Energetics of Quantum Brownian Oscillators

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Outline

Introduction

- Recall that the problem of classical Brownian motion deals with the motion of a suspended particle in a fluid – A prototypical example of a microscopic system + bath scenario.
- Quantum Brownian motion refers to the dissipative dynamics of a (quantum) particle that is coupled with a (quantum) heat bath [Weiss, Quantum Dissipative Systems, 2nd ed., World Scientific (1999)].
- Full Hamiltonian:

$$H = H_{\mathrm{S}} + H_{\mathrm{B}} + H_{\mathrm{SB}}. \tag{1}$$

- Two ways to approach the problem:
  1. Heisenberg-picture formalism, i.e., based on (reduced) Heisenberg equations for the system observables.
  2. Schrödinger-picture formalism, i.e., based on a master equation describing the dynamics of the (reduced) density operator.
- Here we focus on the Heisenberg-picture formalism.

Independent-Oscillator Model

- One can model the heat bath as being composed of an infinite number of independent quantum oscillators; taking a bilinear system-bath coupling, the full Hamiltonian reads as [Feynman-Vernon (1963), Ford-Kac-Mazur (1965), Caldeira-Leggett (1981)]

$$H = \frac{p^2}{2m} + \frac{m\omega_0^2 x^2}{2} + \sum_{j=1}^{N} \left[\frac{p_j^2}{2m_j} + \frac{m_j\omega_j^2}{2} \left(q_j - \frac{c_j}{m_j\omega_j^2} x \right)^2 \right], \qquad (2)$$

where $m, m_j, \omega_0, \omega_j, c_j > 0$, $[x, p] = i\hbar$, and $[q_j, p_k] = i\hbar\delta_{j,k}$.

- Quantum Langevin equation [Ford et al., PRA 37, 4419 (1988)]:

$$m\ddot{x}(t) + \int_0^t \mu(t-t')\dot{x}(t')dt' + m\omega_0^2 x(t) = f(t), \qquad (3)$$

where

$$\mu(\tau) = \sum_{j=1}^{N} \frac{c_j^2}{m_j\omega_j^2} \cos(\omega_j \tau)\Theta(\tau). \qquad (4)$$

Bath-Induced Noise

- In the quantum Langevin equation, $f(t)$ is an operator-valued **noise**:

$$f(t) = \sum_{j=1}^{N} c_j \left[q_j(0)\cos(\omega_j t) + \frac{p_j(0)}{m_j\omega_j}\sin(\omega_j t) \right] - \mu(t)x(0). \quad (5)$$

- Initial distribution:

$$\rho_{\mathrm{B+SB}}(0) = \frac{1}{\Lambda}\exp\left[-\beta \sum_{j=1}^{N} \left\{ \frac{p_j^2(0)}{2m_j} + \frac{1}{2}m_j\omega_j^2 \left(q_j(0) - \frac{c_j x(0)}{m_j\omega_j^2} \right)^2 \right\} \right]. \quad (6)$$

- Statistical properties of the noise:

$$\langle\{f(t), f(t')\}\rangle = \frac{2}{\pi}\int_0^\infty d\omega\hbar\omega\mathrm{Re}[\tilde{\mu}(\omega)]\coth\left(\frac{\hbar\omega}{2k_B T}\right)\cos[\omega(t-t')], \quad (7)$$

$$\langle[f(t), f(t')]\rangle = \frac{2}{i\pi}\int_0^\infty d\omega\hbar\omega\mathrm{Re}[\tilde{\mu}(\omega)]\sin[\omega(t-t')]. \quad (8)$$

Mean Energies

- The mean kinetic and potential energies are obtained by equal-time velocity and position correlation functions. In the steady state, we get the mean kinetic and potential energies as

$$E_k = \lim_{t\to\infty} \frac{m}{2}\langle \dot{x}(t)\dot{x}(t)\rangle, \qquad E_p = \lim_{t\to\infty} \frac{m\omega_0^2}{2}\langle x(t)x(t)\rangle. \tag{9}$$

