Two paradigmatic systems governed by temperature dependent Hamiltonians

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We analyze two paradigmatic systems, linear harmonic oscillator (LHO) and two-level system (TLS) coupled to a heat bath, while their transition frequency is determined by the temperature of the heat bath. We study processes in which the temperature is changed, directly affecting the dynamical and thermodynamic properties of the systems. Study of the equilibrium thermodynamic properties of the LHO and TLS is presented. In the equilibrium situation we focus on basic thermodynamic variables and their temperature dependence. Assuming different temperature dependences of the systems' transition frequency we study behavior of von Neumann entropy and the heat capacities during quasireversible changes of the bath temperature. Such study can be understood as an extension of [1] to different forms of the effective Hamiltonian and different model systems.

The analysis of the quadratic coupling of LHO in the spirit of [2]:

$$\hat{H}_0 = \frac{\hat{P}^2}{2m} + \frac{m\omega_0^2}{2}\hat{X}^2 \quad \hat{H}_I(T) = \frac{mf(T)}{2}\hat{X}^2 \quad \hat{H}(T) \equiv \frac{\hat{P}^2}{2m} + \frac{m\omega(T)^2}{2}\hat{X}^2$$

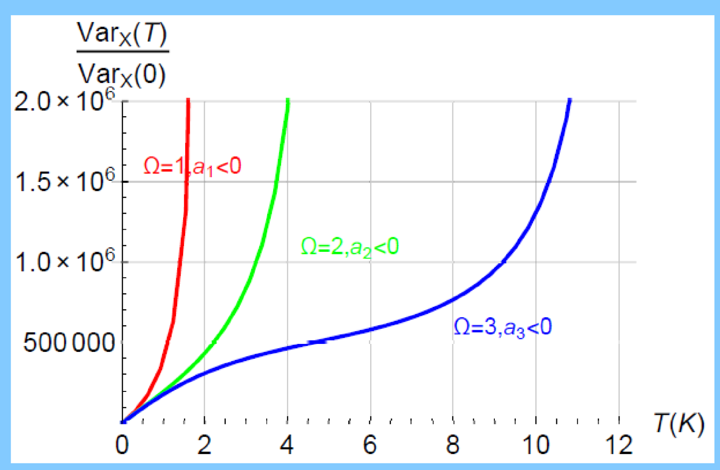
Assumption: $\omega(T) = \sqrt{\omega_0^2 + f(T)} = \sqrt{\omega_0^2 + \sum_{k=0}^{\Omega} a_k T^k}$ $\quad \hat{\rho} = \frac{\exp[-\hat{H}/k_B T]}{Z} = \exp\left[\frac{F-\hat{H}}{k_B T}\right]$

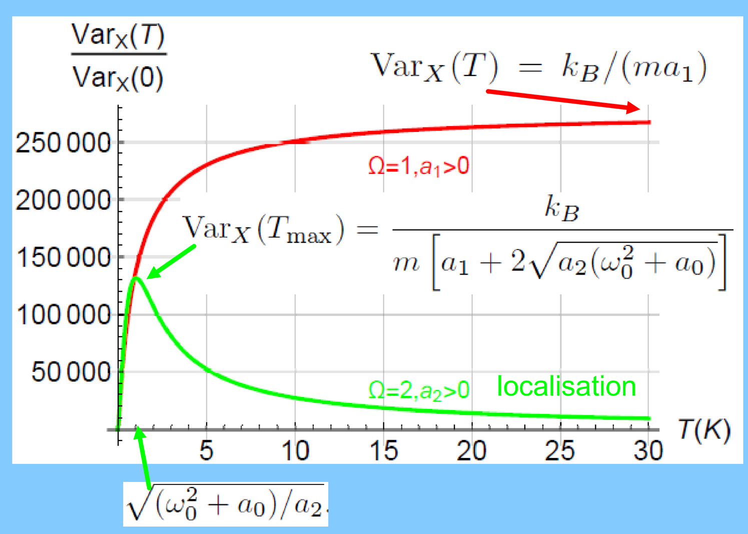
The mechanical characteristics:

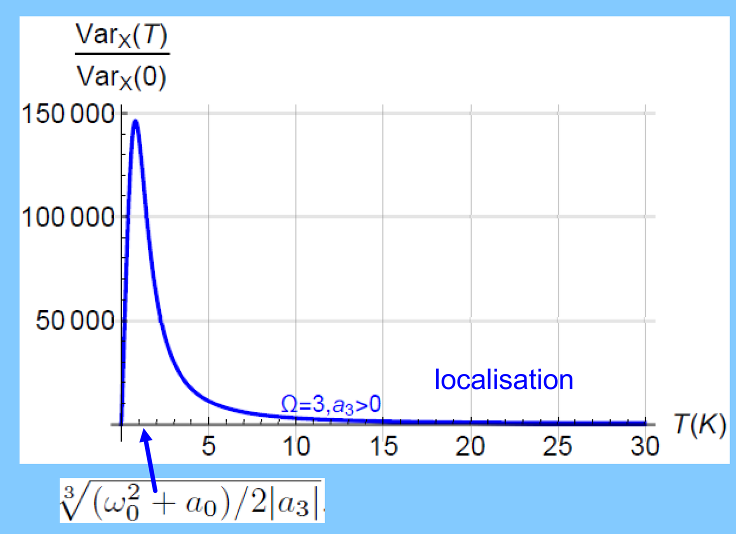
$$\mathrm{Var}_X(T) \approx \frac{k_B T}{m\omega(T)^2}$$

$$\mathrm{Var}_P(T) \approx m k_B T$$

$$\frac{\partial\,\mathrm{Var}_X(T)}{\partial T} = \frac{k_B(\omega_0^2 + a_0 - a_2T^2 - 2a_3T^3)}{m\omega(T)^4}$$





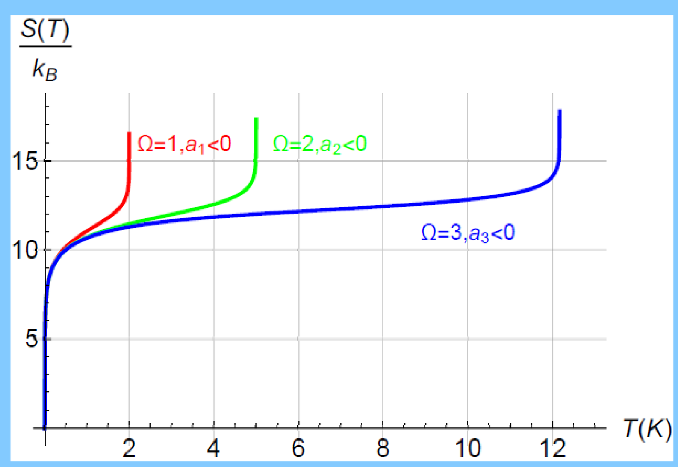


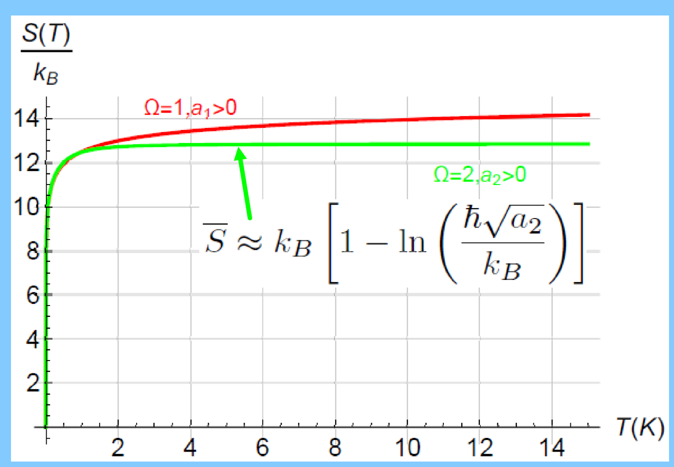
The thermodynamic characteristics:

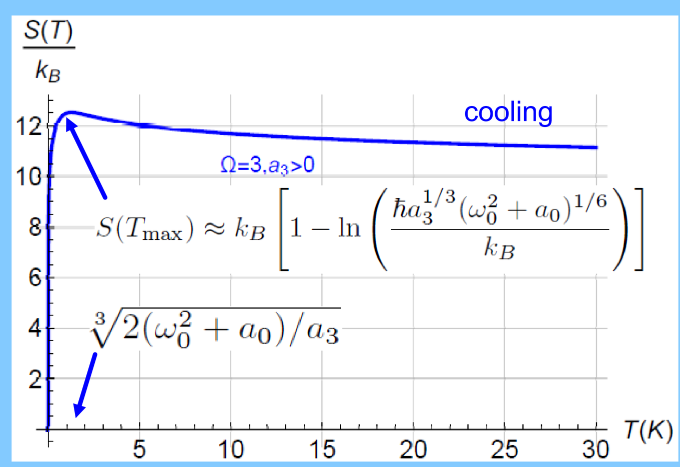
von Neumann entropy:

$$S \approx k_B\left[1 - \ln\left(\frac{\hbar\omega(T)}{k_B T}\right)\right]$$

$$\frac{\partial S(T)}{\partial T} = k_B\frac{2(\omega_0^2 + a_0) + a_1T - a_3T^3}{2T\omega(T)^2}$$



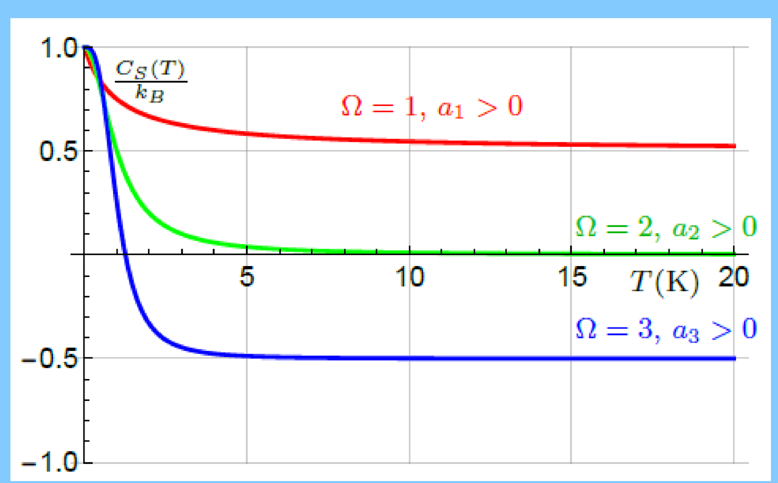




heat capacities:

$$C_S(T) = T\frac{\partial S}{\partial T}$$

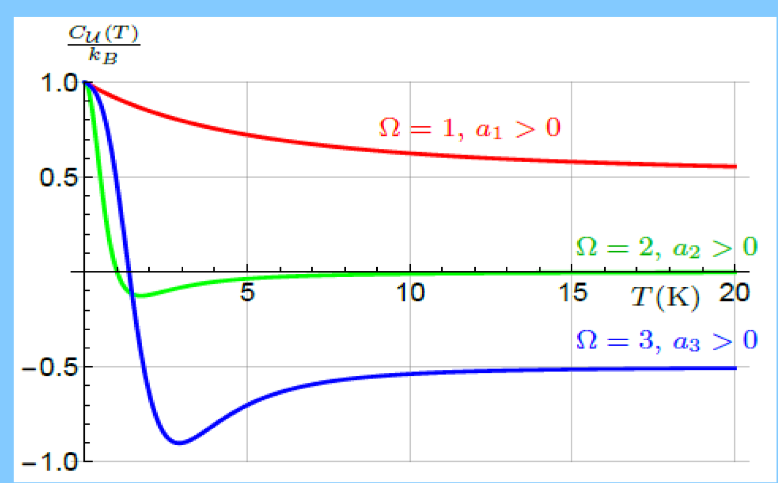
$$C_S \approx k_B(1 - \Omega/2)$$



[2]: $\mathcal{U} = \langle\hat{H}_{\mathrm{tot}}\rangle - \langle\hat{H}_{\mathrm{B}}\rangle$

OR

$$C_{\mathcal{U}}(T) = \frac{\partial}{\partial T}(TC_S)$$



localisation \ cooling	YES	NO
YES	$\Omega = 3,\ a_3 > 0$	$\Omega = 2,\ a_2 > 0$
NO	$\emptyset$	$\Omega \leq 3,\ a_3 < 0$; $\Omega = 1,\ a_1 > 0$

