Grand canonical Gibbs state for systems with non-commuting charges

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[N Yunger Halpern, Ph Faist, J Oppenheim, AW;
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Basic question in thermodynamics:

What is a thermal bath?

(To model equilibrium; free resource; ...)

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Outline

0. Systems with conserved quantities:

   Grand canonical state & Jaynes principle

1. Approximate microcanonical route

2. Resource theoretic route: passivity

3. Discussion

0. Conserved quantities

System: Hilbert space $\mathcal{H}$ (implicit) with Hamiltonian $H = Q_0$ and other observables $Q_1, \ldots, Q_c$ (aka "charges").

Note: Q_j do not have to commute with each other, nor with the Hamiltonian!

[Examples: Particle numbers; directional spin observables; ...]

However, assume them to be extensive in composite systems (more later).

0. ...and Gibbs states

Max-entropy principle [Jaynes, Phys. Rev. 1957]:

Given only the expectation values

$$v_j = \langle Q_j \rangle = \mathrm{Tr}\, \rho Q_j,$$

most rational state assignment is the one maximizing the von Neumann entropy

$$S(\rho) = -\mathrm{Tr}\, \rho \log \rho.$$

Has Grand Canonical Gibbs (GCG) form

$$\gamma(v) = \frac{1}{Z} \exp(-\beta H - \Sigma_j \mu_j Q_j),$$

$$Z = \mathrm{Tr} \exp(-\beta H - \Sigma_j \mu_j Q_j).$$

Grand canonical Gibbs (GCG) form:

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Expectation values $v=(v_0, v_1, \ldots, v_c)$ and the $(\beta, \mu_1, \ldots, \mu_c)$ determine each other one-to-one; "chemical potentials" $-\mu_j/\beta$.

* Why expectation values?
* Why entropy?

Give two justifications of GCG from first principles: one microcanonical (equilibrium), the other resource theoretic (passivity).

1. Microcanonical route

(From now on: only $\mathcal{H}$ and one other charge Q)

Let the system be in contact with many replicas of itself - quantities extensive:

$$\bar{\mathcal{H}} = \frac{1}{n}\sum_{t=1}^{n} \mathcal{H}^{(t)}, \quad \bar{Q} = \frac{1}{n}\sum_{t=1}^{n} Q^{(t)}.$$

Well-known, simple case: $[\mathcal{H}, Q] = 0$, so that $\mathcal{H}$ and Q are simultaneously diagonalized, and so $\overline{\mathcal{H}}$ and $\overline{Q}$.

Now: Let $\mathcal{M}$ simultaneous eigenspace of $\overline{\mathcal{H}}$ and $\overline{Q}$ with eigenvalues E and N, resp. Microcanonical state Ω = uniform density on $\mathcal{M}$.

It follows that single-site states

$$\Omega_t = Tr_{\neq t}\, \Omega \text{ are } \approx \gamma(E,N)!$$

Single-site states $\Omega_t = \mathrm{Tr}_{\neq t}\, \Omega$ are $\approx \gamma(\mathcal{E},\mathcal{N})$!

$$D(\Omega_t \| \gamma(\mathcal{E},\mathcal{N})) = \mathrm{Tr}\, \Omega_t \log \Omega_t - \mathrm{Tr}\, \Omega_t \log \gamma(\mathcal{E},\mathcal{N})$$

$$= - S(\Omega_t)$$

$$= - \log Z - \beta \mathcal{H}^{(t)} - \mu Q^{(t)}$$

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$$= \beta\mathcal{E} + \mu\mathcal{N}$$

$$= \langle \beta\mathcal{H} + \mu Q \rangle_{\gamma(\mathcal{E},\mathcal{N})}$$

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$$\frac{1}{n}\sum_{t=1}^{n} D(\Omega_t \| \gamma(\mathcal{E},\mathcal{N})) = -\frac{1}{n}\sum_{t=1}^{n} S(\Omega_t) + \underbrace{\log Z + \langle \beta \vec{\mathcal{H}} + \mu \vec{\mathcal{Q}} \rangle_{\Omega}}$$

$$= S(\gamma(\mathcal{E},\mathcal{N})) - \frac{1}{n}\sum_{t=1}^{n} S(\Omega_t)$$

$$\leq S(\gamma(\mathcal{E},\mathcal{N})) - \frac{1}{n} S(\Omega)$$

$$= S(\gamma(\mathcal{E},\mathcal{N})) - \frac{1}{n} \log |\mathcal{M}|$$

$$= o(1)$$

Leading order of $|\mathcal{M}|$ from combinatorics…

If $[\mathcal{H}, Q] \neq 0$, $\mathcal{H}$ and Q now don't have joint eigenspaces ⚡

However, $[\bar{\mathcal{H}}, \bar{Q}] = O(1/n)$, so for large n expect "almost commutation"...

