PHYSICAL REVIEW E **73**, 025107(R) (2006)

Quantum lubrication: Suppression of friction in a first-principles four-stroke heat engine

Tova Feldmann and Ronnie Kosloff[1]
[1]*Department of Physical Chemistry, Hebrew University, Jerusalem 91904, Israel*
(Received 14 September 2005; published 22 February 2006)

A quantum model of a heat engine resembling the Otto cycle is employed to explore strategies to suppress frictional losses. These losses are caused by the inability of the engine's working medium to follow adiabatically the change in the Hamiltonian during the expansion and compression stages. By adding external noise to the engine frictional losses can be suppressed.

DOI: 10.1103/PhysRevE.73.025107 PACS number(s): 05.70.Ln, 07.20.Pe

I. INTRODUCTION

Working conditions of real heat engines are far from the ideal reversible limit. Their performance is restricted by irreversible losses due to heat transport, heat leaks, and also friction. Actual working devices tend to optimize the performance by balancing the losses with maximizing work [1]. For engines producing finite power, irreversible losses are unavoidable. High-performance engines are therefore constructed from materials that reduce heat resistivity while minimizing heat leaks. In addition, lubricants are employed to reduce frictional losses. The present study explores quantum lubricants, schemes to reduce the frictional irreversible losses and thus enhance the performance of the quantum heat engine.

Quantum models of heat engines based on first principles are remarkably similar to their macroscopic counterparts [2,3]. These engines extract heat from a hot bath of temperature T_h and eject heat to a cold bath of temperature T_c. The irreversible losses due to the finite rate of heat transport have been linked to their quantum origin [4–7]. Optimal performance strategies lead to solutions where the working fluid never reaches thermodynamical equilibrium with the heat baths. Performance curves can be directly compared to those obtained in finite-time thermodynamics that employ phenomenological heat-transport laws [8,9].

Friction is the punishment for compressing or expanding the working medium too fast. In a quantum engine, compression and/or expansion is a change in an external field described by a parametrically time-dependent Hamiltonian of the working medium. Whenever the control Hamiltonian does not commute with the internal Hamiltonian of the working medium, the rapid change in the external field does not allow the state of the working medium to follow adiabatically the instantaneous energy levels [10–12]. As a result both coherences and additional energy becomes stored in the working medium. The dissipation of this additional energy in the cold bath together with the inevitable decoherence is the quantum analog of friction. The key to quantum lubrication is to suppress the creation of off-diagonal terms in the energy representation.

The quantum four-stroke Otto cycle is chosen to demonstrate the lubrication effect. The working medium is composed from interacting two-level systems. Accordingly, the uncontrolled internal Hamiltonian becomes ($\hbar=1$)

$$\hat{\mathbf{H}}_{int} = 2^{-3/2}J(\hat{\boldsymbol{\sigma}}_x^1 \otimes \hat{\boldsymbol{\sigma}}_x^2 - \hat{\boldsymbol{\sigma}}_y^1 \otimes \hat{\boldsymbol{\sigma}}_y^2) \equiv J\hat{\mathbf{B}}_2, \tag{1}$$

where $\hat{\boldsymbol{\sigma}}$ represents the spin-Pauli operators and J scales the strength of the interparticle interaction [10,11]. The external control Hamiltonian is chosen as

$$\hat{\mathbf{H}}_{ext} = 2^{-3/2}\omega(t)\left(\hat{\boldsymbol{\sigma}}_z^1 \otimes \hat{\mathbf{I}}^2 + \hat{\mathbf{I}}^1 \otimes \hat{\boldsymbol{\sigma}}_z^2\right) \equiv \omega(t)\hat{\mathbf{B}}_1, \tag{2}$$

where $\omega(t)$ represents the external field. The total Hamiltonian becomes

$$\hat{\mathbf{H}} = \omega(t)\hat{\mathbf{B}}_1 + \mathrm{J}\hat{\mathbf{B}}_2, \tag{3}$$