- Solving the quantum Langevin equation, we find

$$E_k(T) = \frac{2m}{\pi}\int_0^\infty \mathrm{Im}[\alpha(\omega)]\omega\epsilon_k(\omega, T)d\omega, \tag{10}$$

$$E_p(T) = \frac{2m\omega_0^2}{\pi}\int_0^\infty \frac{\mathrm{Im}[\alpha(\omega)]}{\omega}\epsilon_p(\omega, T)d\omega, \tag{11}$$

$$\epsilon_{k,p}(\omega, T) = \frac{\hbar\omega}{4}\coth\left(\frac{\hbar\omega}{2k_B T}\right), \tag{12}$$

$$\alpha(\omega) = [m(\omega_0^2 - \omega^2) - i\omega\tilde{\mu}(\omega)]^{-1}. \tag{13}$$

Quantum Energy Partition

- We define the (probability distributions)

$$P_k(\omega) = \frac{2m}{\pi}\mathrm{Im}[\alpha(\omega)]\omega, \qquad P_p(\omega) = \frac{2m\omega_0^2}{\pi}\frac{\mathrm{Im}[\alpha(\omega)]}{\omega}, \tag{14}$$

which satisfy $P_{k,p}(\omega) \geq 0$, $\forall\omega \in [0,\infty)$ and $\int_0^\infty P_{k,p}(\omega)d\omega = 1$.

- This allows us to write

$$E_{k,p}(T) = \int_0^\infty \epsilon_{k,p}(\omega, T)P_{k,p}(\omega)d\omega, \tag{15}$$

- The thermally-averaged energies arise as a sum of contributions from bath oscillators with different frequencies with $\epsilon_{k,p}(\omega, T)P_{k,p}(\omega)d\omega$ being the contribution from bath oscillators in the frequency range from ω to $\omega + d\omega$.

- In the classical limit, we have $\epsilon \to k_B T/2$, which gives

$$E_{k,p}(T) = \frac{k_B T}{2}\int_0^\infty P_{k,p}(\omega)d\omega = \frac{k_B T}{2}. \tag{16}$$

Illustrative Example: Ohmic Dissipation

- Let us adopt the Ohmic model of dissipation in which we have $\mu(t) = 2m\gamma\delta(t)$ or equivalently, $\tilde{\mu}(\omega) = m\gamma$.
- This gives
$$P_k(\omega) = \frac{2\omega^2}{\pi}\frac{\gamma}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}, \tag{17}$$
and
$$P_p(\omega) = \frac{2\omega_0^2}{\pi}\frac{\gamma}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}, \tag{18}$$
which can be observed to be positive definite and may be verified by explicit integration to be normalized.
- Note, however, that for the Ohmic dissipation model, the mean kinetic energy diverges; this is regularized by imposing a finite memory timescale in the dissipation kernel. One choice is $\mu(t) \sim e^{-\omega_{\mathrm{cut}} t}$, which is called the Drude model.

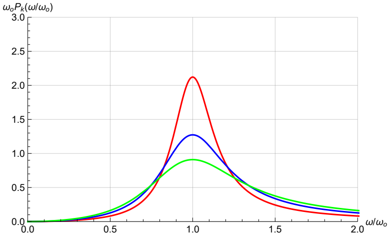


Figure: $\omega_0 P_k(\omega/\omega_0)$ for $\gamma = 0.3\omega_0$ (red), $\gamma = 0.5\omega_0$ (blue) and $\gamma = 0.7\omega_0$ (green).

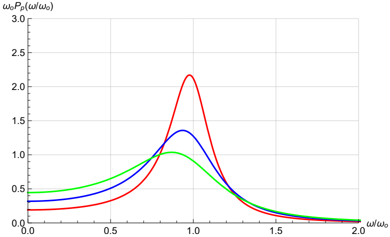


Figure: $\omega_0 P_p(\omega/\omega_0)$ for $\gamma = 0.3\omega_0$ (red), $\gamma = 0.5\omega_0$ (blue) and $\gamma = 0.7\omega_0$ (green).