Indeed, [Ogata, J Func. Anal. 2013] proved that there exist $\hat{\mathcal{H}} = \hat{Q}_0$ and $\hat{Q}_j$ that commute, and $\| \bar{Q}_j - \hat{Q}_j \| \to 0$ for $n \to \infty$.

Operator norm, i.e. largest singular value

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Can exploit this to construct an approximate microcanonical (a.m.c.) subspace consisting of the "almost-eigenstates" of the observables.

Say that ρ is almost *E*-eigenstate of $\bar{H}$, if it has most of its amplitude in the eigenvalue band $[E \pm \eta]$, i.e. $\mathrm{Tr}\, \rho \Pi_E^\eta \geq 1-\delta$.

Projector onto eigenspaces of $\bar{H}$ with eigenvalues $E \pm \eta$.

Say that ρ is almost E-eigenstate of $\mathcal{H}$, if it has most of its amplitude in the eigenvalue band $[E \pm \eta]$, i.e. $Tr\, \rho \Pi_E^\eta \geq 1-\delta$.

Approximate microcanonical (a.m.c.) subspace $\mathcal{M}$ in $\mathcal{H}^{\otimes n}$ (with projector P) satisfies:

(i) Every state ω supported on $\mathcal{M}$ is an almost-eigenstate of $\mathcal{H}$ and Q: $Tr\, \omega \Pi_E^\eta \geq 1-\delta$ & $Tr\, \omega \Pi_N^\eta \geq 1-\delta$.

(ii) Every almost-eigenstate ω of $\mathcal{H}$ & Q, i.e. $Tr\, \omega \Pi_E^{\eta'} \geq 1-\delta'$ & $Tr\, \omega \Pi_N^{\eta'} \geq 1-\delta'$, has large overlap with $\mathcal{M}$: $Tr\, \omega P \geq 1-\varepsilon$.

Approximate microcanonical (a.m.c.) subspace consists of precisely the *almost-eigenstates* of the observables; parameters $(\varepsilon,\eta,\eta',\delta,\delta')$ 😬

For instance in the commuting case, $P=\Pi_{E}^{\eta}\Pi_{N}^{\eta}$ is a.m.c. subspace for large enough n, with parameters $(\varepsilon,\eta,\eta'=\eta,\delta,\delta'=\varepsilon/2)$.

Approximate microcanonical (a.m.c.) subspace consists of precisely the almost-eigenstates of the observables; parameters $(\varepsilon, \eta, \eta', \delta, \delta')$ 😬

Result 1: For consistent values of $\mathcal{E}$ & $\mathcal{N}$ [i.e. there is a $\gamma(\mathcal{E},\mathcal{N})$], $\varepsilon > 2\delta' > 0$, $\eta > \eta' > 0$ and $\delta > 0$, and large enough n, there exists a non-zero a.m.c. subspace $\mathcal{M}$.

Idea: Approximate $\bar{H}$, $\bar{Q}$ by $\hat{H}$, $\hat{Q}$, and let P be the product of the almost-eigenstate projections of those with values $\mathcal{E}$, $\mathcal{N}$ $(\pm\eta)$

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Result 1': Using only information theory ideas, can get $\varepsilon > \mathrm{poly}(n)\delta' > 0$, and $\delta > 0$ exp. small in n; furthermore, $\eta > \eta' > 0$ can be as small as $O((\log n)/\sqrt{n})$ [AW, in preparation].

& permutation symmetric!

Result 2: Given an a.m.c. subspace $\mathcal{M}$ with projector P and uniform density Ω, for most t, $\Omega_t \approx \gamma(E,N)$.