where $\Omega(t)=\sqrt{\omega^2+J^2}$ defines the temporary energy scale. At various times $\hat{\mathbf{H}}(t)$ does not commute with itself since $[\hat{\mathbf{B}}_1,\hat{\mathbf{B}}_2]\equiv\sqrt{2}i\hat{\mathbf{B}}_3\neq 0$, $[\hat{\mathbf{B}}_3=2^{-3/2}(\hat{\boldsymbol{\sigma}}_y^1\otimes\hat{\boldsymbol{\sigma}}_x^2+\hat{\boldsymbol{\sigma}}_x^1\otimes\hat{\boldsymbol{\sigma}}_y^2)]$. The set of operators $\{\hat{\mathbf{B}}\}$ forms a closed orthogonal Lie algebra. In addition, $(\hat{\mathbf{B}}_k\cdot\hat{\mathbf{B}}_j)=\mathrm{tr}\,\{\hat{\mathbf{B}}_k^\dagger\hat{\mathbf{B}}_j\}=\delta_{kj}$ and $\mathrm{tr}\,\{\hat{\mathbf{B}}_k\}=0$. The irreversible equations of motion for this set are $d\hat{\mathbf{B}}/dt=i[\hat{\mathbf{H}},\hat{\mathbf{B}}]+\mathcal{L}_D^*(\hat{\mathbf{B}})$ where $\mathcal{L}_D^*$ is the dissipative Liouville superoperator defined in Eq. (9). A thermodynamical description requires that the set of variables $\{\mathbf{b}(t)\}=\{\langle\hat{\mathbf{B}}\rangle\}$ should be closed to the dynamics generated on all branches of the engine's cycle.

The energy balance of the engine is composed of the heat flow and power

$$\frac{dE}{dt} = \mathcal{P} + \dot{\mathcal{Q}}, \tag{4}$$

where $\mathcal{P}=\langle\partial\hat{\mathbf{H}}/\partial t\rangle=\dot{\omega}\langle\hat{\mathbf{B}}_1\rangle$, and $\dot{\mathcal{Q}}=\langle\mathcal{L}_D^*(\hat{\mathbf{H}})\rangle$.

The state of the working medium $\hat{\boldsymbol{\rho}}$ can be reconstructed from five thermodynamical variables $b_{\mathbf{k}}=\langle\hat{\mathbf{B}}_k\rangle$ composed of the expectation of the three operators in the Lie algebra and two additional ones, $\hat{\mathbf{B}}_4=2^{-3/2}(\hat{\boldsymbol{\sigma}}_z^1\otimes\hat{\mathbf{I}}^2)-\hat{\mathbf{I}}^1\otimes\hat{\boldsymbol{\sigma}}_z^2)$ and $\hat{\mathbf{B}}_5=\frac{1}{2}\hat{\boldsymbol{\sigma}}_z^1\otimes\hat{\boldsymbol{\sigma}}_z^2$ [11], leading to

$$\hat{\boldsymbol{\rho}} = \frac{1}{N}\mathbf{I} + \sum_{\mathbf{k}} b_{\mathbf{k}}\hat{\mathbf{B}}_k. \tag{5}$$

