The third law as a single inequality

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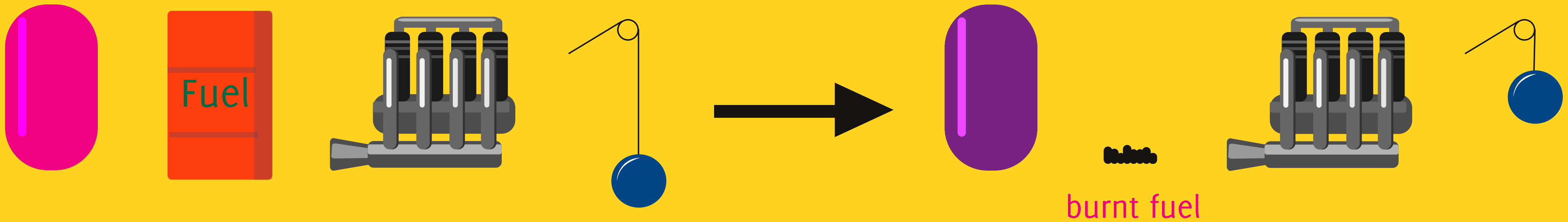
Second Law

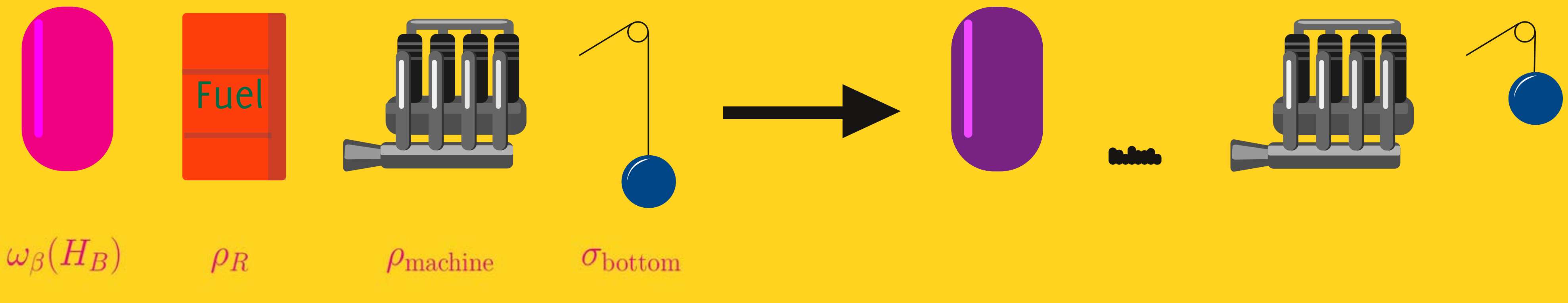
2nd Law of thermodynamics (in its most convenient form for this talk):

"It is impossible to extract work, in a complete cycle, with the sole effect of cooling a heat reservoir"

Work extraction

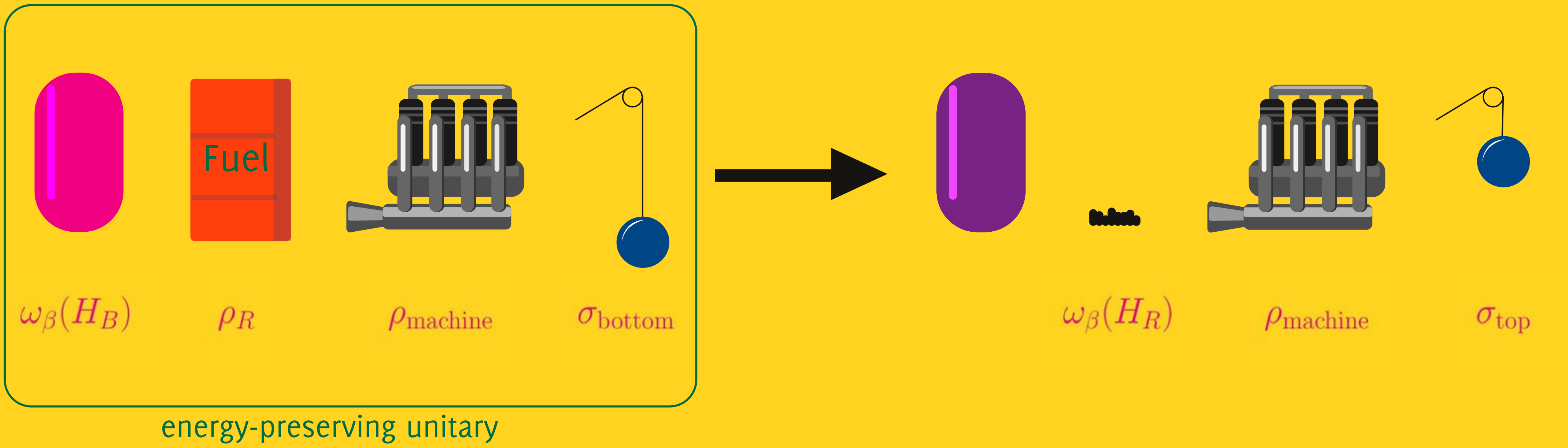


Second Law: Quantification in quantum language



Thermal state: $\omega_\beta(H) = \frac{e^{-\beta H}}{Z_\beta}$

Second Law: Quantification in quantum language



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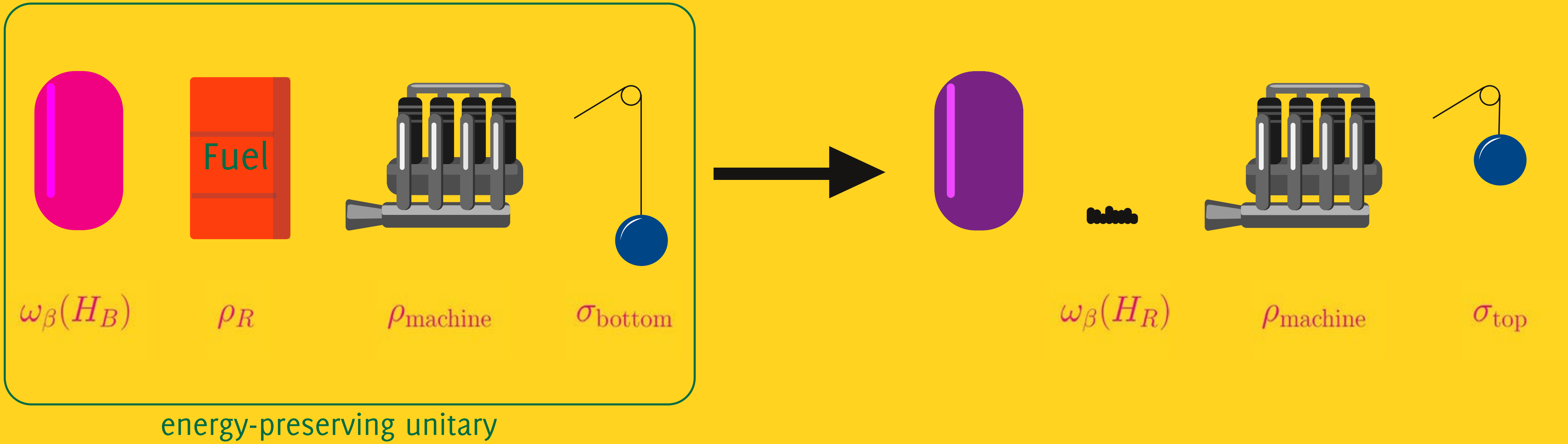
Second Law: Quantification in quantum language



$$\text{Max. Work} = \text{FreeEnergy}_\beta(\rho_R, H_R) - \text{FreeEnergy}_\beta(\omega_\beta(H_R), H_R)$$

$$\propto D\left(\rho_R \| \omega_\beta(H_R)\right)$$

Thermal state: $\omega_\beta(H) = \frac{\mathrm{e}^{-\beta H}}{Z_\beta}$

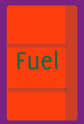
Relative entropy: $D(\rho\|\sigma) = \mathrm{tr}(\rho \log(\rho)) - \mathrm{tr}(\rho \log(\sigma))$

Second Law (work extraction)

No work can be extracted from a heat bath only.

