathbf{L} \mathbf{C} \right)(t) = \left( -\Gamma - 2 \omega - \Gamma \right) \left( \mathbf{L} \mathbf{C} \right)(t). \quad (6)$$

The equations of motion (4), (5) and (6) can be solved in closed form for certain special choices of $\omega(t)$ (cf. section below) and numerically for any given functions $\omega(t)$ and time allocation to the branches. After a few cycles, the refrigerator settles down to a periodic limit cycle [17], which allows to calculate the cooling power $R_c = Q_c / \tau$ from the expectations of $\mathbf{H}, \mathbf{L}, \mathbf{C}$.

**Optimization of the cooling rate.** — For sufficiently low $T_c$, the rate limiting branch of our cycle is cooling the working medium to a temperature below $T_c$ ($A \rightarrow D$ along the expansion adiabat). As $T_c \rightarrow 0$, the total cycle time $\tau$ is of the order of the time of this cooling adiabat, $\tau_{hc}$, which tends to infinity.

Quantum friction is completely eliminated if the adiabat proceeds quasistatically with $\mu \ll 1$. This leads to a scaling law $R_c \propto T^\delta$ with $\delta \geq 3$. It turns out however that it is not the only frictionless way to reach the final state at energy $E_D = (\omega_e/\omega_h) E_A$. We describe two other possibilities which require less time and result in improved scaling, $\delta = 2$ and $\delta = 3/2$, respectively.

The first frictionless solution to eq. (4) is obtained for $\mu = const$, by changing the time variable to $\theta = \int_0^t \omega(t') dt'$. Then factoring out the term $\mu \theta$ and diagonalizing the time independent part with the eigenvalues $\lambda_0 = 0$ and $\lambda_\pm = \pm \Omega$ where $\Omega = \sqrt{\mu^2 - 4}$ leads to the adiabatic propagator $U_\theta$ of $\mathbf{H}, \mathbf{L}, \mathbf{C}$:

$$U_\theta(t) = \frac{\omega(t)}{\omega(0) \Omega^2} \begin{pmatrix} \mu^2 c - 4 & \mu \Omega s & 2 \mu (c - 1) \\ \mu \Omega s & \Omega^2 c & 2 \Omega s \\ -2 \mu (c - 1) & -2 \Omega s & \mu^2 - 4c \end{pmatrix}, \quad (7)$$

where $c = \cosh(\Omega \theta)$, $s = \sinh(\Omega \theta)$ and $\theta(t) = -\log(\omega(0)/\omega(t))/\mu$.

The cycle propagator becomes the product of the segment propagators $U_{hc} = U_t U_{hc} U_0 U_\theta$, where $U_{hc} U_\theta$ is obtained from eq. (5) and eq. (6) on the isochores.

The energy change on the expansion adiabat is the key for the optimal solution: $A \rightarrow D$:

$$E_D = \frac{1}{2} \hbar \omega_c \frac{1}{\Omega^2} \left( \mu^2 \cosh(\Omega \theta_c) - 4 \right), \quad \theta_c = -\frac{1}{\mu} \log(C), \quad (8)$$

where $C = \frac{\omega_e}{\omega_h}$ is the compression ratio and equilibration is assumed at the end of the hot isochore $E_A = \frac{1}{2} \hbar \omega_h$ for $\omega_h \rightarrow \infty$. For very fast expansion $\mu \rightarrow \infty$, $E_D = \frac{1}{2} \hbar \omega_c$ which becomes larger than $E_{eq}^c$ therefore the cooling stops due to friction. For the limit of infinite time $\mu \rightarrow 0$ leading to the frictionless result characterized by constant $n$ and $S_F$.