The occupation probability p_n of the energy level n defines the energy entropy

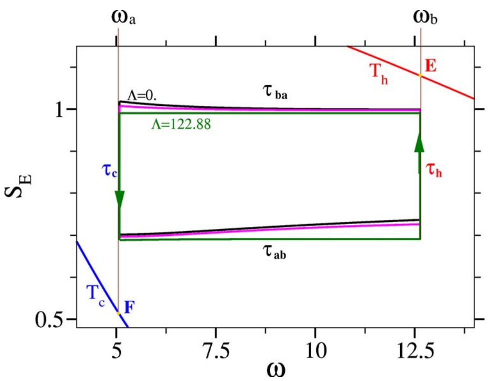

FIG. 1. (Color online) Three cycles of the heat engine in the $(\omega,\mathcal{S}_E)$ plane (dimensional units $\hbar=1,k_b=1$). The common values are: $J=2.0$, $T_h=7.5$, $T_c=1.5$, $\omega_a=5.083\,64$, $\omega_b=12.6355$, heat-transfer rates $\Gamma_h=\Gamma_c=1.167\,48$, and dephasing rates $\gamma_h=-0.05$, $\gamma_c=-0.06$. $\Lambda_{ba}=\Lambda_{ab}=0$ [Eq. (11)] for the unlubricated cycle (black), $\Lambda_{ba}=1.28$, $\Lambda_{ab}=0.64$ for the intermediate cycle (red), and $\Lambda_{ba}=122.88$, $\Lambda_{ab}=61.44$ for the strongly lubricated cycle (green). The time allocations on the different branches correspond to the optimal engine's power, when $\Lambda_{ba}=\Lambda_{ab}=0$. The optimal time allocations are $\tau_h=1.0795, \tau_{ba}=0.01478$, $\tau_c=1.0088$, and $\tau_{ab}=0.0069$. The points **E** and **F** represent the equilibrium points of the hot and cold isochores.

$$\mathcal{S}_E=-\sum_n p_n \ln p_n. \tag{6}$$

If $[\hat{\boldsymbol{\rho}},\hat{\mathbf{H}}]\neq 0$ then this entropy is different from the von Neumann entropy,

$$\mathcal{S}=-\,\mathrm{tr}\,\{\hat{\boldsymbol{\rho}}\ln\hat{\boldsymbol{\rho}}\}, \tag{7}$$

and $\mathcal{S}_E\geqslant\mathcal{S}$. The difference between $\mathcal{S}_E$ and $\mathcal{S}$ is a signature of friction [12]. The external entropy production is a measure of the irreversible dissipation to the hot and cold baths,

$$\Delta S^u=-\left(\frac{\mathcal{Q}_h}{T_h}+\frac{\mathcal{Q}_c}{T_c}\right)\geqslant 0, \tag{8}$$

where $\mathcal{Q}_h$ and $\mathcal{Q}_c$ are the heat dissipated to the hot or cold baths, respectively.

II. THE CYCLE OF OPERATION

A four-stroke cycle of operation is studied. As shown in Fig. 1 this cycle includes (i) an adiabatic expansion branch where an external field is chosen to decrease linearly from ω_b to ω_a in a time τ_{ba}; (ii) a cold isochoric branch where heat is transferred from the working medium to the cold bath (T_c) in a time τ_c; (iii) an adiabatic compression branch where an external field is increased linearly from ω_a to ω_b in a time τ_{ab}; and (iv) a hot isochoric branch where heat is transferred from the hot bath at temperature T_h to the working medium in a time τ_h.

This cycle is a quantum model of the macroscopic Otto cycle. The control parameters are the time allocations on the different branches, the total cycle time, and the extreme values of the external field.

The cycle of the engine becomes a sequence of four completely positive maps that define the different branches. Eventually this sequence closes upon itself. Repetition of the sequence of controls leads to steady-state operational conditions or a limit cycle [12]. The map $\mathcal{U}_k$ relates the initial set of these operators to their final values for each of the engine branches. These maps are obtained by solving the equations of motion for the set of operators $\{\hat{\mathbf{B}}\}$. The overall cycle map is the product of the individual maps of each branch $\mathcal{U}=\mathcal{U}_{ab}\mathcal{U}_c\mathcal{U}_{ba}\mathcal{U}_h$ [11,12].

On the isochores the maps $\mathcal{U}_{h/c}$ are generated by the completely positive generator $\mathcal{L}^*$ [13] with the dissipative term $\mathcal{L}_D^*$, which leads to thermal equilibrium;

$$\mathcal{L}_D^*(\hat{\mathbf{B}})=k_\downarrow\left(\hat{\mathbf{L}}_+\hat{\mathbf{B}}\hat{\mathbf{L}}_- -\frac{1}{2}\{\hat{\mathbf{L}}_+\hat{\mathbf{L}}_-,\hat{\mathbf{B}}\}\right)+k_\uparrow\left(\hat{\mathbf{L}}_-\hat{\mathbf{B}}\hat{\mathbf{L}}_+ -\frac{1}{2}\{\hat{\mathbf{L}}_-\hat{\mathbf{L}}_+,\hat{\mathbf{B}}\}\right). \tag{9}$$