Q: How much work from a given resource?

A: Ruled by free energy difference

$D\left(\rho_R \| \omega_\beta(H_R)\right) = D($ 

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Third Law (cooling)

No cooling to zero temperature with finite resources: time, fuel, steps...

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Third Law (cooling)

No cooling to zero temperature with finite resources: time, fuel, steps...

Q: How cold using a given resource?

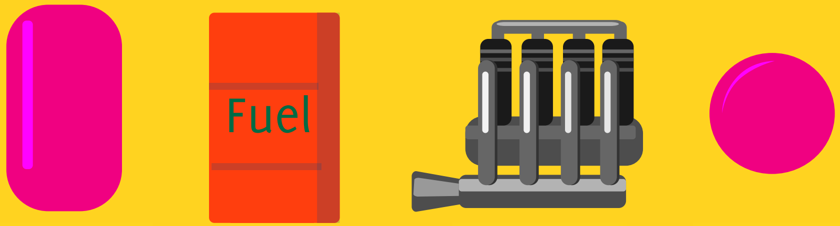
A: Ruled by **vacancy**

$\mathcal{V}_\beta(\rho_R, H_R) := D\left(\omega_\beta(H_R)\|\rho_R\right)$

$= D($  $\|$ 

$)$

Abstract problem of cooling



$\omega_\beta(H_B)$ ρ_R ρ_{machine} $\omega_\beta(H_T)$

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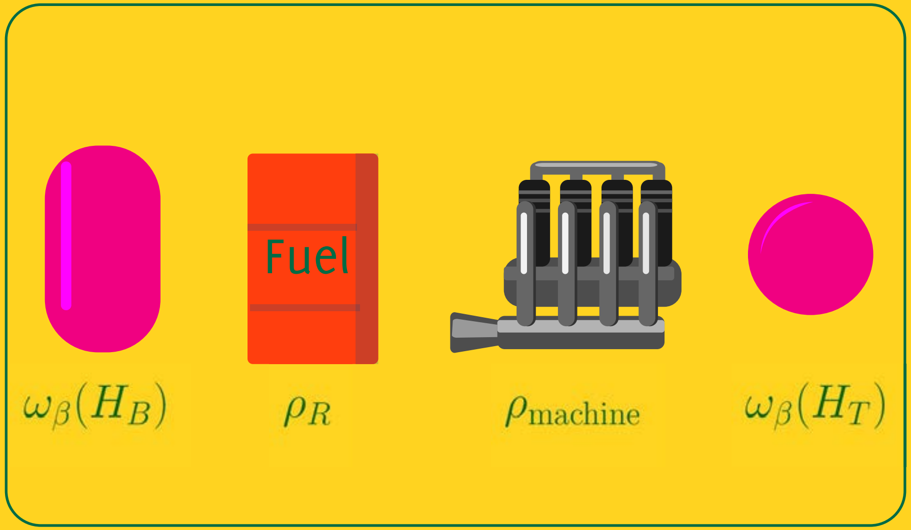

energy-preserving unitary U

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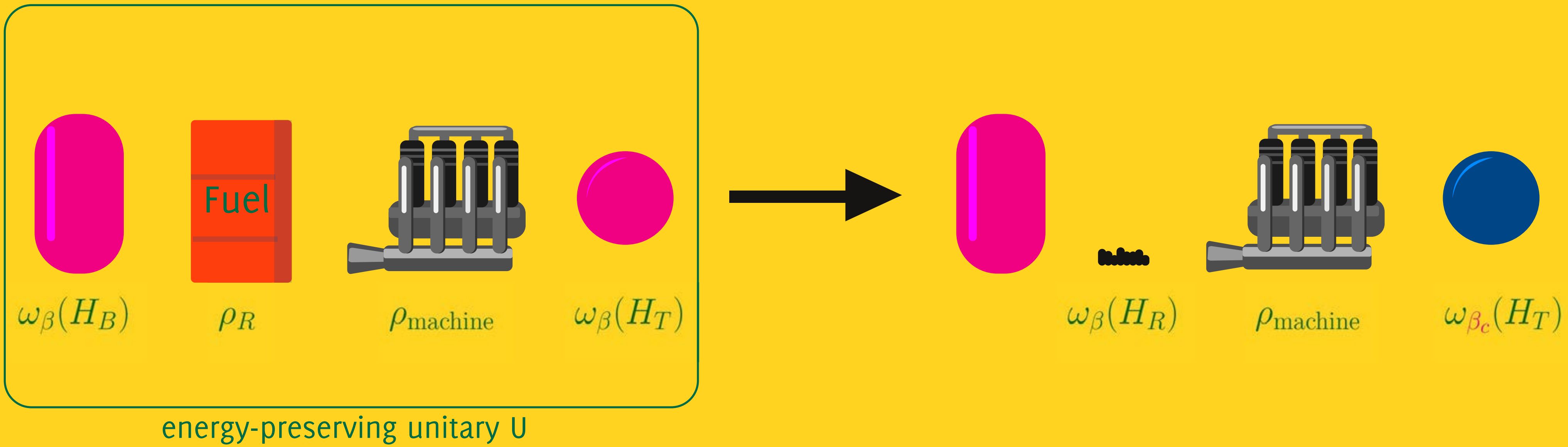

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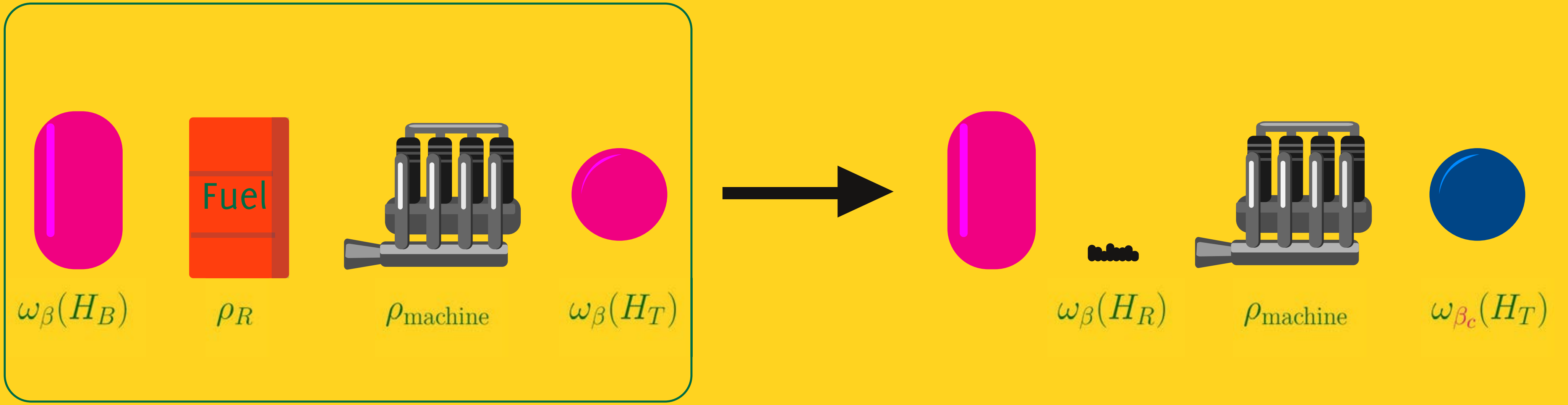

energy-preserving unitary U

Formal optimization problem

$$
\begin{aligned}
&\max_{U, H_B, \rho_{\mathrm{machine}}, H_{\mathrm{machine}}} \beta_c \\
\text{s.t.} \quad & [U, H_B + H_R + H_{\mathrm{machine}} + H_T] = 0 \\
& \rho_{\mathrm{machine}} \otimes \omega_{\beta_c}(H_T) = \mathrm{Tr}_{BR}\left(U \omega_\beta(H_B) \otimes \rho_R \otimes \rho_{\mathrm{machine}} \otimes \omega_\beta(H_T) U^\dagger \right)
\end{aligned}
$$

More on this condition in Markus P. Mueller's talk

Main results (informal overview)

A **necessary** condition for cooling is:

$$\mathcal{V}_\beta(\rho_R, H_R) \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T).$$

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For low enough target temperature and quasi-classical resources with full rank, a **sufficient** condition for cooling is:

$$\mathcal{V}_\beta(\rho_R, H_R) - \text{Error Term} \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T).$$

The error term is **additive** over independent systems and vanishes for large classes of resource. Also for any fixed resource if the target temperature goes to zero.