Then $E_D = \frac{1}{2} \hbar \omega_c$ which is the ground state of the oscillator. At this limit since $\tau \rightarrow \infty$, $R_c = 0$. The surprising point is that we can find an additional frictionless point where $n_c = n_h$, when $\cosh(\Omega \theta_c) = 1$. Then $\mu < 2$ and $\Omega$ becomes imaginary leading to the critical points

$$\mu^* = -\sqrt{\frac{2 \log(C)}{4 \pi^2 + \log(C)^2}}, \quad (9)$$

$$\tau_{hc}^* = (1 - C)/(\mu^* \omega_h). \quad (10)$$

Asymptotically as $T_c \rightarrow 0$ and $\omega_e \rightarrow 0$, the critical terms approach $\mu^* \rightarrow 2$ and with it the time allocation $\tau_{hc}^* = \frac{1}{\omega_e} - 1$. This frictionless solution with a minimum time allocation $\tau_{hc}$ scales as the inverse frequency $\omega_c^{-1}$ which is better than the quasistatic limit where $\tau_{hc} \propto \omega_c^{-2}$. As we see, it leads to $\delta = 2$.

Inspired by these findings, we sought the minimum time frictionless solution. The resulting optimal control problem [19] is solvable leading to a second closed-form solution. The optimal trajectory is of the bang-bang form with three jumps

$$\omega(t) = \begin{cases} \omega_h, & \text{for } t = 0, \\
\omega_c, & \text{for } 0 < t \leq \tau_1, \\
\omega_h, & \text{for } \tau_1 < t \leq \tau_{hc}, \\
\omega_c, & \text{for } t = \tau_{hc}, \\
\end{cases} \quad (11)$$

where $\tau_1 + \tau_2 = \tau_{hc}$ and the times $\tau_1 = \frac{1}{2 \omega_h} \arccos\left( \frac{\omega_e^2 + \omega_h^2}{(\omega_c + \omega_h)^2} \right)$ and $\tau_2 = \frac{1}{2 \omega_h} \arccos\left( \frac{\omega^2 + \omega_h^2}{(\omega_c + \omega_h)^2} \right)$ are chosen such that the number operator is preserved $n_\tau = n_1$. The minimum time allocation for $\omega_e \rightarrow 0$ which is appropriate for $T_c \rightarrow 0$ becomes $\tau_{hc}^* = \frac{1}{\omega_c^{\frac{1}{2}}}$, which is better than the solution in eq. (10). As we show below, it leads to $\delta = 3/2$.

The derivation of this optimum is based on constructing an optimal control Hamiltonian, which then is found to be linear in the control $u = \Omega / \omega_h$ (the details are found in ref. [19]). The Pontryagin maximality principle then dictates maximal or minimal frequency at any point in
the trajectory, with instant jumps between them. This is because in this case one can exclude “singular” segments, where \( v \) varies. The number of jumps and their sequence is then determined by the boundary conditions (\( \omega = \omega_R \) for \( t = 0 \) and so on), and the degrees of freedom. Thus, the above solution is derived for the case where the frequency is constrained to remain between \( \omega_R \) and \( \omega_c \) at all times.

Both frictionless solutions lead to an upper bound on the optimal cooling rate of the form

\[
R_c \leq A \omega^\nu n_c^{e\nu}, \quad (12)
\]

where \( A \) is a constant and the exponent \( \nu \) is either \( \nu = 2 \) for the \( \mu = \) const solution or \( \nu = \frac{3}{2} \) for the three-jump solution. Optimizing \( R_c \) with respect to \( \omega_c \) leads to a linear relation between \( \omega_c \) and \( T_c \), \( h_\omega = \kappa k_B T_c \). The constant \( \kappa = 2 + \mathcal{P}(-2e^{-2}) \approx 1.6 \) for \( \nu = 2 \) and \( \kappa = 3/2 + \mathcal{P}(-3/2e^{-3/2}) \approx 0.87 \) for \( \nu = \frac{3}{2} \), where \( \mathcal{P} \) is the product-log function.