Proof even more info theoretic now:

$$\frac{1}{n}\sum_{t=1}^{n} D(\Omega_t \| \gamma(E,N)) \leq S(\gamma(E,N)) - \frac{1}{n} S(\Omega) + O(\eta)$$

Observe that $\omega = \gamma(E,N)^{\otimes n}$ is an almost-eigenstate for E, N ($\pm\eta$), and hence has high probability on P. By Schumacher quantum data compression,

$$S(\Omega) = \log |\mathcal{M}| \geq n\, S(\gamma(E,N)) - O(\sqrt{n}).$$

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$$\leq O(1/\sqrt{n}) + O(\eta).$$

In general, $\mathcal{M}$ may not be permutation symmetric, so need average over Ω_t.

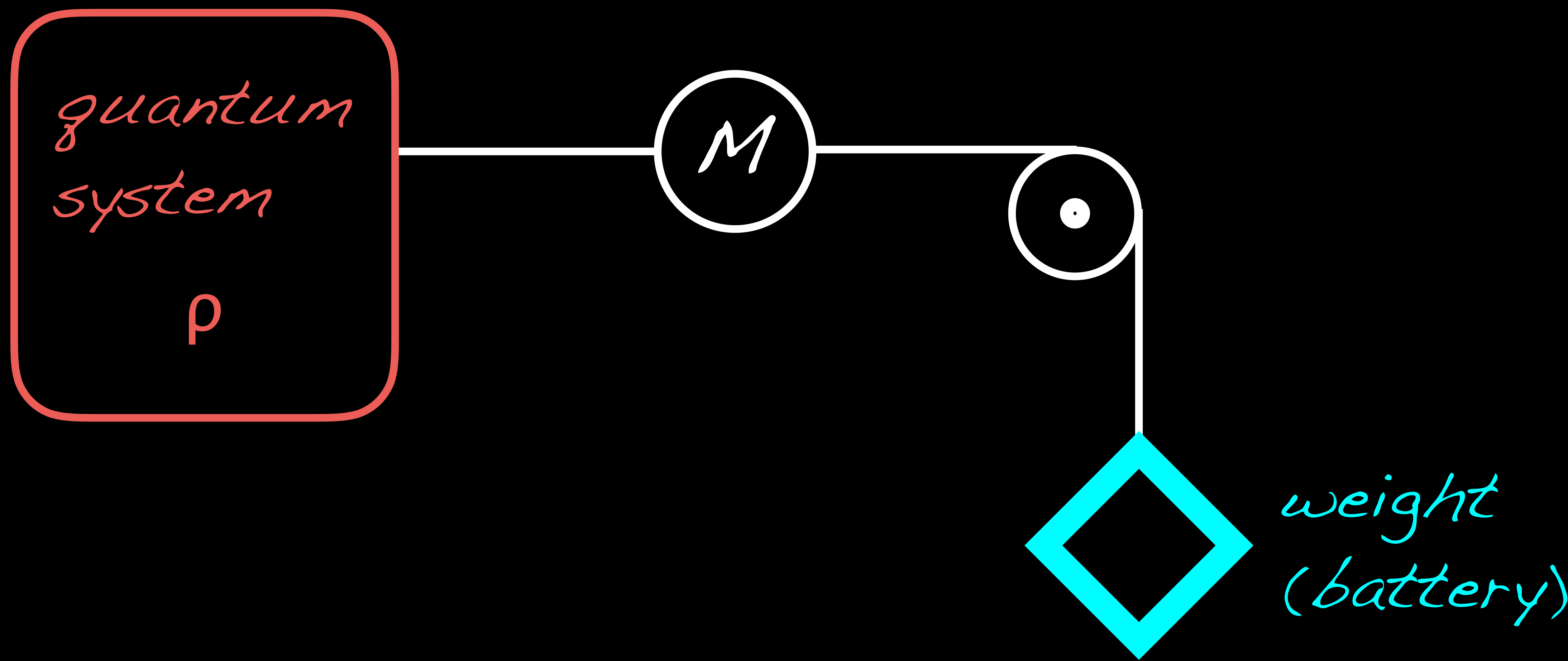
2. Resource theory: passivity

Justify Gibbs states as the unique "completely passive" states, from which no work can ever be extracted [Pusz/Woronowicz, CMP 1978; Lenard, J Stat. Phys. 1978].

This is the only way in which you can draw thermal states for free from the bath. It also defines temperature: $e^{-\beta \mathcal{H}}$

Redo this here under conservation of the charges Q_j ...

Recall P-W-L model: Couple the system to a weight to extract work.



- Can effect any $\mathcal{U}$ on $\mathcal{H}$ (suitable interaction with weight conserves energy)
- $\Delta E = \mathrm{Tr}\, \rho H - \mathrm{Tr}\, U \rho U^{\dagger} H$ is translated into (expected) raising of the weight.