Two Notions of Energy

- The mean energy can be defined as $E(T) = E_k(T) + E_p(T)$, which coincides with $\langle H_{\mathrm{S}} \rangle$ averaged over the ensemble of bath-induced noise.
- Alternatively, one can define an 'internal energy' as

$$\begin{aligned} U(T) &= \langle H \rangle_{\rho_H} - \langle H_{\mathrm{B}} \rangle_{\rho_{H_{\mathrm{B}}}}, \\ &= \frac{\mathrm{Tr}(e^{-H/k_B T} H)}{Z} - \frac{\mathrm{Tr}(e^{-H_{\mathrm{B}}/k_B T} H_{\mathrm{B}})}{Z_{\mathrm{B}}}. \end{aligned} \tag{19}$$

- Explicitly, we have $\tilde{U}(T) = \langle H \rangle_{\rho_H}$ and $U_{\mathrm{B}}(T) = \langle H_{\mathrm{B}} \rangle_{\rho_{H_{\mathrm{B}}}}$, where

$$U_{\mathrm{B}}(T) = \sum_{j=1}^{N} \frac{\hbar\omega_j}{2} \coth\left(\frac{\hbar\omega_j}{2k_B T}\right), \quad \tilde{U}(T) = \sum_{k=0}^{N} \frac{\hbar\Omega_k}{2} \coth\left(\frac{\hbar\Omega_k}{2k_B T}\right), \tag{20}$$

where $\{\omega_j\}$ are the heat-bath frequencies and $\{\Omega_k\}$ are the normal-mode frequencies of the coupled system+bath.

Partition of Internal Energy

- It follows that the internal energy may be expressed as

$$U(T) = \frac{1}{\pi}\int_0^\infty \epsilon(\omega, T)\mathrm{Im}\left[\frac{d}{d\omega}\ln[\alpha(\omega)]\right]d\omega, \tag{21}$$

where $\epsilon(\omega, T) = \epsilon_k(\omega, T) + \epsilon_p(\omega, T) = \frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_B T}\right)$.

- Some straightforward manipulations reveal that

$$\frac{1}{\pi}\mathrm{Im}\left[\frac{d}{d\omega}\ln\alpha(\omega)\right] \tag{22}$$
$$= \sum_{k=0}^{N}\left[\delta(\omega-\Omega_k)+\delta(\omega+\Omega_k)\right] - \sum_{j=1}^{N}\left[\delta(\omega-\omega_j)+\delta(\omega+\omega_j)\right],$$

which is positive definite and normalized [J. K., Ghosh, and Bandyopadhyay, Physica A 599, 127466 (2022)].

Energy Functions Vs γ

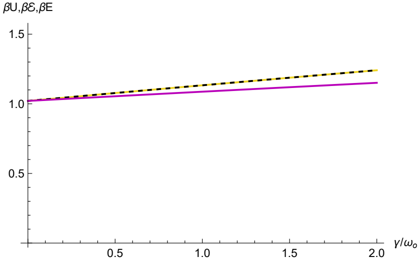


Figure: Dimensionless energy functions βU (black-dashed), $\beta\mathcal{E}$ (yellow-solid), and βE (violet-solid) for the dissipative quantum oscillator as a function γ/ω_0, for $\alpha = \beta\hbar\omega_0 = 0.5$ and $\omega_{\rm cut} = 10\omega_0$; here $\mu(t) \sim e^{-\omega_{\rm cut} t}$ and $\mathcal{E}$ is the energy function found from the partition function obtained via Euclidean path integrals. We have taken $\omega_0 = 1$.