The operators $\hat{\mathbf{L}}_\pm=(1/\sqrt{2}\Omega)(\omega\hat{\mathbf{B}}_2-J\hat{\mathbf{B}}_1\pm i\Omega\hat{\mathbf{B}}_3)$ are the raising and/or lowering operators of $\hat{\mathbf{H}}$, $[\hat{\mathbf{H}},\hat{\mathbf{L}}_\pm]=\pm\sqrt{2}\Omega\hat{\mathbf{L}}_\pm$. Thermal equilibrium is obtained by forcing detailed balance $k_\uparrow/k_\downarrow=e^{-\Omega/\sqrt{2}T}$ ($k_B=1$). The rate of equilibration becomes $\Gamma=k_\uparrow+k_\downarrow$. $\mathcal{L}_D^*$ also degrades the off-diagonal elements of $\hat{\boldsymbol{\rho}}_e$, interpreted either as decoherence or as dephasing. The dephasing time T_2 becomes identical to the energy equilibration time $T_2=T_1=1/\Gamma$. The dissipation also has to eliminate the additional energy accumulated on the adiabat. Degrading the coherences causes the frictional process to become irreversible [11,12]. The interaction of the working medium with the bath can also be elastic. These encounters will scramble the phases conjugate to the energy, and the associated decay time is termed pure dephasing (T_2^*). In Lindblad's formulation it becomes $\mathcal{L}_{De}^*(\hat{\mathbf{B}})=-\gamma[\hat{\mathbf{H}},[\hat{\mathbf{H}},\hat{\mathbf{B}}]]$ and $T_2^*=1/2\gamma\Omega^2$. Note that elastic medium cannot transfer or absorb heat.

On the adiabats, the varying field $\omega(t)$ causes an explicit time dependence of $\hat{\mathbf{H}}$ $(d\hat{\mathbf{B}}/dt)=i[\hat{\mathbf{H}}(t),\hat{\mathbf{B}}]$. Since the energy eigenvalues change, even if initially $[\hat{\boldsymbol{\rho}},\hat{\mathbf{H}}]=0$ the state $\hat{\boldsymbol{\rho}}$ will develop off-diagonal terms in the energy frame [cf. Eq. (B6) in Ref. [12]]. The effect on the external power $\mathcal{P}=\dot{\omega}b_1$ is made explicit by decomposing $\mathcal{P}$ to diagonal and off-diagonal terms in the energy representation,

$$\mathcal{P}=\frac{\dot{\Omega}}{\Omega}\langle\hat{\mathbf{H}}\rangle-\frac{\dot{\omega}J}{\Omega}\sqrt{2}\langle\hat{\mathbf{L}}_+ +\hat{\mathbf{L}}_-\rangle. \tag{10}$$

The first diagonal term represents the power required to compress or decompress the working fluid $\mathcal{P}^{field}=(\dot{\Omega}/\Omega)\langle\hat{\mathbf{H}}\rangle$, the second term in Eq. (10) is the additional power required to drive the working fluid in a finite rate $\mathcal{P}^{friction}-(\dot{\omega}J/\Omega)\sqrt{2}\langle\hat{\mathbf{L}}_+ +\hat{\mathbf{L}}_-\rangle$, interpreted as the power invested against friction; therefore it vanishes when $J=0$ or $\dot{\omega}=0$ [14].

III. QUANTUM LUBRICATION

A good lubricant should be able to increase the overall optimal power of the engine. The insight that energy coher-

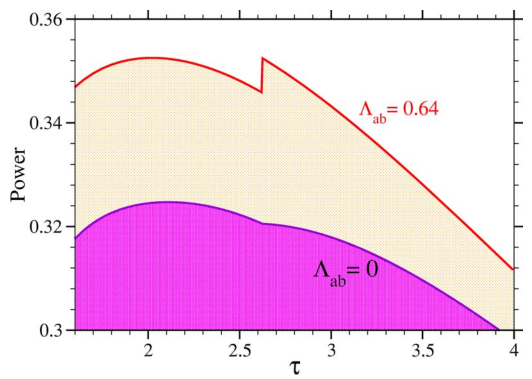

FIG. 2. (Color online) The optimal power $\mathcal{P}$ as function of cycle time τ with and without the quantum lubricant. The optimization is with respect to the time allocations for $\Lambda_{ba}=\Lambda_{ab}=0$ (lower line). The power with the lubrication $\Lambda_{ba}=1.28\Lambda_{ab}=0.64$ (top line). All the other parameters are as in Fig. 1.