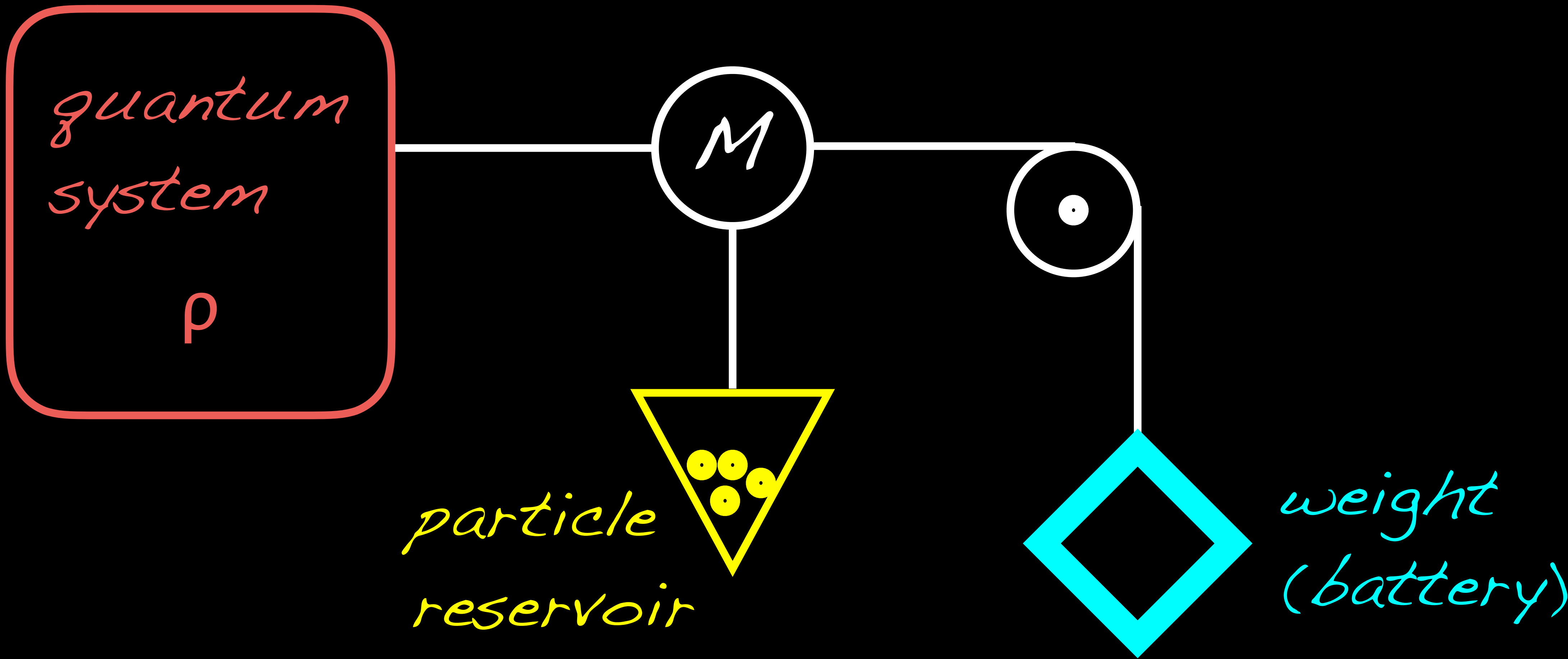
Def: State ρ is *passive* if for all U, $\Delta E \leq 0$.
It is *completely passive* if $\rho^{\otimes n}$ is passive w.r.t. $\vec{H}$, for all n.

Easy to see that passivity is equivalent to $[\rho, H] = 0$, and population $p(E)$ of energy E is non-increasing with growing E.

P-W-L prove: ρ is completely passive iff it is of Gibbs form $\gamma(E) = \frac{1}{Z} \exp(-\beta H)$.

[Cf. also Alicki/Fannes, PRE 2013]

How to bring charges into play?



Need a battery for each kind of charge, including energy. Can still do any unitary on the system using a suitable "reference frame" state in the batteries to enforce global conservation.

