Constant of motion identifying ESQPTs

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What does ESQPT mean?

- Hamiltonian depending on an external parameter, $\mathcal{H}(\lambda)$.

Definition of ESQPT

An ESQPT is a non-analyticity of the level density and/or the level flow in the plane $E \times \lambda$.

- Generalization of QPT to excited states.

Typical features of QPT

- Non-analyticity at a critical value, λ_c.
- Two different phases separated by λ_c.

Example: Rabi/Dicke models

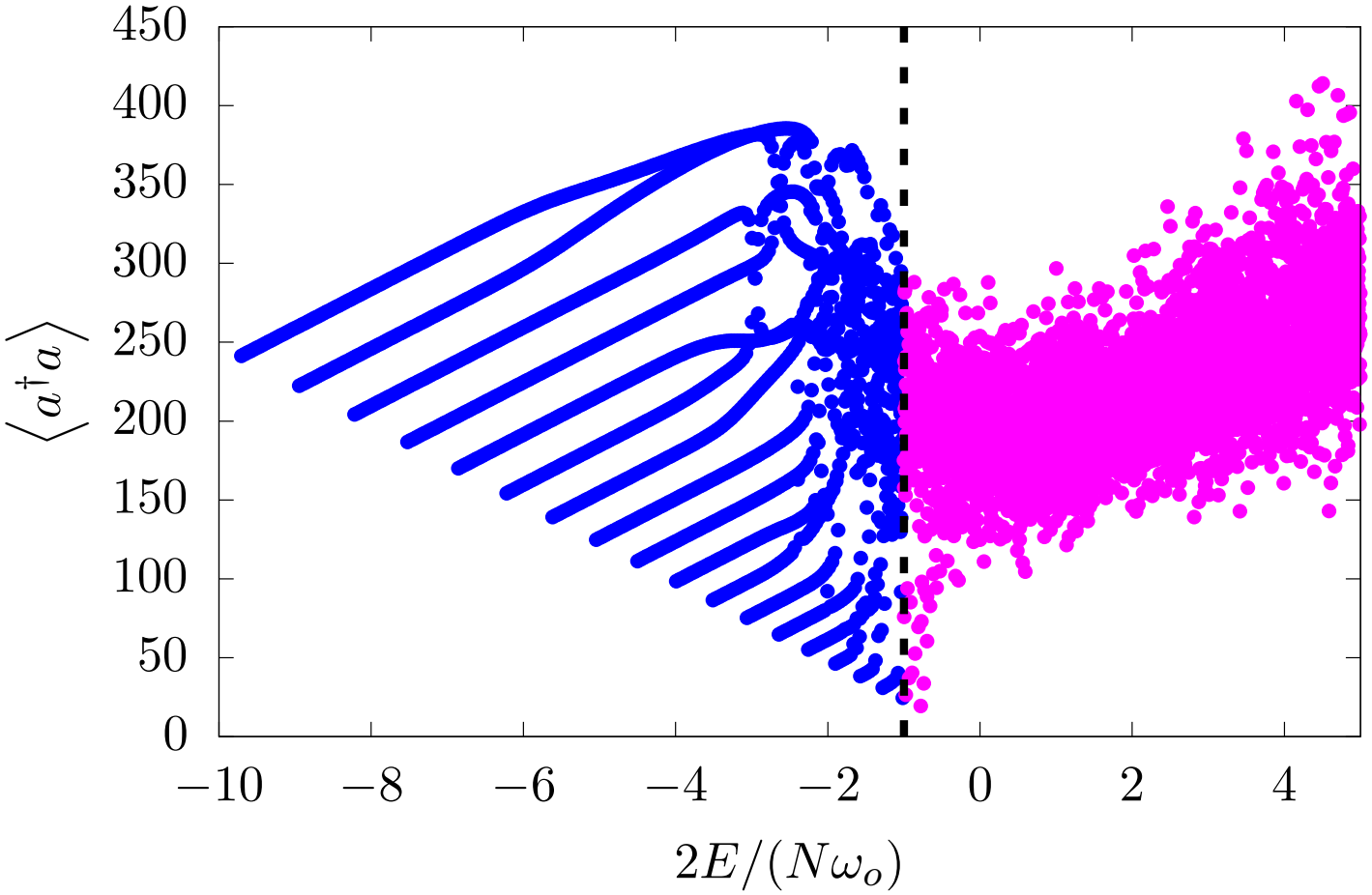
$$\mathcal{H} = \omega_o J_z + \omega a^\dagger a + \frac{2\lambda}{\sqrt{N}} J_x \left(a + a^\dagger\right), \quad \lambda_c = \frac{\sqrt{\omega_o \omega}}{2}$$