Energy Functions Vs $\hbar\omega_0/k_B T$

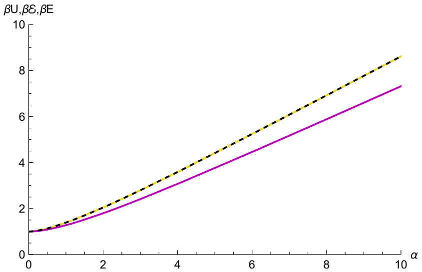


Figure: Dimensionless energy functions βU (black-dashed), $\beta\mathcal{E}$ (yellow-solid), and βE (violet-solid) for the dissipative quantum oscillator, as a function $\alpha = \beta\hbar\omega_0$, for $\gamma = \omega_0$ and $\omega_{\rm cut} = 10\omega_0$; here $\mu(t) \sim e^{-\omega_{\rm cut} t}$ and $\mathcal{E}$ is the energy function found from the partition function obtained via Euclidean path integrals. We have taken $\omega_0 = 1$.

Weak-Coupling Limit

- At weak system-bath coupling, the initial density matrix is factorizable as $\rho(0) = \rho_{\mathrm{S}}(0) \otimes \rho_{\mathrm{B}}(0)$, as in the Born approximation.
- The weak-coupling limit corresponds to[1] $\gamma \to 0^+$, in which one finds [Ghosh and Dattagupta, Physica A 129926 (2024)]

$$E_k = E_p = \int_0^\infty \delta(\omega - \omega_0) \frac{\hbar\omega}{4} \coth\left(\frac{\hbar\omega}{2k_B T}\right) d\omega = \frac{\hbar\omega_0}{4} \coth\left(\frac{\hbar\omega_0}{2k_B T}\right). \tag{23}$$

- Markovian-noise approximation (for $\tilde{\mu}(\omega) = m\gamma$):

$$\langle\{f(t), f(t')\}\rangle = 2m\gamma\hbar\omega_0 \coth\left(\frac{\hbar\omega_0}{2k_B T}\right)\delta(t - t'). \tag{24}$$

- Eq. (24) matches exactly with that presented in [Agarwal, Phys. Rev. A 4, 739 (1971)] obtained from a Born-Markov master equation.

[1] Physically this means $\gamma << \omega_0$.

Dissipative Diamagnetism: Model

- Relevant Hamiltonian (in 3D) [Dattagupta and Singh, Phys. Rev. Lett. 79, 961 (1997)]:

$$H = \frac{(\mathbf{p} - \frac{e}{c}\mathbf{A})^2}{2m} + \frac{m\omega_0^2 \mathbf{r}^2}{2} + \sum_j \left[\frac{\mathbf{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left(\mathbf{q}_j - \frac{c_j}{m_j \omega_j^2} \mathbf{r} \right)^2 \right]. \quad (25)$$

- Here $\mathbf{p} = (p_x, p_y, p_z)$ and $\mathbf{r} = (x, y, z)$ are the three-dimensional momentum and position operators, $\mathbf{p}_j$ and $\mathbf{q}_j$ are the corresponding variables for the jth bath oscillator and $\mathbf{A}$ is the vector potential.

- Corresponding quantum Langevin equation:

$$m\ddot{\mathbf{r}}(t) + \int_0^t \mu(t - t')\dot{\mathbf{r}}(t')dt' - \frac{e}{c}(\dot{\mathbf{r}}(t) \times \mathbf{B}) + m\omega_0^2 \mathbf{r} = \mathbf{f}(t), \quad (26)$$

  where $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mu(t)$ is defined in the same way as before.

- $\mathbf{f}(t)$ is now a three-component operator-valued quantum noise.