[1512.01189 & Guryanova et al., 1512.01190]

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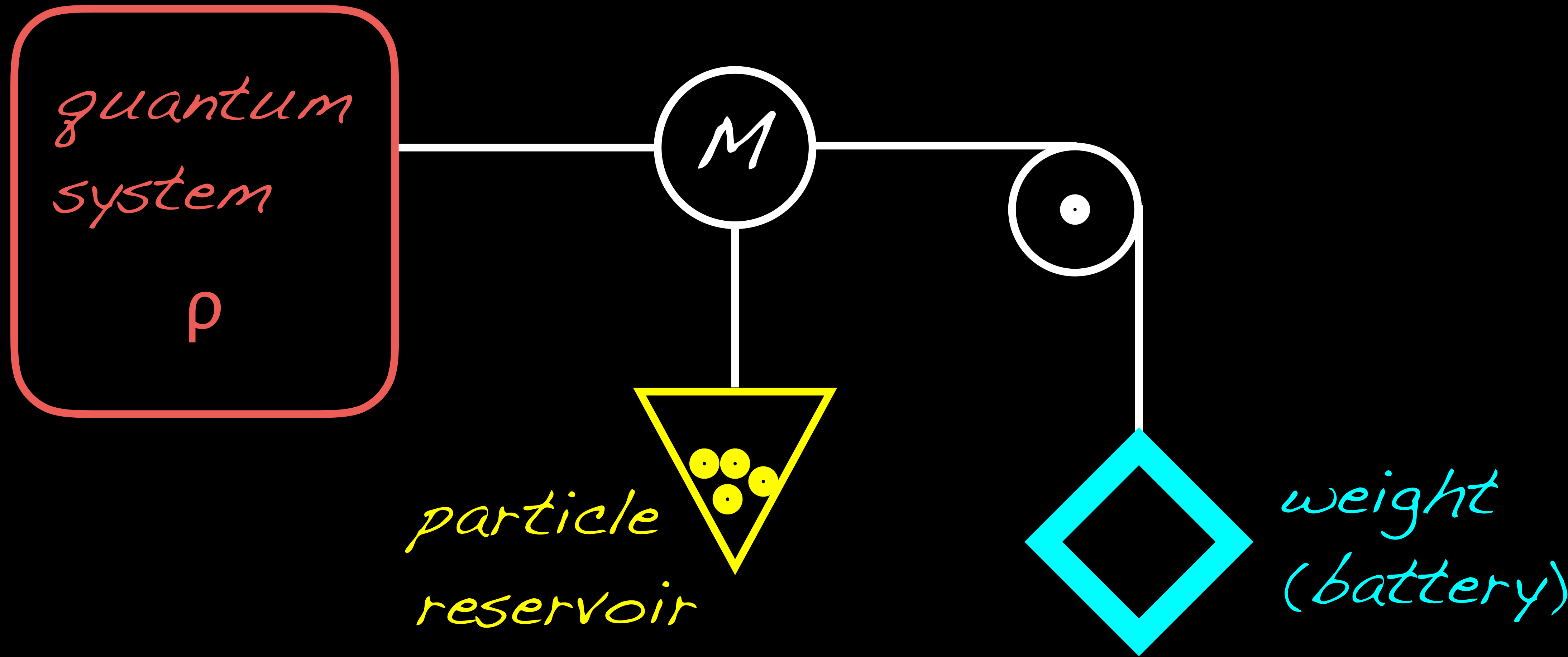

However, turns out that having access to infinitely many $\gamma(E,N)$, can trade H for Q freely subject to $\beta \Delta E + \mu \Delta N \leq 0$. If you find that surprising, consider that $\gamma(E,N)$ is not completely passive for H...

[1512.01189 & *Guryanova et al.*, 1512.01190]