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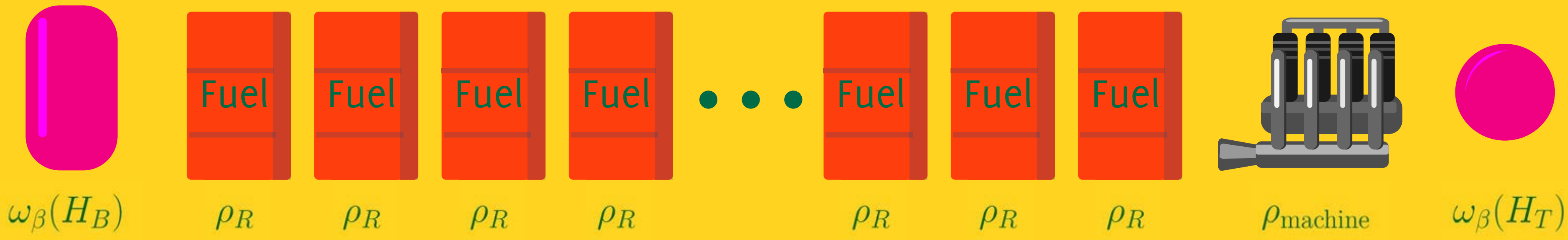
Third law follows since vacancy of target diverges as target temperature goes to zero.

i.i.d. resources



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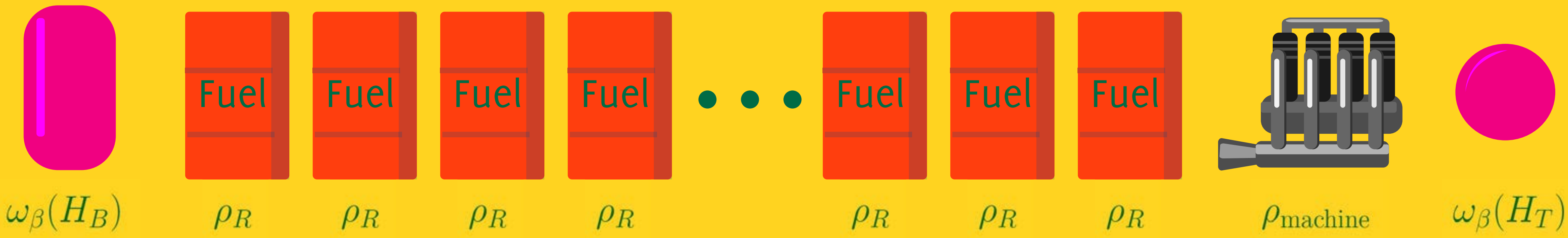

Vacancy and error term are **additive**:

$$\mathcal{V}_\beta(\rho \otimes \sigma, H_1 \otimes \mathbf{1} + \mathbf{1} \otimes H_2) = \mathcal{V}_\beta(\rho, H_1) + \mathcal{V}_\beta(\sigma, H_2).$$

Necessary and sufficient number of resources are given by:

$$n^{\text{necc.}} \geq \frac{\mathcal{V}_\beta(\text{target,final})}{\mathcal{V}_\beta(\text{resource,initial})}, \qquad n^{\text{suff.}} \leq \frac{\mathcal{V}_\beta(\text{target,final})}{\mathcal{V}_\beta(\text{resource,initial}) - \text{Error Term}}.$$

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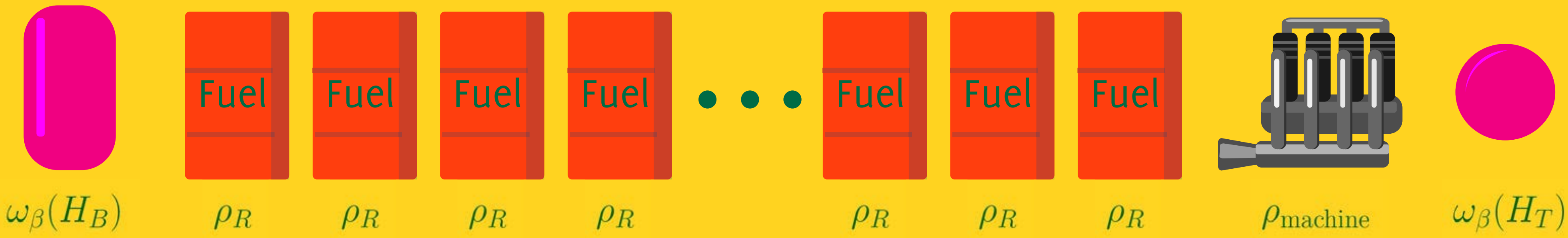

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As target temperature approaches absolute zero $\frac{n^{\text{necc.}}}{n^{\text{suff.}}} \longrightarrow 1.$

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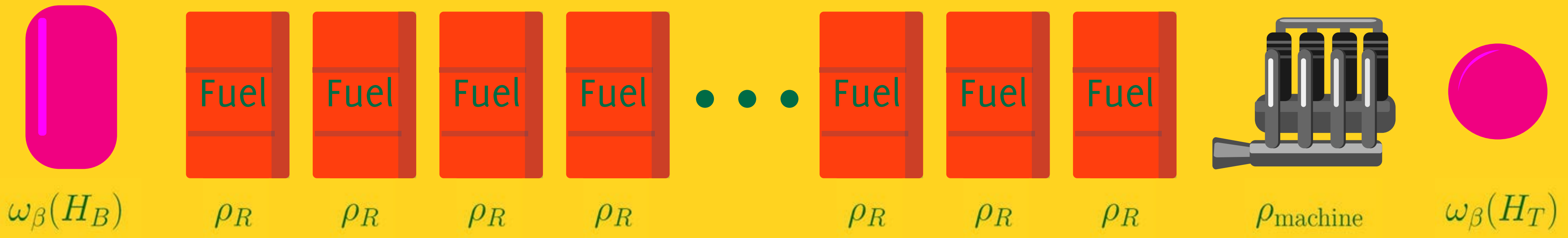

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The smallest possible achievable temperature with n resource copies fulfills:

$$\lim_{n\to\infty} nT_c^{(n)} = \frac{E_\beta(H_T)}{\mathcal{V}_\beta(\rho_R, H_R)}.$$

Similar results for qubit as target system by Janzing et al, 2000.