Energy in Dissipative Diamagnetism

- Performing analogous calculations, we can show that for $\mathbf{B} = (0, 0, B)$ [J.K., Ghosh, and Bandyopadhyay, Phys. Rev. E 104, 064112 (2021); Physica A 625, 128993 (2023)]

$$\langle \mathrm{K.E.} \rangle = \frac{\langle (\mathbf{p} - e\mathbf{A}/c)^2 \rangle}{2m} = \int_0^\infty \epsilon_k(\omega, T) P_k(\omega) d\omega, \tag{27}$$

$$\langle \mathrm{P.E.} \rangle = \frac{\langle m\omega^2 \mathbf{r}^2 \rangle}{2} = \int_0^\infty \epsilon_p(\omega, T) P_p(\omega) d\omega. \tag{28}$$

- Here $\epsilon_k(\omega, T) = \epsilon_p(\omega, T) = \frac{3\hbar\omega}{4} \coth\left(\frac{\hbar\omega}{2k_B T}\right)$ are the thermally-averaged kinetic and potential energies of each three-dimensional bath oscillator.

- $P_k(\omega)$ and $P_p(\omega)$ are probability distributions (too complicated to explicitly write here).

- Thus, we have the quantum counterpart of energy equipartition theorem in three dimensions, in the presence of a magnetic field.

Probability Distributions for Drude Dissipation: Dependence on Magnetic Field

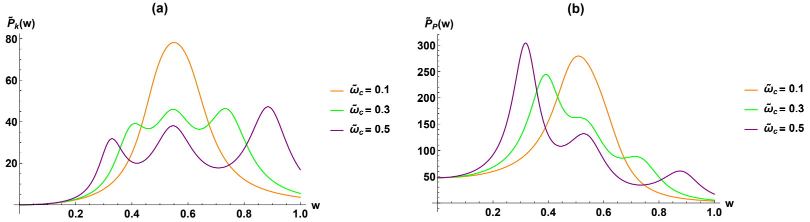
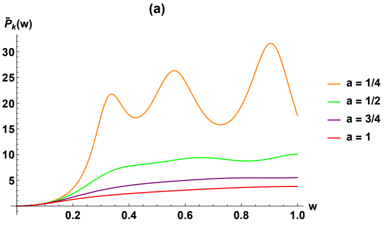


Figure: Variation of (a) $\tilde{P}_k(\mathrm{w}) = \omega_{\mathrm{cut}} P_k(\omega/\omega_{\mathrm{cut}})$ and (b) $\tilde{P}_p(\mathrm{w}) = \omega_{\mathrm{cut}} P_p(\omega/\omega_{\mathrm{cut}})$ as a function of re-scaled thermostat oscillator frequencies $\mathrm{w} = \omega/\omega_{\mathrm{cut}}$ for Drude dissipation with selected values of $\tilde{\omega}_c = \omega_c/\omega_{\mathrm{cut}}$ while keeping $\omega_0/\omega_{\mathrm{cut}} = 0.5$ and $\gamma/\omega_{\mathrm{cut}} = 0.2$.

Probability Distributions for Drude Dissipation: Dependence on Damping Strength



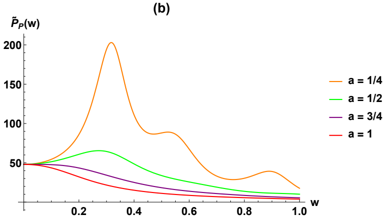


Figure: Variation of (a) $\tilde{P}_k(\mathrm{w}) = \omega_{\mathrm{cut}} P_k(\omega/\omega_{\mathrm{cut}})$ and (b) $\tilde{P}_p(\mathrm{w}) = \omega_{\mathrm{cut}} P_p(\omega/\omega_{\mathrm{cut}})$ as a function of re-scaled thermostat oscillator frequencies $\mathrm{w} = \omega/\omega_{\mathrm{cut}}$ for Drude dissipation with selected values of $a = \gamma/\omega_{\mathrm{cut}}$ while keeping $\omega_0/\omega_{\mathrm{cut}} = 0.5$ and $\omega_c/\omega_{\mathrm{cut}} = 0.5$.