$$\lambda < \lambda_c \quad \longrightarrow \quad \text{Normal phase} \longrightarrow \begin{cases} \langle a^\dagger a \rangle = 0 \\ \langle J_z \rangle = -N/2 \end{cases}$$

$$\lambda > \lambda_c \quad \longrightarrow \quad \text{Superradiant phase} \longrightarrow \begin{cases} \langle a^\dagger a \rangle > 0 \\ \langle J_z \rangle > -N/2 \end{cases}$$

ESQPT in the Rabi/Dicke models

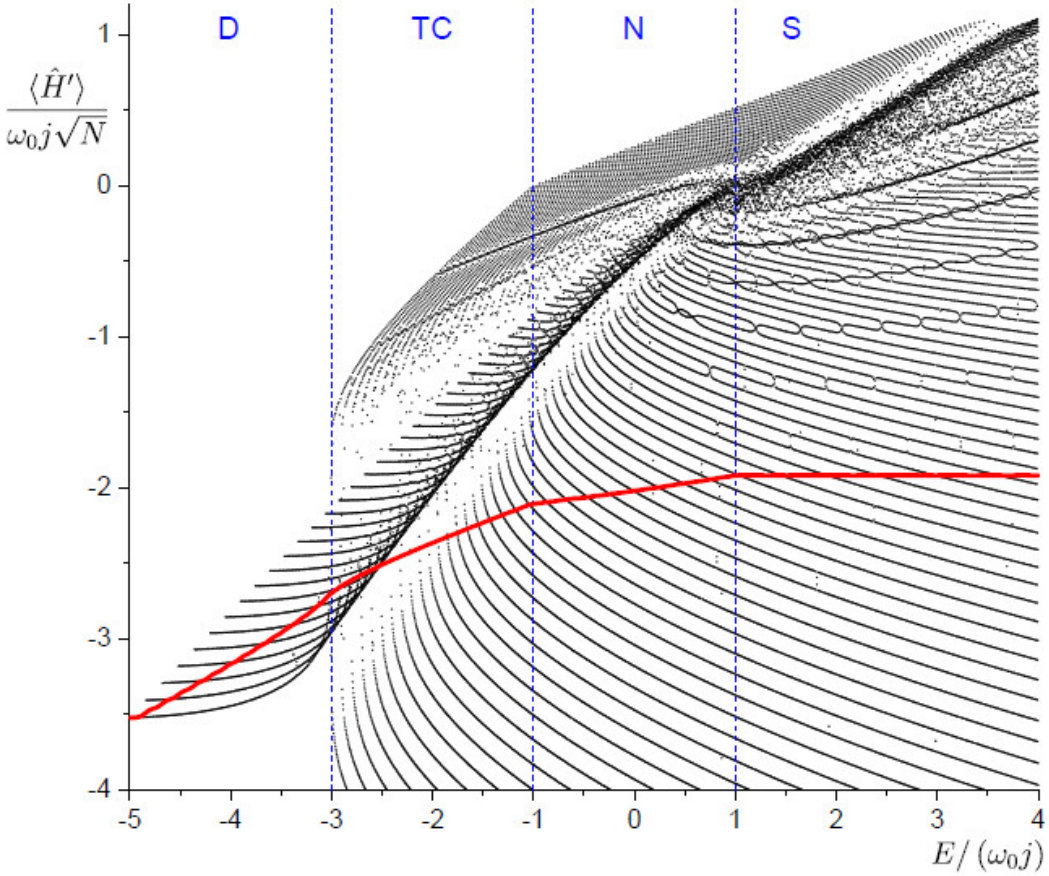
For $\lambda > \lambda_c$, critical energy at $E_c = -N\omega_o/2$



No clear differences between $E < E_c$ and $E > E_c$

What does ESQPT mean?