Once the time allocation on the adiabats is set, the time allocation on the isochores is optimized using the method of ref. [14]:

\[
R^*_c = \frac{e^z}{1+e^{z}} \Gamma h_\omega (n_c^{eq} - n_h^{eq}), \quad (13)
\]

where \( z = \Gamma_B T_R = \Gamma_c \tau_c \) and \( z \) is determined by the equation \( 2z + (\Gamma_B T_R + \tau_c) = 2\sinh(z) \). For the limit \( T_c \to 0 \), \( \tau_c \) is large therefore \( z \) is large leading to

\[
R^*_c \approx \frac{\Gamma(\tau_c + \tau_h)}{(1+\Gamma(\tau_c + \tau_h))^2} \Gamma h_\omega (n_c^{eq} - n_h^{eq}). \quad (14)
\]

At high compression ratio \( \omega_h \gg \omega_c \) and if in addition \( \omega_c \ll \Gamma \) we obtain

\[
R^*_c \approx \Gamma h_\omega \sqrt{n_c^{eq}}, \quad (15)
\]

for the \( \mu = \) const frictionless solution, and

\[
R^*_c \approx \frac{1}{2} \Gamma h_\omega \sqrt{n_c^{eq}}, \quad (16)
\]

for the three-jump frictionless solution. Due to the linear relation between \( \omega_c \) and \( T_c \), eqs. (15) and (16) determine the exponent \( \delta \). We obtain \( \delta = 3 \) for the quasistatic scheduling, \( \delta = 2 \) for the constant \( \mu \) frictionless scheduling and \( \delta = \frac{3}{2} \) for the three-jump frictionless scheduling.

To check the optimization assumptions a numerical procedure was applied to maximize the cooling rate by adjusting the times on the four branches for a given choice of scheduling function and the external constraints on the cycle. These constraints are the coupling \( \Gamma \), the temperatures \( T_c \) and \( T_h \), and the frequencies \( \omega_c \) and \( \omega_h \).

The cooling rate optimizations employed random time allocations to the different cycle segments augmented by a guided-search algorithm. The choice of scheduling function \( \omega(t) \) determines the exponent of the scaling in \( R_c \propto T^\delta \). The optimal cooling rate for linear and exponential scheduling functions are shown in fig. 2. As a final numerical corroboration, we tried a multistep genetic algorithm allowing piecewise variation of \( \omega(t) \). The algorithm converged to a cooling rate very close to the optimal three-jump solution.

Two main observations have led to the optimal exponents as \( T_c \to 0 \), the first is that the time allocation on the expansion adiabat sets the scaling and the second is that the frictionless cycles have superior performance. Figure 2 also shows the results of numerical optimizations for the two frictionless schedules. At low temperatures the time allocated to the adiabats dominates and scales as \( \tau_c \propto 1/T_c \) for the \( \mu = \) const schedule and \( \tau_c \propto 1/T_c^2 \) for the three-jump schedule. Since \( Q_c \) for all cases is linear with \( T_c \), the asymptotic cooling rate approaches \( R_c \propto T_c^\delta \) and \( R_c \propto T_c^{3/2} \), respectively.

**Discussion and conclusion.** – The optimal quantum refrigerator in the quest to reach the absolute zero temperature shows a linear scaling of \( Q_c^* \) with \( \omega_c \) and \( T_c \). This scaling is the minimum to eliminate the divergence of the entropy generated on the cold bath. If the energy level spacing \( h_\omega \) cannot follow \( T_c \), the refrigerator will be limited by a minimum temperature. If the level spacing follows \( T_c \), the scaling of the cycle time is dominated by the scheduling function \( \omega(t) \) on the adiabats. The best results were obtained for the three-jump frictionless solutions which give \( \tau \propto \omega_c^{1/2} \). The three-jump scheduling is the minimum time frictionless solution [19]. We conjecture that the time required by any cooling cycle is limited by the adiabatic expansion [5]. The critical exponent is composed from the linear relation \( Q_c \propto T_c \) and the scaling of the minimum cycle time \( T_c^{-1/2} \). Our conjecture therefore implies that the unattainability principle is a
consequence of dynamical considerations and is limited by the exponent $R_{\text{opt}}^c \propto T_c^{3/2}$.

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We want to thank T. Feldmann for support and crucial discussions. This work was supported by the Israel Science Foundation, The Fritz Haber center is supported by the Minerva Gesellschaft für die Forschung, GmbH München, Germany. PS gratefully acknowledges the hospitality of the Hebrew University of Jerusalem and the Technical University of Chemnitz.

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