Variation of Mean Kinetic Energy

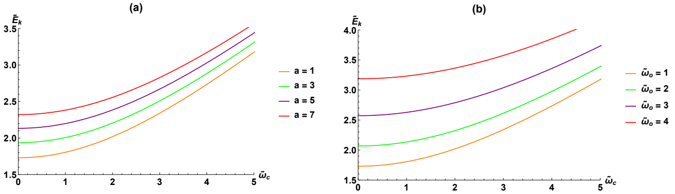


Figure: Variation of $\tilde{E}_k = \beta E_k$ as a function of the re-scaled magnetic field $\tilde{\omega}_c = \omega_c/\omega_{\rm cut}$ with (a) $\omega_0/\omega_{\rm cut} = 1$, $\beta\hbar\omega_{\rm cut} = 1$ for different values of $a = \gamma_0/\omega_{\rm cut}$ and (b) $\gamma_0/\omega_{\rm cut} = 1$, $\beta\hbar\omega_{\rm cut} = 1$ for different values of $\tilde{\omega}_0 = \omega_0/\omega_{\rm cut}$.

$$E_k = \frac{3}{2\beta} + \frac{2}{\beta}\sum_{n=1}^{\infty}\frac{A_n \times B_n + (\omega_c\nu_n)^2}{A_n^2 + (\omega_c\nu_n)^2} + \frac{1}{\beta}\sum_{n=1}^{\infty}\frac{B_n}{A_n} \tag{29}$$

where $A_n = \nu_n^2 + \omega_0^2 + \frac{\nu_n\gamma_0\omega_{\rm cut}}{\nu_n+\omega_{\rm cut}}$ and $B_n = \omega_0^2 + \frac{\nu_n\gamma_0\omega_{\rm cut}}{\nu_n+\omega_{\rm cut}}$.

Variation of Mean Potential Energy

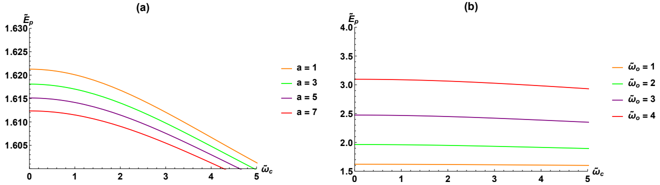


Figure: Variation of $\tilde{E}_p = \beta E_p$ as a function of the re-scaled magnetic field $\tilde{\omega}_c = \omega_c/\omega_{\rm cut}$ with (a) $\omega_0/\omega_{\rm cut} = 1$, $\beta\hbar\omega_{\rm cut} = 1$ for different values of $a = \gamma_0/\omega_{\rm cut}$ and (b) $\gamma_0/\omega_{\rm cut} = 1$, $\beta\hbar\omega_{\rm cut} = 1$ for different values of $\tilde{\omega}_0 = \omega_0/\omega_{\rm cut}$.

$$E_p = \frac{3}{2\beta} + \frac{2\omega_0^2}{\beta}\sum_{n=1}^{\infty}\frac{A_n}{A_n^2 + (\omega_c\nu_n)^2} + \frac{\omega_0^2}{\beta}\sum_{n=1}^{\infty}\frac{1}{A_n} \qquad (30)$$

Energy Functions Vs γ

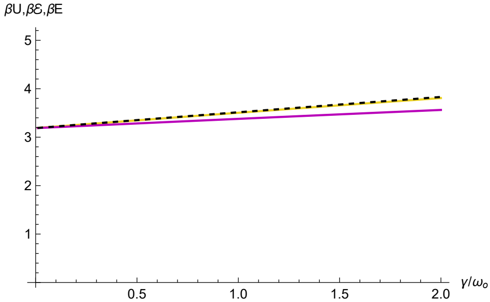


Figure: Dimensionless energy functions βU (black-dashed), $\beta\mathcal{E}$ (yellow-solid), and βE (violet-solid) for the dissipative magneto-oscillator, as a function γ/ω_0, for $\alpha = \beta\hbar\omega_0 = 0.5$, $\omega_c = 2.5\omega_0$, and $\omega_{\rm cut} = 10\omega_0$. We have taken $\omega_0 = 1$.