D. Janzing, P. Wocjan, R. Zeier, R. Geiss, and T. Beth, Int. J. Th. Phys. 39, 2717 (2000)

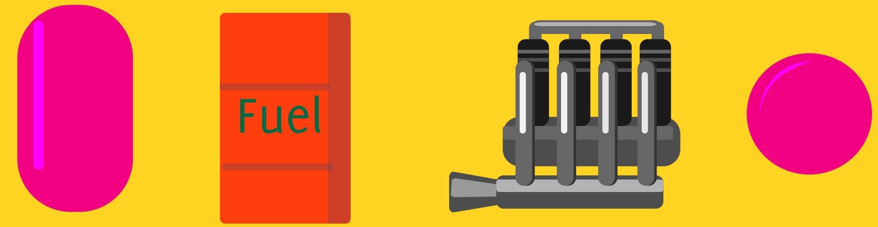
i.i.d. resources

Occupation probability of ground-state increases **exponentially** with number of resources. Worst-case bound shows:

$$p_0 \geq 1 - de^{-n\mathcal{V}_\beta(\text{Resource,initial})\frac{\Delta}{E_\beta}}, \quad n \gg 1.$$

- Δ : Gap above ground-state of target
- d : Dimension of target

thermal resources (non-i.i.d.)



$\omega_\beta(H_B)$ $\omega_{\beta_R}(H_R)$ ρ_{machine} $\omega_\beta(H_T)$

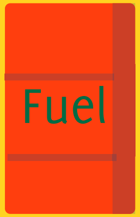
Vacancy can be expressed in terms of free energies:

$$\mathcal{V}_\beta(\omega_{\beta_R}(H_R), H_R) = \beta_R \left[F_{\beta_R}(\omega_\beta(H_R), H_R) - F_{\beta_R}(\omega_{\beta_R}(H_R), H_R)\right].$$

Since free energies are extensive, so is the vacancy for thermal many-body systems. The scaling results for i.i.d. systems transfer similarly.

Non-equilibrium free energy: $F_\beta(\rho, H) := \mathrm{Tr}(\rho H) - \frac{1}{\beta} S(\rho)$

thermal resources: vanishing error term



$\omega_{\beta_R}(H_R)$

Lemma:

For any thermal resource that is warmer than the heat bath and whose thermal energy $\beta \mapsto E_\beta(H_R)$ is **convex**, the error term in the sufficient condition vanishes.

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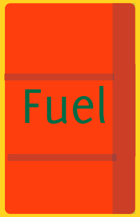

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Systems for which this is true:

- Two-level systems
- Any system with equidistant energy-levels
- Arbitrary networks of harmonic oscillators (quasi-free bosonic system)
- Quasi-free fermionic systems
- Any system whose heat capacity increases monotonically with temperature (i.e., generic, large many-body systems)

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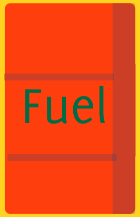

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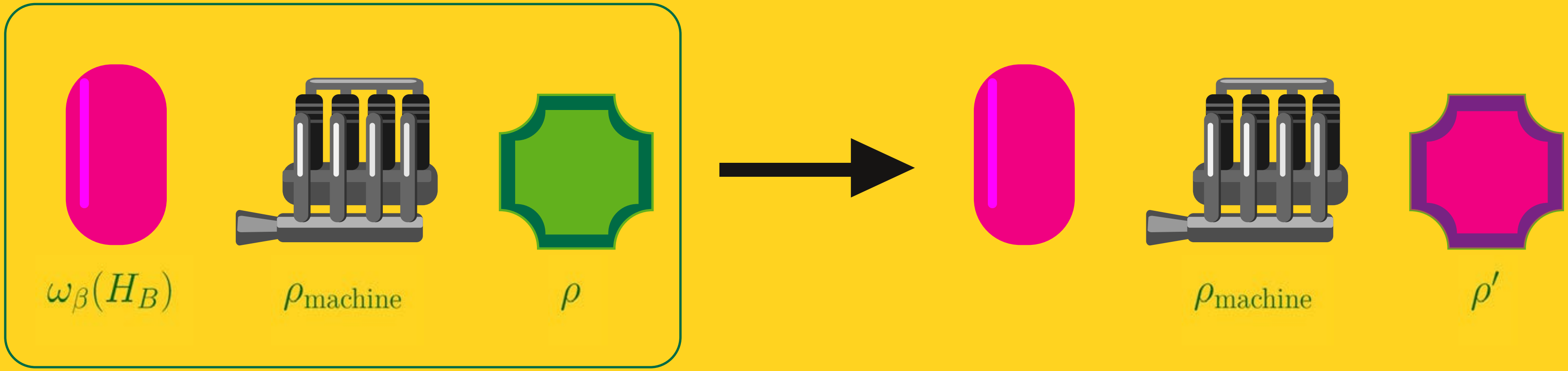
In all these cases $\mathcal{V}_\beta(\rho_R, H_R) \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T)$ is **necessary** and **sufficient**.

Towards proof: General properties of vacancy



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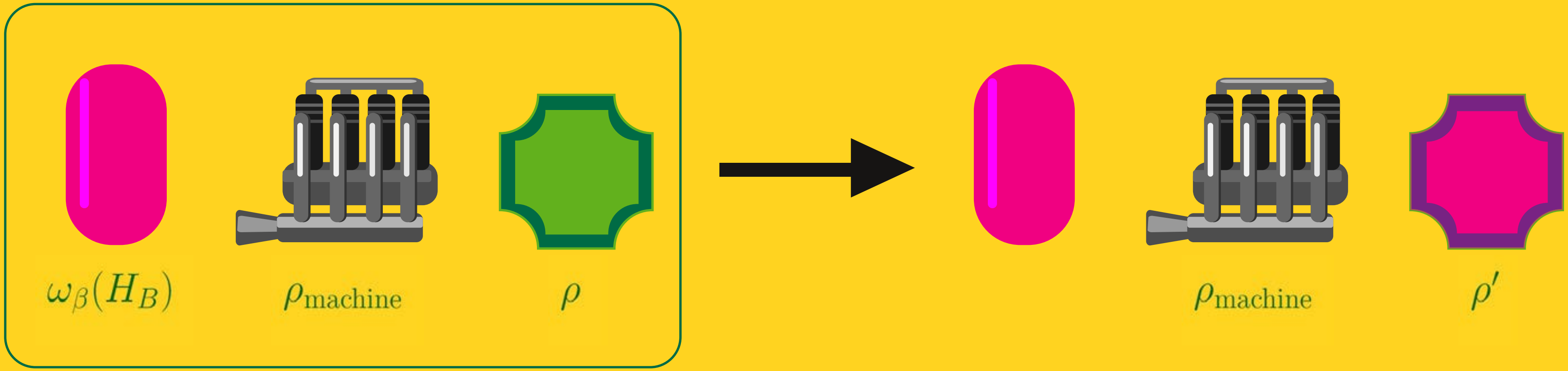


- Vacancy is **monotonic** under such **catalytic thermal operations**:

$$\mathcal{V}_\beta(\rho, H) \geq \mathcal{V}_\beta(\rho', H).$$

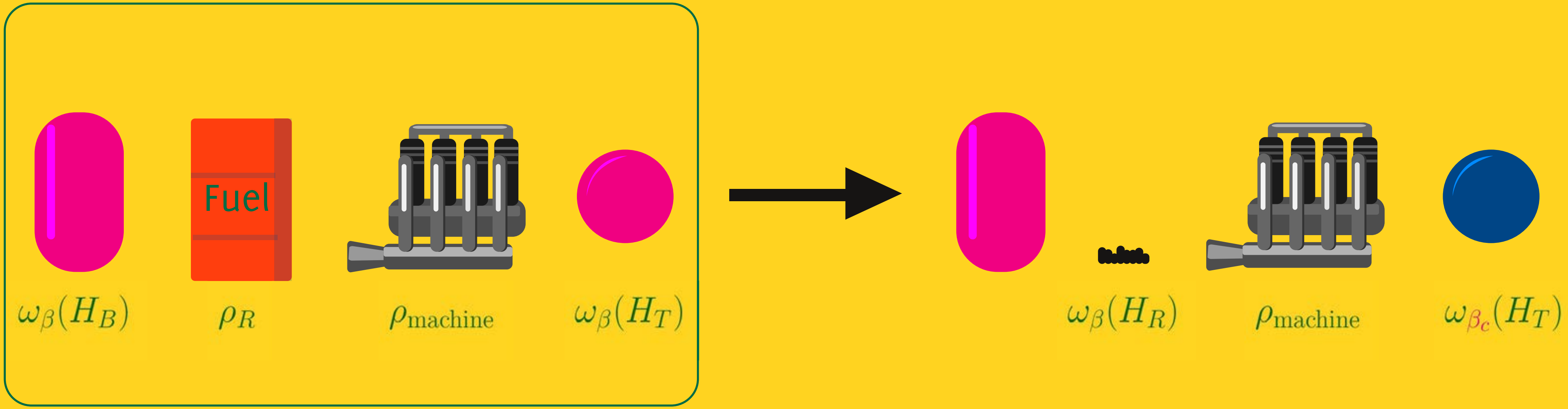
- Vacancy is **additive**:

$$\mathcal{V}_\beta(\rho \otimes \sigma, H_1 \otimes \mathbf{1} + \mathbf{1} \otimes H_2) = \mathcal{V}_\beta(\rho, H_1) + \mathcal{V}_\beta(\sigma, H_2).$$