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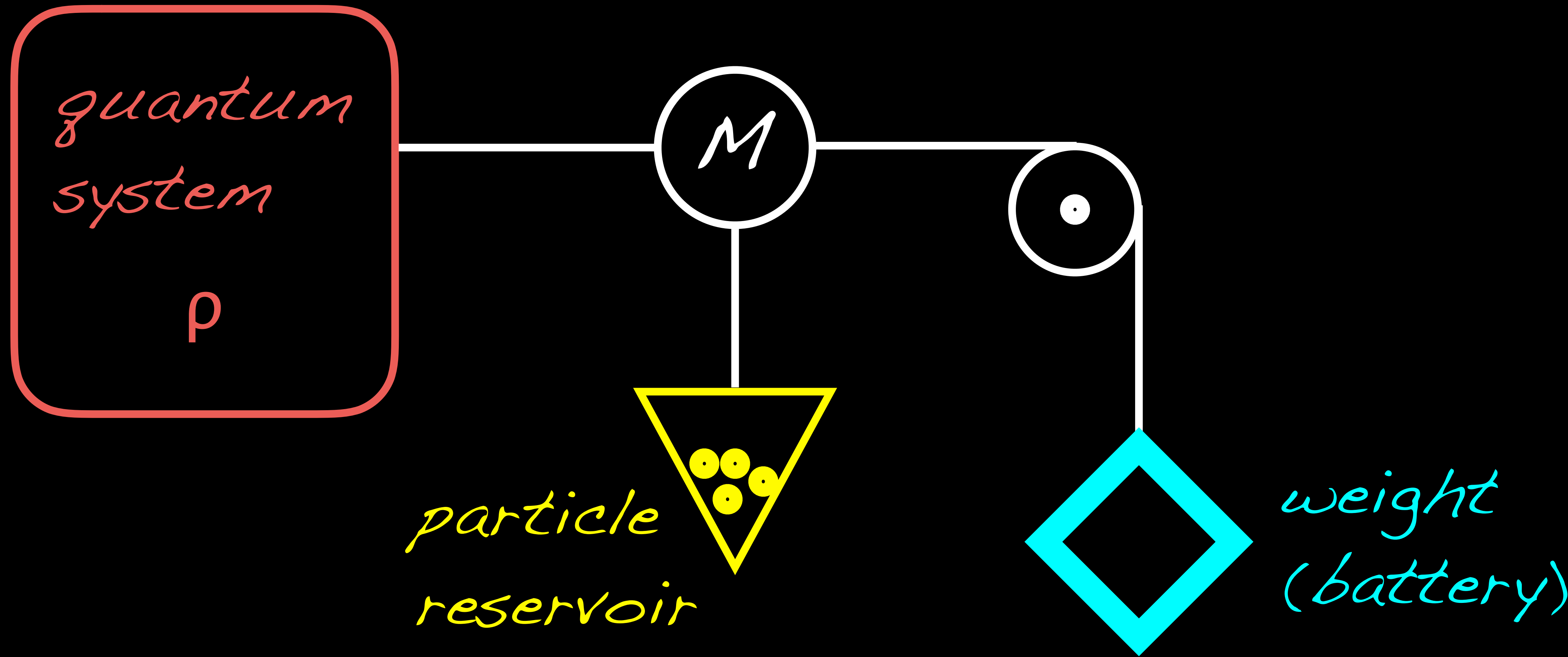

For passivity theory: Constrain allowed operations to $\Delta N = 0$, i.e. no change of the charges on the batteries.

In fact: Want $\mathcal{U}$ acting on $\mathcal{H}$ to conserve Q (all Q_j).

[AW, in preparation]

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- Clearly a problem when $[\mathcal{H},Q]\neq 0$: $[\mathcal{U},Q]=0$ would mean that we cannot work in the energy eigenbasis...(?)
- Even have a problem when $[\mathcal{H},Q]=0$: let E_α and N_α be the $\mathcal{H}$ and Q eigenvalues in joint eigenbasis $|\alpha\rangle$, and assume the N_α to be incommensurate. Then on n copies, allowed $\mathcal{U}$ must automatically conserve the energy!

[AW, in preparation]

Motivates the following new rules:

Def: On n copies, allow asymptotically charge conserving unitaries, i.e.

$$\| \overline{Q} - U^\dagger \overline{Q} U \| \to 0.$$

(Equivalent to saying that if ρ is eigen-state of Q, then $U\rho U^\dagger$ is an almost-eigenstate.)

[AW, in preparation]

Motivates the following new rules:

Def: On n copies, allow asymptotically charge conserving unitaries, i.e.
$\| \overline{Q} - U^\dagger \overline{Q} U \| \to 0$.

Result 3: The GCG states $\gamma(E,N)$ are asymptotically passive, meaning that no rate of work per copy can be extracted under asymptotically charge conserving U.
(This follows already from [Guryanova et al., 1512.01190] under $\Delta N \to 0$.)