Energy Functions Vs $\hbar\omega_0/k_BT$

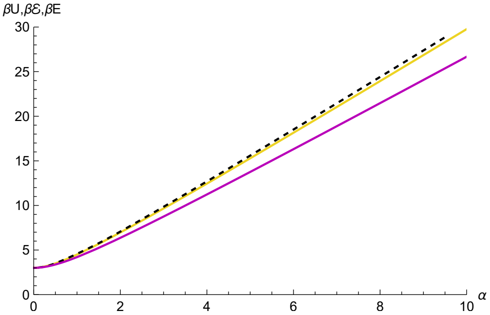


Figure: Dimensionless energy functions βU (black-dashed), $\beta\mathcal{E}$ (yellow-solid), and βE (violet-solid) for the dissipative magneto-oscillator, as a function $\alpha = \beta\hbar\omega_0$, for $\gamma = \omega_0$, $\omega_c = 2.5\omega_0$, and $\omega_{\rm cut} = 10\omega_0$. We have taken $\omega_0 = 1$.

Ongoing Work: Ericsson Cycle for Magnetic Work

- One can utilize the case of dissipative cyclotron motion as a heat engine (**Collaboration with A. Ghosh, S. Dattagupta, S. Chaturvedi, and M. Bandyopadhyay**).
- In an ongoing project, we are investigating the effect of different system and environmental parameters on the behavior of the efficiency of an Ericsson Cycle:

$$
\begin{array}{ccccccc}
B_1, T_h & & \text{Isothermal} & & B_2, T_h \\
 & 1 & \longrightarrow & 2 & \\
\text{Iso-}B & \uparrow & & \downarrow & \text{Iso-}B \\
 & 4 & \longleftarrow & 3 & \\
B_1, T_c & & \text{Isothermal} & & B_2, T_c
\end{array}
$$

$$B_2 > B_1, \quad T_h > T_c$$

Preliminary Results 1

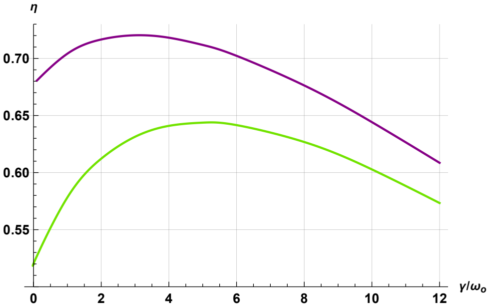


Figure: Plot of efficiency η as a function of γ/ω_0 for $T_c/\omega_0 = 0.002$ (purple) and 0.003 (green). We have used $\omega_{c,1}/\omega_0 = 0.1$, and for computing the energy differences, we have used $\omega_{\rm cut}/\omega_0 = 1000$.

Preliminary Results 2

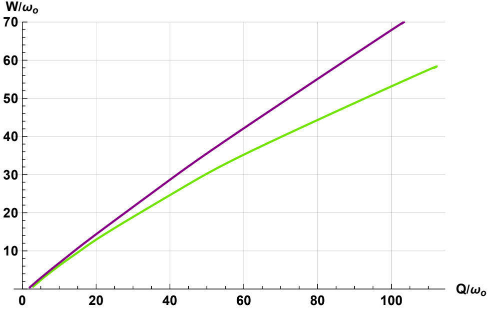


Figure: Plot of rescaled work done W/ω_0 as a function of the rescaled heat input Q/ω_0 for $T_c/\omega_0 = 0.002$ (purple) and 0.003 (green). We have used $\omega_{c,1}/\omega_0 = 0.1$, and for computing the energy differences, we have used $\omega_{\rm cut}/\omega_0 = 1000$.

Thank You!