The analysis of the TLS behavior:

$$C_S(T) = T\frac{\partial S(T)}{\partial T} \quad C_{\mathcal{U}}(T) = \frac{\partial\mathcal{U}(T)}{\partial T} \quad C_{\mathcal{U}}(T) \neq \frac{\partial}{\partial T}(TC_S)$$

$$\hat{\rho} = \exp\left[\frac{F - \hat{H}(T)}{k_B T}\right]$$

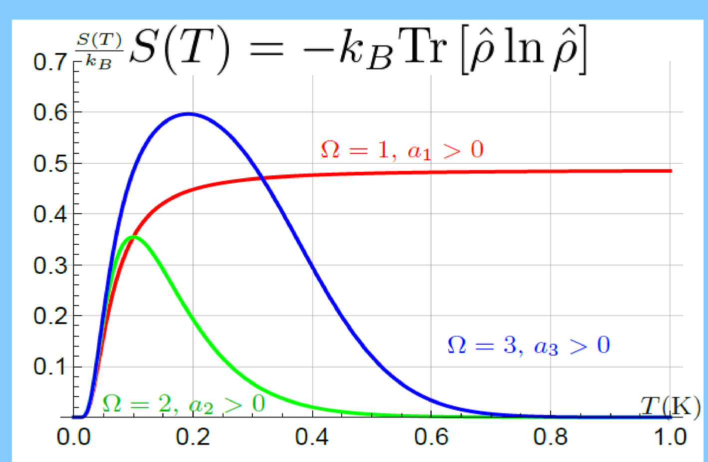
$$\hat{H}(T) = \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \frac{\hbar f(T)}{2}\hat{\sigma}_x$$

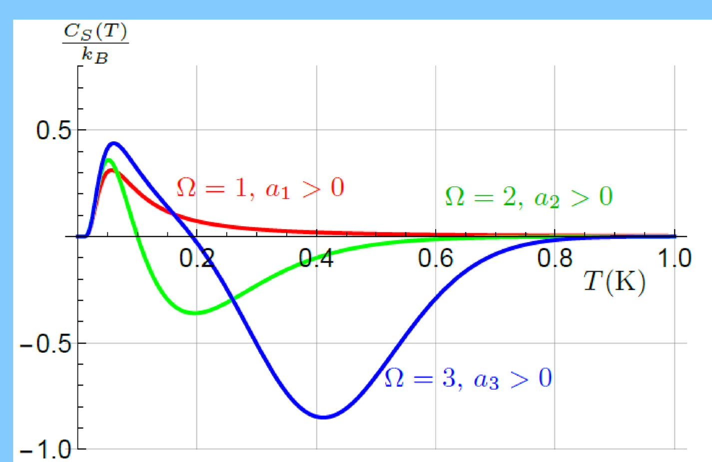
$$\mathcal{U}(T) = \left\langle\hat{H}(T)\right\rangle - T\left\langle\frac{\partial\hat{H}(T)}{\partial T}\right\rangle$$