Idea I: susceptibilities

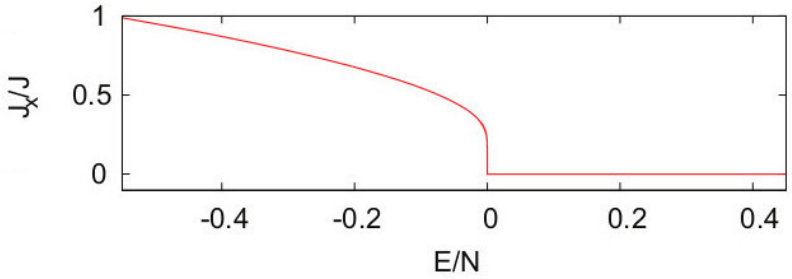


P. Cejnar, P. Stránský, M. Macek, and M. Kloc, J. Phys. A **54**, 133001 (2021)

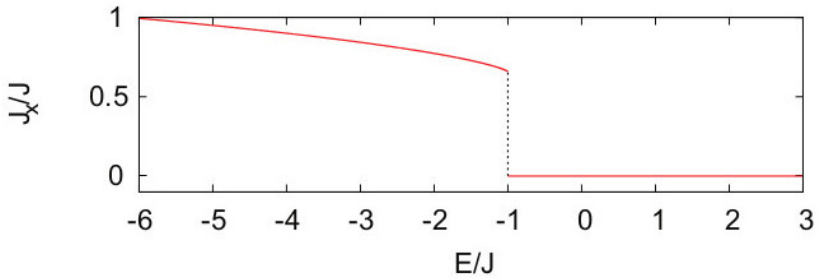
What does ESQPT mean?

Idea II: symmetry-breaking order parameter

LMG model



Dicke model



R. Puebla and A. R., EPL **104**, 50007 (2013)

What does ESQPT mean?

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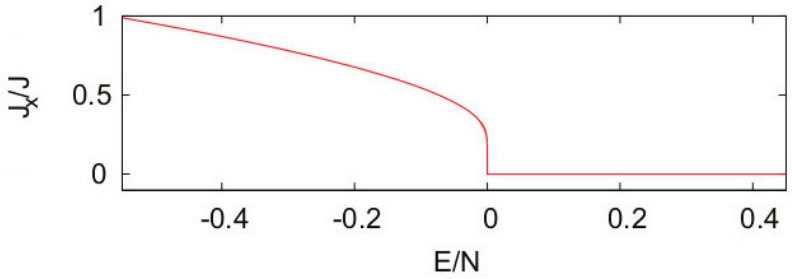

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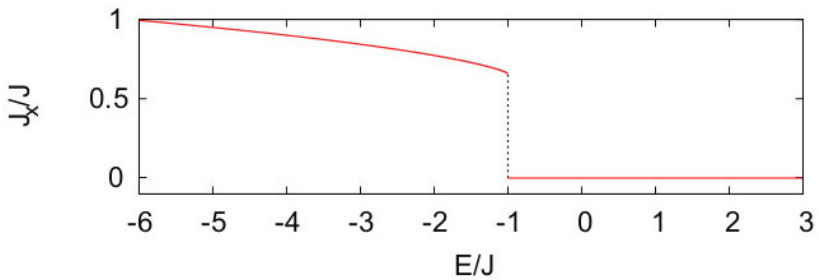