ences leads to frictional losses suggests that forcing the cycle trajectory to follow adiabatically the instantaneous energy levels will be beneficial.

The quantum "lubricant" has to suppress the creation of the energy coherences on the adiabats. Formally this can be described by a generator of dephasing in the equations of motion for the set $\{\hat{\mathbf{B}}\}$ on the adiabat,

$$\frac{d\hat{\mathbf{B}}}{dt} = i[\hat{\mathbf{H}},\hat{\mathbf{B}}] - \Lambda[\hat{\mathbf{H}},[\hat{\mathbf{H}},\hat{\mathbf{B}}]] \tag{11}$$

and Λ is the dephasing lubricating coefficient.

The success of this approach is shown in Fig. 2. As a reference the optimal power of the engine as a function of cycle time is shown in the vicinity of the global power maximum. Each point on the graph is optimized with respect to the time allocations on the four branches of the cycle using a random search procedure. Employing these time allocations, the power of the engine is recalculated with the addition of the lubricating term on the adiabats $\Lambda \neq 0$. It is clear in Fig. 2 that in the interval of cycle times near the maximum power the lubricated engine outperforms the optimal solutions of the reference engine. The lubricated maximum power point also moves to shorter cycle times.

For longer time allocations on the adiabats where less external power is consumed to overcome the friction, the performance enhancement due to dephasing decreased, eventually leading to a crossover where dephasing on the adiabats decreased the power. For larger J values we also found that dephasing was not able to improve the performance.

Figure 3 shows the accumulated work against friction $\mathcal{W}^{friction}=\int\mathcal{P}^{friction}dt=\int\sqrt{2}(\dot{\omega}J/\Omega)\langle\hat{\mathbf{L}}_{+}+\hat{\mathbf{L}}_{-}\rangle dt$ [cf. Eq. (10)] as a function of time on the adiabat for a increasing dephasing parameter. The main point is that increasing dephasing eliminates the work against friction. This improvement saturates once $\mathcal{W}^{friction}$ is eliminated.

Another consequence of the quantum lubrication is that the energy entropy $\mathcal{S}_E$ does not increase on the adiabats as can be seen in Fig. 1. As a result the energy entropy $\mathcal{S}_E$ approaches the von Neumann entropy $\mathcal{S}$, Eq. (7). These results establish the principle of quantum lubrication, maintaining the working fluid in a diagonal state in the energy representation.

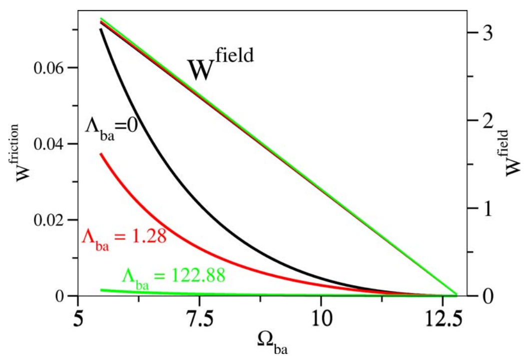

FIG. 3. (Color online) The work performed by the engine on the adiabat $b\to a$ branch, separated into $W^{friction}$ (left scale) and W^{field} (right scale) for different dephasing values as a function of $\Omega_{ba}(t)$. W^{field} has only a weak dependence on the dephasing lubricating value Λ. The cycle parameter values are as in Fig. 1.

Suppression of friction requires a method to synthesize dephasing on the adiabats. The dynamics of the working medium has to be changed from unitary to dissipative. The obvious approach of adding a dissipative bath on the adiabatic branches is difficult to achieve. Such a bath should have only elastic encounters with a system with a time-dependent Hamiltonian.