- Vacancy **vanishes in equilibrium**:

$$\mathcal{V}_\beta(\omega_\beta(H), H) = 0.$$

Necessary condition



Initial Vacancy: $\mathcal{V}_\beta(\rho_R \otimes \omega_\beta(H_T), H_R + H_T) = \mathcal{V}_\beta(\rho_R, H_R).$

Final Vacancy: $\mathcal{V}_\beta(\omega_\beta(H_R) \otimes \omega_{\beta_c}(H_T), H_R + H_T) = \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T).$

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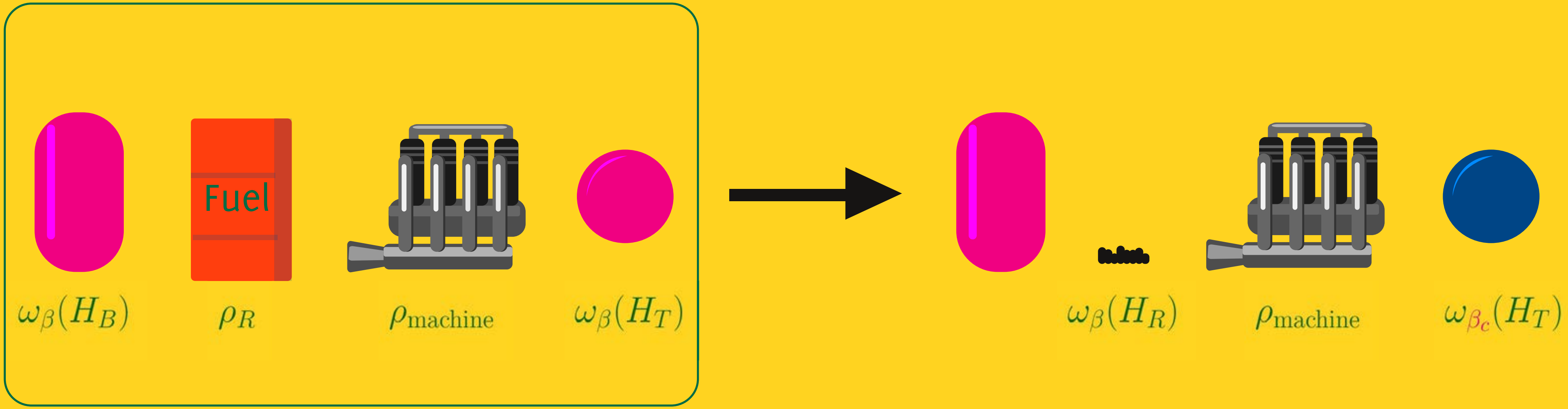

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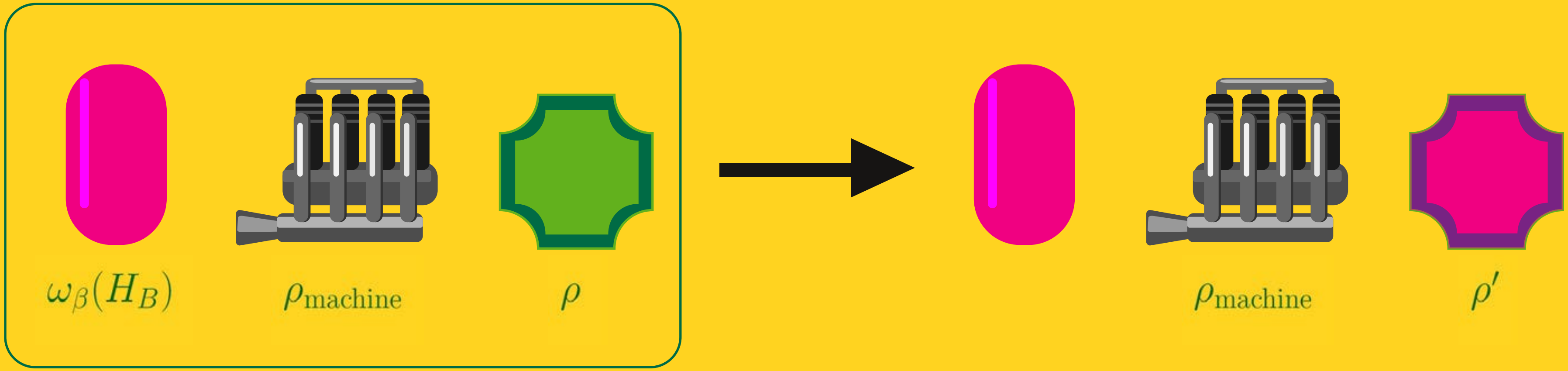
Thus **monotonicity** implies:

$$\mathcal{V}_\beta(\rho_R, H_R) \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T).$$

See also Janzing et al, 2000.

D. Janzing, P. Wocjan, R. Zeier, R. Geiss, and T. Beth, Int. J. Th. Phys. 39, 2717 (2000)

Sufficient condition



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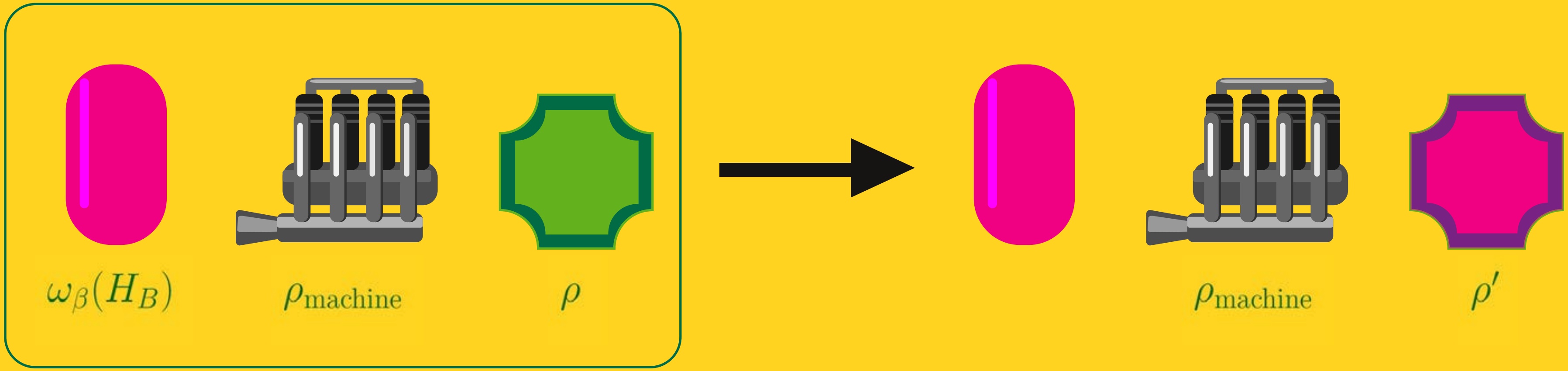


General theorem (Brandao et al, 2015)

Let ρ and ρ' be diagonal in the energy basis. Then ρ can be mapped to ρ' by a catalytic thermal operation if and only if*

$$D_\alpha(\rho, \omega_\beta(H_T)) \geq D_\alpha(\rho', \omega_\beta(H_T)), \qquad \forall \alpha \geq 0,$$

where D_α denote the Rényi divergences.