[AW, in preparation]

Result 4: For any state ρ, the asymptotic rate of work per copy that can be extracted by the allowed operations is $\Delta E = E - E_0$, where $E = \mathrm{Tr}\, \rho \mathcal{H}$, $N = \mathrm{Tr}\, \rho Q$, and $E_0 := \min \mathrm{Tr}\, \sigma \mathcal{H}$ s.t. $S(\sigma) \geq S(\rho)$, $\mathrm{Tr}\, \sigma Q = N$ (= energy of the GCG with same $\langle Q \rangle$ and entropy as ρ). I.e. no non-GCG state is asymptotically passive.

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$$\Delta E = kT\, D(\rho \| \gamma(E_0, N))$$ 🤓

[1512.01189 & 1512.01190; AW, in preparation]

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Justifies $\gamma(E,N)$ as free state in thermodynamic resource theory with conserved quantities; and β, μ as intrinsic properties.

[1512.01189 & 1512.01190; AW, in preparation]

Proof ideas:

In one direction, cannot extract more work because $\omega = U\rho^{\otimes n}U^{\dagger}$ has the same entropy as $\rho^{\otimes n}$, but almost the same expectation of $\vec{Q}$, so $\mathrm{Tr}\,\omega\vec{H}$ is essentially lower bounded by E_0...

Work extraction protocol is fun - it uses a.m.c. subspaces and information theory ideas.

Proof ideas (Work extraction protocol):

1. Construct a.m.c. subspaces $\mathcal{M}$ for $(\underline{E}=\langle H\rangle, \underline{N}=\langle Q\rangle)$ and $\mathcal{M}_0$ for $(\underline{E}_0,\underline{N})$. Both may be assumed to lie inside an a.m.c. $\mathcal{L}$ for $\underline{N}=\langle Q\rangle$ alone: $\mathcal{M} \subset \mathcal{L} \supset \mathcal{M}_0$.

2. $\mathcal{M}$ is a high-probability subspace for $\rho^{\otimes n}$; so we can find inside it a minimal typical subspace $\mathcal{T} \subset \mathcal{M}$, of $\log|\mathcal{T}| \lesssim n\, S(\rho)$.

3. Otoh, $\mathcal{M}_0$ is a high-probability subspace for $\gamma(\underline{E}_0,\underline{N})$, so

$$\log|\mathcal{M}_0| \gtrsim n\, S(\gamma(\underline{E}_0,\underline{N})) = n\, S(\rho).$$

Proof ideas (Work extraction protocol):

1. Construct a.m.c. subspaces $\mathcal{M}$ for $(E=\langle H\rangle, N=\langle Q\rangle)$ and $\mathcal{M}_0$ for (E_0, N). Both may be assumed to lie inside an a.m.c. $\mathcal{L}$ for $N=\langle Q\rangle$ alone: $\mathcal{T} \subset \mathcal{M} \subset \mathcal{L} \supset \mathcal{M}_0$;

$$\log|\mathcal{T}| \lesssim n\, S(\rho);$$

$$\log|\mathcal{M}_0| \gtrsim n\, S(\gamma(E_0, N)) = n\, S(\rho).$$

4. Thus there is an isometry $U : \mathcal{T} \to \mathcal{M}_0$, which we can extend to a unitary U on $\mathcal{L}$, and then trivially (by identity) to the whole space. Check that it does what we want.

3. Discussion

- What we did: GCG states justified as equilibrium states and asymptotically passive states, even when charges do not commute. Tool: a.m.c. subspace.
- [Guryanova et al., 1512.01190] show that in the presence of multiple observables, and free $\gamma(E,N)$, the only quantity obeying a second law is $\beta\mathcal{H}+\mu Q$.
- Can replicate this by composing asymptotically conserving operations.

3. Discussion

- Beginnings of a resource theory: Peculiar due to necessity of batteries that double as reference frame to deal with conservation laws. Seems that we can only deal with work/charge extraction on expectation. Fluctuations?
- However, the many-copy protocols suggest deterministic work/charge extraction - open how to characterize the kind of reference frames needed to implement those unitaries...

3. Discussion

- In fact, it's open even how to think of separate batteries in the non-commuting case – in 1512.01189 have an "integrated battery + reference" for all Q_j, and actually all elements of the Lie algebra generated by them. How to avoid this overkill?

3. Discussion

- A.m.c. subspace a robust extension of microcanonicality to non-commuting quantities. Can we do it also for a general bath (≠ replicas of the system)?
- Can we impose further constraints on the a.m.c. subspace? E.g., would be nice if we could get its projector to commute with at least $\mathcal{H}$...
- Other applications or generalizations of a.m.c. subspaces?