The solution is to employ the external controls of the engine to synthesize the dissipation. The idea comes from the singular bath limit, a bath generated from a system operator coupled to a delta correlated noise $\hat{\mathbf{H}}_{sr}=\hat{\mathbf{A}}_s g(t)$ where $\langle g(t)g(t')\rangle_r=\gamma_g\delta(t-t')$ where the average is taken over the bath fluctuations. The Liouville generator associated with this system bath coupling becomes $\mathcal{L}^*(\hat{\mathbf{X}}) =-(\gamma_g^2/2)[\hat{\mathbf{A}}_s,[\hat{\mathbf{A}}_s,\hat{\mathbf{X}}]]$ [15,16].

To implement such a scheme random noise is added to the external controls of the engine. The implementation divides the adiabat branch into N segments. In each of these segments, the external field ω is constant and is chosen to be (for the $a\to b$ adiabat): $\omega_k=\omega_a+k(\omega_b-\omega_a)/N$ for the kth segment. The short time propagator on the k segment for the set $\hat{\mathbf{B}}$ becomes

$$\mathcal{U}_k\hat{\mathbf{B}} = e^{i\hat{\mathbf{H}}(\omega_k)\Delta t_k}\hat{\mathbf{B}}e^{-i\hat{\mathbf{H}}(\omega_k)\Delta t_k}, \tag{12}$$

where Δt_k is the time interval of the kth segment. At this point random noise is added to the time interval

$$\Delta t_k = \frac{\tau_{ab}}{N}(1+r), \tag{13}$$

where r is a random number with zero mean and variance σ. Expanding the propagator Eq. (12) to second order and averaging over the random noise will lead to the average generator for the k time segment: $\mathcal{L}_k^*(\hat{\mathbf{B}})=i[\hat{\mathbf{H}}(\omega_k),\hat{\mathbf{B}}] -(N\sigma^2/2\tau_{ad})[\hat{\mathbf{H}}(\omega_k),[\hat{\mathbf{H}}(\omega_k),\hat{\mathbf{B}}]]$. In the limit when $N\to\infty$

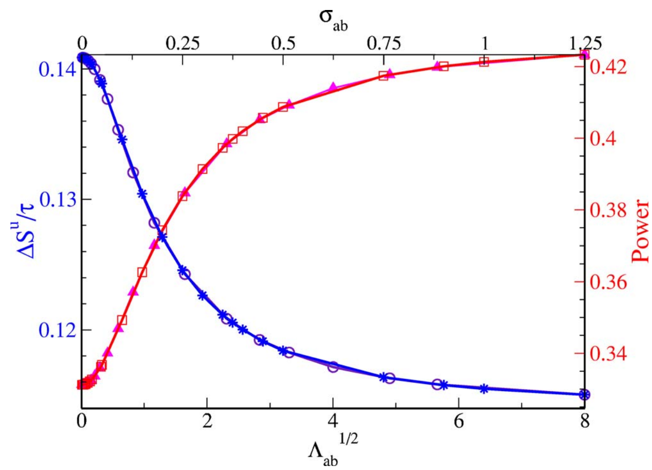

FIG. 4. (Color online) Power (right scale, red online) and entropy production (left scale, blue online) as a function of the dephasing parameter $\Lambda_{ab}^{1/2}$ and the variance, σ_{ab} of the random fluctuations of the time segment on the adiabats (upper scale). The dephasing synthesis results are represented by stars and filled triangles. The empty circles and squares represent the dephasing dynamics. The calculations were performed with $\Lambda_{ab}/\Lambda_{ba}=\sigma_{ab}/\sigma_{ba}$.

this average propagator becomes identical to Eq. (11) provided $\sigma=\sqrt{2\tau_{ad}\Lambda/N}$.

The addition of random noise means that the individual cycle has to be replaced by the average performance on many cycles. As a result, only an average cycle time can be defined. This noisy lubrication procedure was simulated with $N=200$ on both adiabats. The power and other thermodynamic variables were calculated as an average of 2000 cycles. Convergence was checked by continuing this averaging 1000 additional times.