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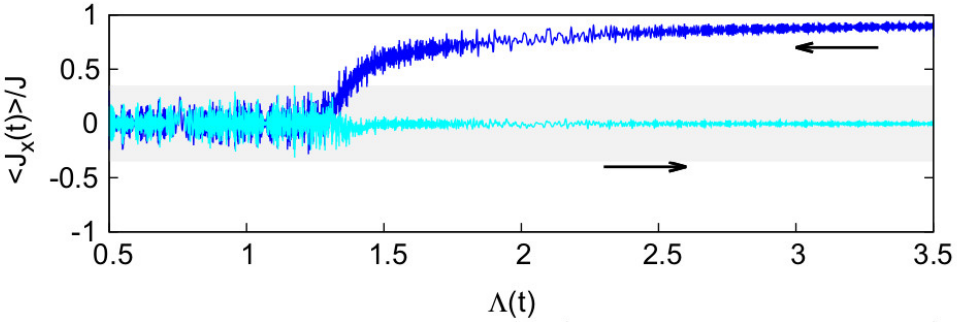
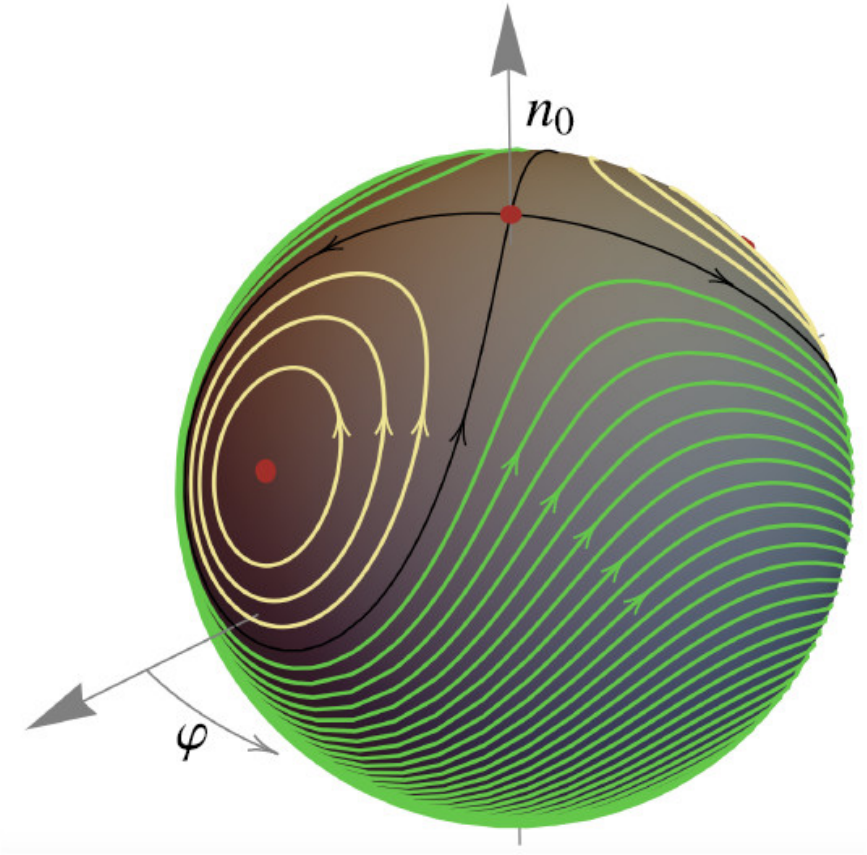


R. Puebla and A. R., Phys. Rev. E **92**, 012101 (2015).

What does ESQPT mean?