* Omitting some detail about the use of the machine/catalyst. See our paper or talk to me for detailed discussion of this point.

F. G.S. L. Brandao, M. Horodecki, N. H. Y. Ng, J. Oppenheim, and S. Wehner. "The second laws of quantum thermodynamics". PNAS 112 (2015)

A technical Lemma

For any target Hamiltonian and environment temperature, there exists a critical inverse tempreature β_{critical} , such that for all $\beta_c > \beta_{\text{critical}}$ and all $0 \leq \alpha \leq \delta(\beta_c)$, the Renyi-divergence

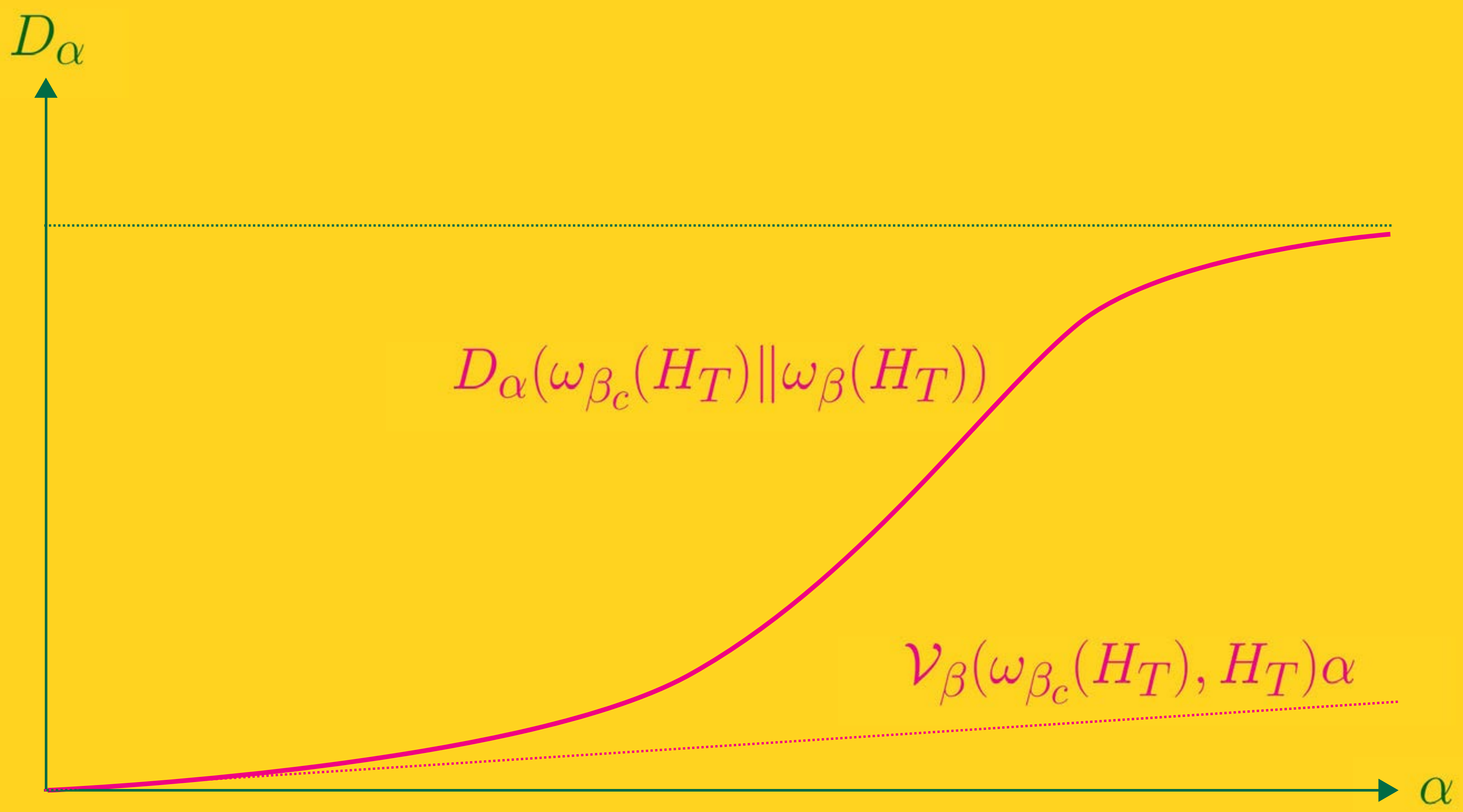
$$\alpha \mapsto D_\alpha(\omega_{\beta_c}(H_T) \| \omega_\beta(H_T))$$

is **concave**.

The critical value $\delta(\beta_c)$ is given by

$$\delta(\beta_c) = \frac{\log(Z_\beta)}{\mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T)} < 1.$$

Sufficient condition: Proof sketch



$$D_\alpha(\rho_R\|\omega_\beta(H_R)) \geq D_\alpha(\omega_{\beta_c}(H_T)\|\omega_\beta(H_T)) \quad \forall\alpha \geq 0.$$

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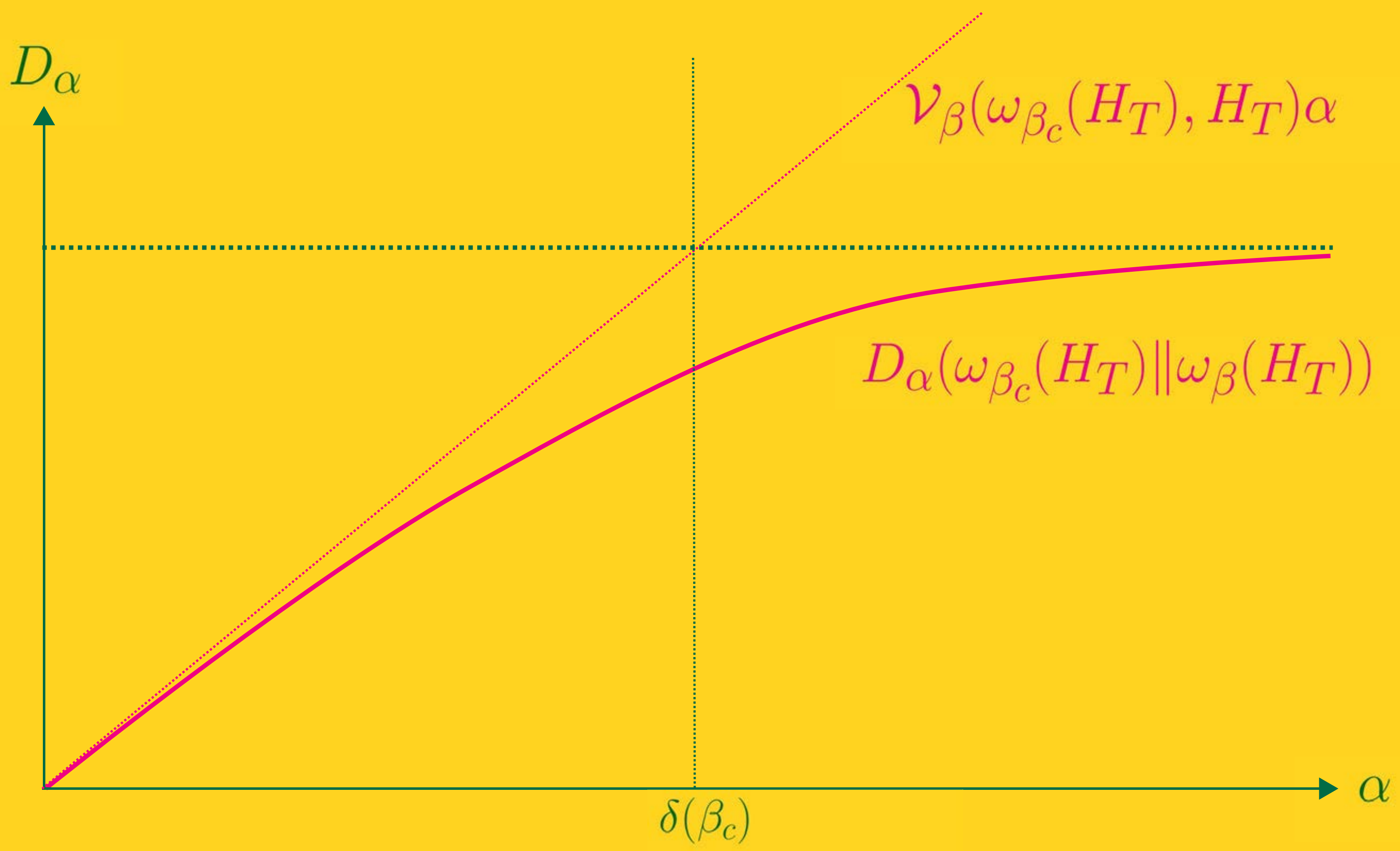