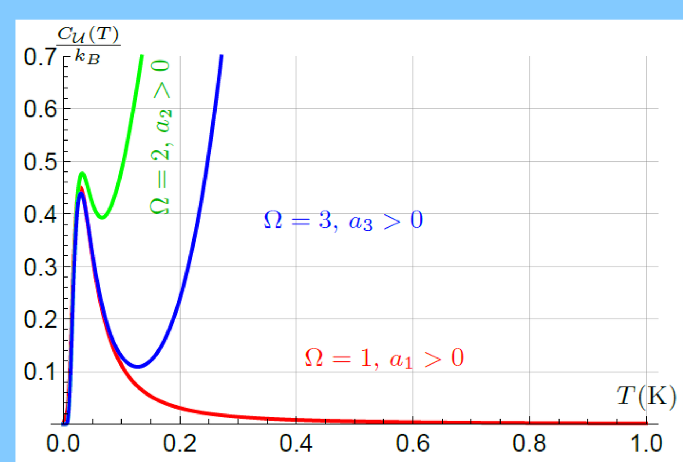
$$f(T) = \sum_{k=1}^{\Omega} a_k T^k$$

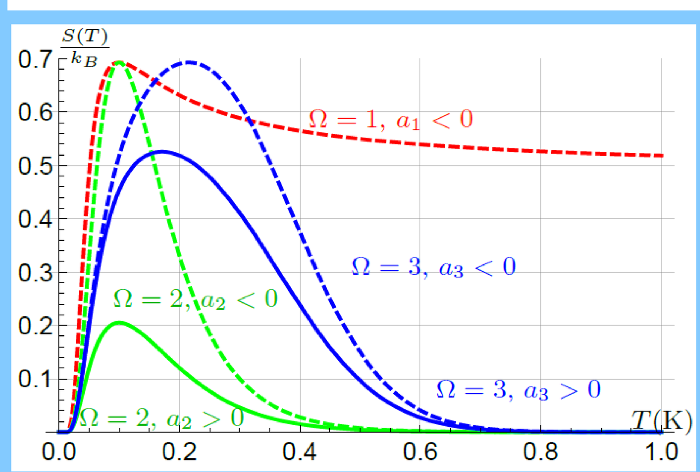
$$\langle\bullet\rangle \equiv \mathrm{Tr}\,[\hat{\rho}\,\bullet]$$

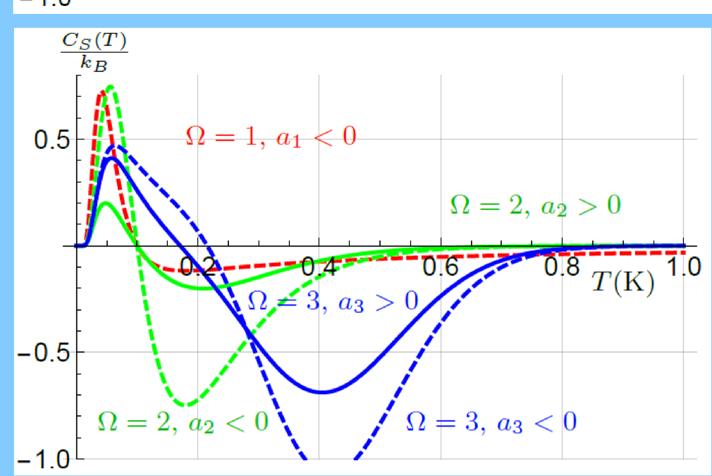
$$\hat{H}(T) = \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \frac{\hbar f(T)}{2}\hat{\sigma}_z$$

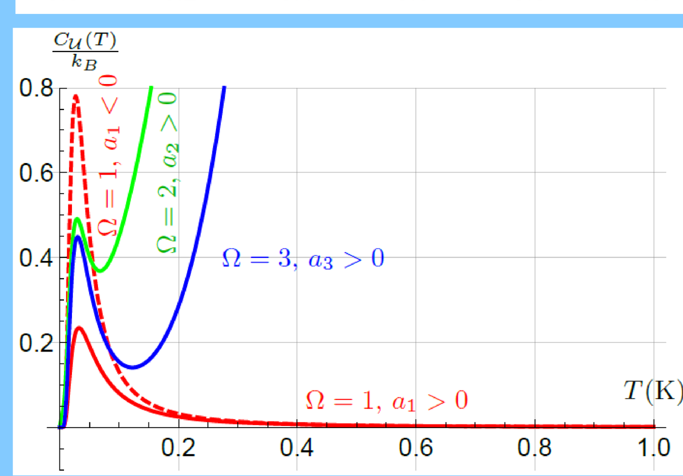












Conclusions:

cooling	NO	YES
$\hat{\sigma}_x$	$\Omega = 1$	the rest
$\hat{\sigma}_z$	$\Omega = 1,\ a_1 > 0$	the rest

- we have studied a LHO and TLS coupled to its surroundings by a bath temperature *T* - dependent force
- LHO position variance can diverge, saturate, or decrease (localisation effect) with increasing bath temperature
- LHO von Neumann entropy can as well diverge, saturate, or decrease (cooling effect) with increasing bath temperature
- LHO entropic and thermodynamic heat capacity can be negative allowing to „witness“ system-bath strong coupling
- TLS von Neumann entropy can as well saturate at lower value, or decrease (cooling effect) with increasing bath temperature
- TLS entropic heat capacity can be negative allowing to witness system-bath strong coupling
- TLS thermodynamic heat capacity is positive, can diverge; does it allow for witnessing system-bath strong coupling by such divergence?

References: [1] M. Kolář, A. Ryabov, and R. Filip, Phys. Rev. A 95, 042105 (2017).
[2] U. Seifert, Phys. Rev. Lett. 116, 020601 (2016); P. Talkner and P. Hanggi, Phys. Rev. E94, 022143 (2016).
[3] W. Greiner, *et. al.*, Thermodynamics and Statistical Mechanics, Springer (1997).

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