Figure 4 compares the power $\mathcal{P}$ and entropy production per cycle, $\Delta S^u/\tau$ calculated by the two methods for the time allocations of the maximum power point. It is clear that the results obtained by imposing dephasing on the adiabats Eq. (11) are identical to the dephasing synthesis Eq. (12). The signature of lubrication is the reduction of entropy production which accompanies the increase in power. This is contrary to optimizing the power with respect to heat transport. In that case the increase in output power is accompanied by an increase in entropy production [14]. The choice of the procedure to generate dephasing is unique. For example, adding the random noise to the frequency ω_k at each time segment has been tested. The performance of the engine only became worse. The reason is that such a term leads to the dissipative generator $\mathcal{L}_D(\hat{\mathbf{A}})=-(\gamma_g/2)[\hat{\mathbf{B}}_1,[\hat{\mathbf{B}}_1,\hat{\mathbf{A}}]]$, which does not eliminate the off-diagonal elements in the energy representation.

The present study should be related to other recent work. For example, adding mechanical noise to a quantum refrigerator has been shown experimentally to cool atoms in a magnetic trap [17]. It seems that the mechanism involves inducing nonunitary dynamics. Contrary to the present study, in other scenarios coherence can be beneficial. Without violating the second law, Scully *et al.* [18] showed that additional work can be extracted from the coherences in a quantum heat engine.

To summarize, frictional losses are caused whenever $[\hat{\mathbf{H}}_{ext},\hat{\mathbf{H}}_{int}]\neq 0$. Then the fast dynamics induces coherences in the energy frame. The essence of quantum lubrication is suppressing the generation of these off-diagonal elements in the energy representation. The present model demonstrates how externally induced noise can achieve this task.

ACKNOWLEDGMENTS

This work was supported by the Israel Science Foundation. We want to thank Lajos Diósi, David Tannor, and Peter Salamon for many helpful discussions, and Moshe Goldstein for the random number generator.

[1] P. Salamon, J. D. Nulton, G. Siragusa, T. R. Andersen, and A. Limon, Energy **26**, 307 (2001).
[2] T. D. Kieu, Phys. Rev. Lett. **93**, 140403 (2004).
[3] K. H. Hoffmann, Ann. Phys. **10**, 79 (2002).
[4] Eitan Geva and Ronnie Kosloff, J. Chem. Phys. **96**, 3054 (1992).
[5] Eitan Geva and Ronnie Kosloff, J. Chem. Phys. **97**, 4398 (1992).
[6] Tova Feldmann, Eitan Geva, Ronnie Kosloff, and Peter Salamon, Am. J. Phys. **64**, 485 (1996).
[7] Eitan Geva and Ronnie Kosloff, J. Chem. Phys. **104**, 7681 (1996).
[8] F. Curzon and B. Ahlborn, Am. J. Phys. **43**, 22 (1975).
[9] P. Salamon, A. Nitzan, B. Andresen, and R. S. Berry, Phys. Rev. A **21**, 2115 (1980).
[10] Ronnie Kosloff and Tova Feldmann, Phys. Rev. E **65**, 055102(R) (2002).
[11] Tova Feldmann and Ronnie Kosloff, Phys. Rev. E **68**, 016101 (2003).
[12] Tova Feldmann and Ronnie Kosloff, Phys. Rev. E **70**, 046110 (2004).
[13] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976).
[14] Tova Feldmann and Ronnie Kosloff, Phys. Rev. E **61**, 4774 (2000).
[15] V. Gorini and A. Kossakowski, J. Math. Phys. **17**, 1298 (1976).
[16] R. S. Ingarden and A. Kossakowski, Ann. Phys. **89**, 451 (1975).
[17] M. Kumakura, Y. Shirahata, Y. Takasu, Y. Takahashi, and T. Yabuzaki, Phys. Rev. A **68**, 021401(R) (2003).
[18] M. O. Scully, M. S. Zubairy, G. S. Agarwal, and H. Walther, Science **299**, 862 (2003).