$$D_\alpha(\rho_R\|\omega_\beta(H_R)) \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T)\alpha \quad \forall 0 \leq \alpha \leq \delta(\beta_c).$$

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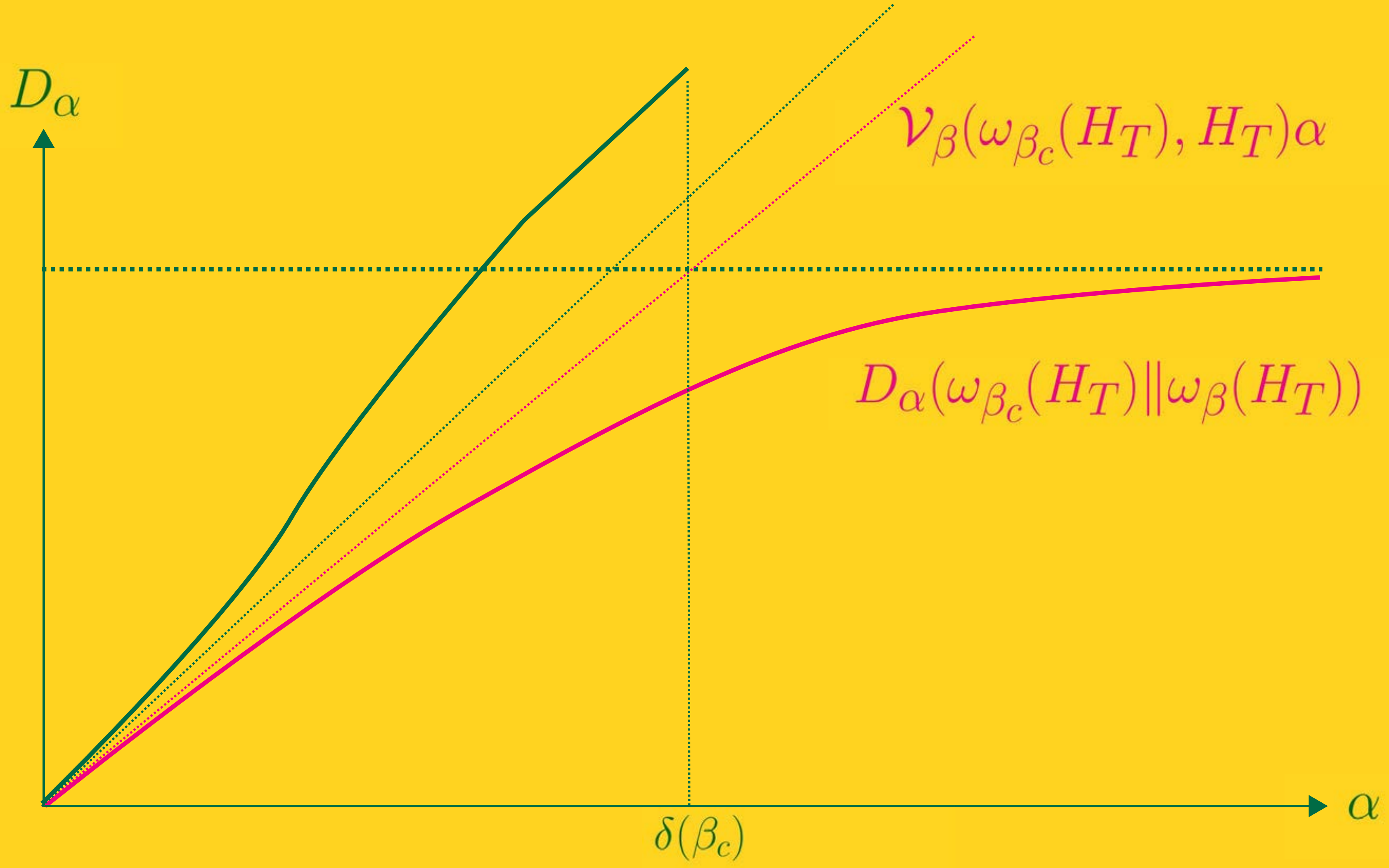

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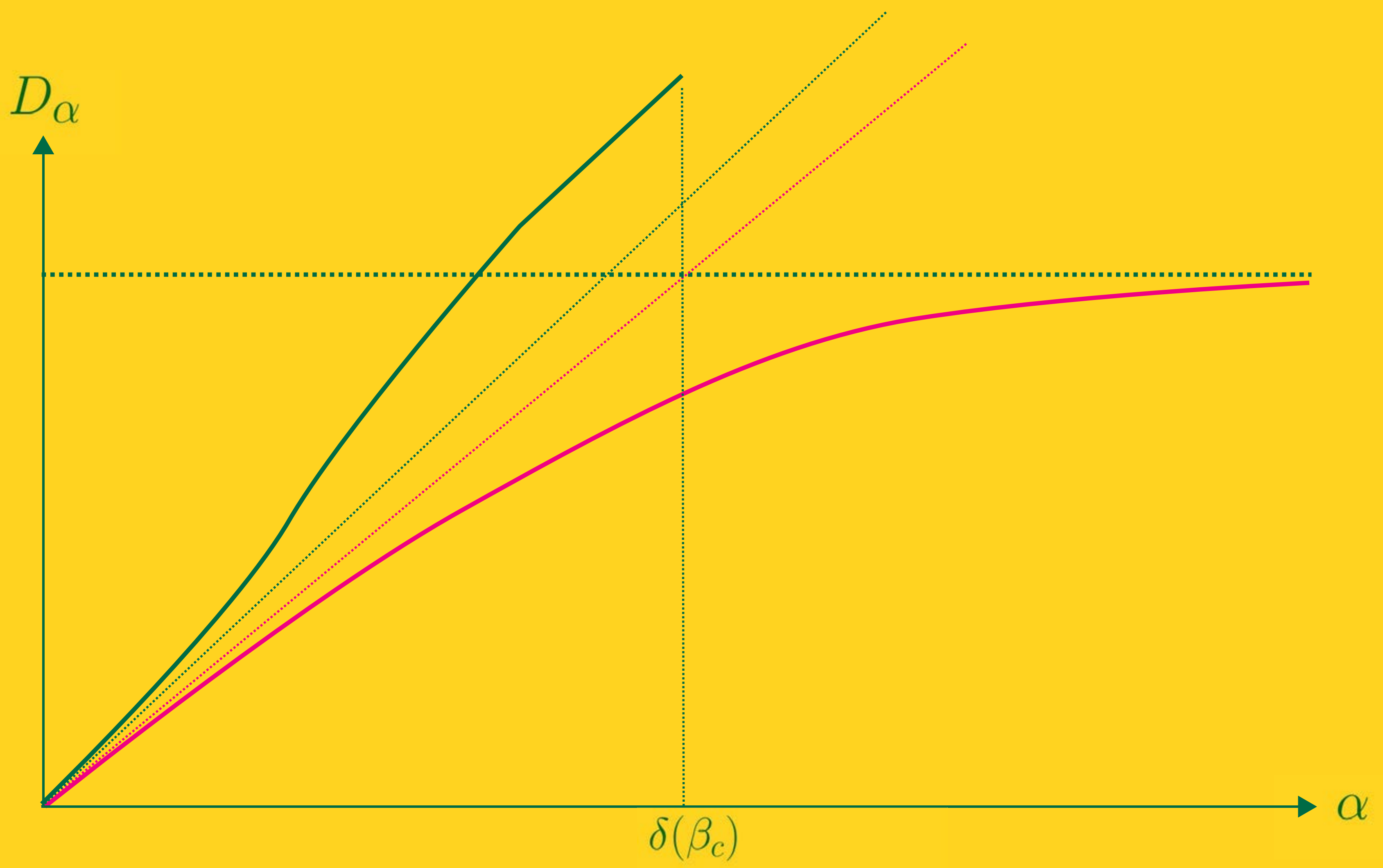

$$\mathcal{V}_\beta(\rho_R, H_R)\alpha - k\alpha^2 \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T)\alpha \quad \forall 0 \leq \alpha \leq \delta(\beta_c)$$

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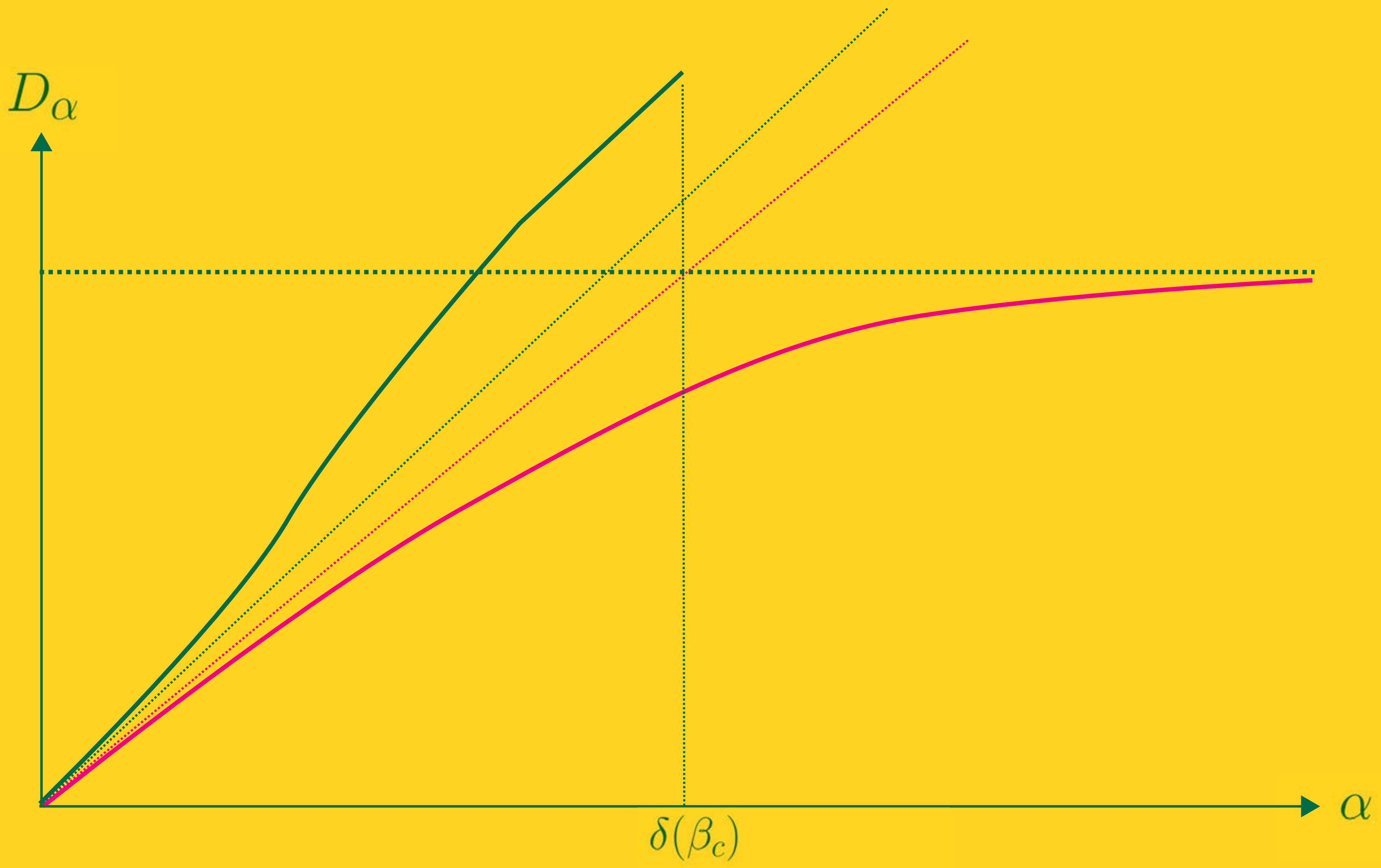

$$\mathcal{V}_\beta(\rho_R, H_R) - k\delta(\beta_c) \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T)$$

Summary

- We derived general necessary and sufficient conditions for low-temperature cooling using non-equilibrium resources.

- For large classes of non-i.i.d resources the necessary and sufficient condition for cooling a target to very low temperature is given by:

$$\mathcal{V}_\beta(\rho_R, H_R) \geq \mathcal{V}_\beta(\omega_{\beta_c}(H_T), H_T).$$

- Thus, low temperature cooling is essentially determined by the single quantity

$$\mathcal{V}_\beta(\rho, H) := D(\omega_\beta(H) \| \rho).$$

- Similar to work extraction, which is quantified by the non-equilibrium free energy

$$\Delta F_\beta(\rho, H) := \mathrm{k_B} T D(\rho \| \omega_\beta(H)).$$

Open Problems

- Understand general properties of vacancy.
- Do we really need the catalyst/cyclic machine? Can we bound the vacancy required in the catalyst independent of the target temperature?
- Get better estimates for error term and prove that it vanishes under more general conditions.
- Connect this resource theoretic approach to physical cooling mechanisms like laser-cooling.
- Quantum coherence in the resource states.

Thanks!

arXiv:1701.07478
Phys. Rev. X 7, 041033 (2017)

Some references and related work:

D. Janzing, P. Wocjan, R. Zeier, R. Geiss, and T. Beth, "Thermodynamic Cost of Reliability and Low Temperatures: Tightening Landauer's Principle and the Second Law" Int. J. Th. Phys. 39, 2717 (2000)

L. Masanes and J. Oppenheim. "A general derivation and quantification of the third law of thermodynamics". Nature Comm. 8 (2017)

J. Scharlau and M. P. Mueller. "Quantum Horn's lemma, finite heat baths, and the third law of thermodynamics" (2016). arXiv: 1605.06092.

R. Silva, G. Manzano, P. Skrzypczyk, and N. Brunner. "Performance of autonomous quantum thermal machines: Hilbert space dimension as a thermodynamic resource" (2016). arXiv:1604.04098.

F. G.S. L. Brandao, M. Horodecki, N. H. Y. Ng, J. Oppenheim, and S. Wehner. "The second laws of quantum thermodynamics". PNAS 112 (2015)