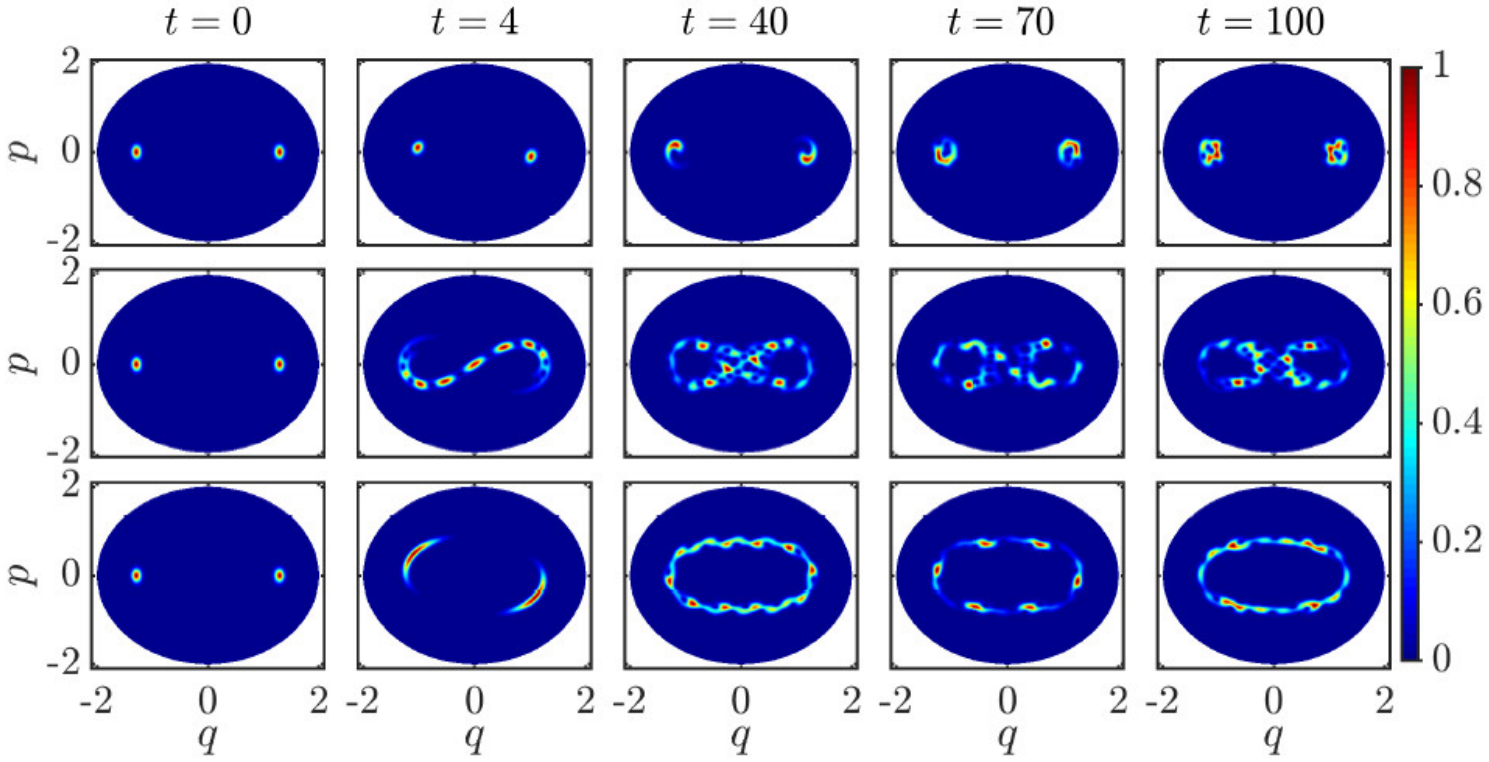
Idea III: Topology of classical orbits



P. Feldmann, C. Klempt, A. Smerzi, L. Santos, and M. Gessner, arXiv:2011.02823 (2020)

What does ESQPT mean?

Idea IV: Husimi functions



Q. Wang and F. Perez-Bernal, arXiv:2011.11932 (2020)

Relying on the classical phase space

LINK BETWEEN ESQPTS AND CLASSICAL MECHANICS

There is a fixed point of the classical Hamiltonian flow at the critical energy of an ESQPT:

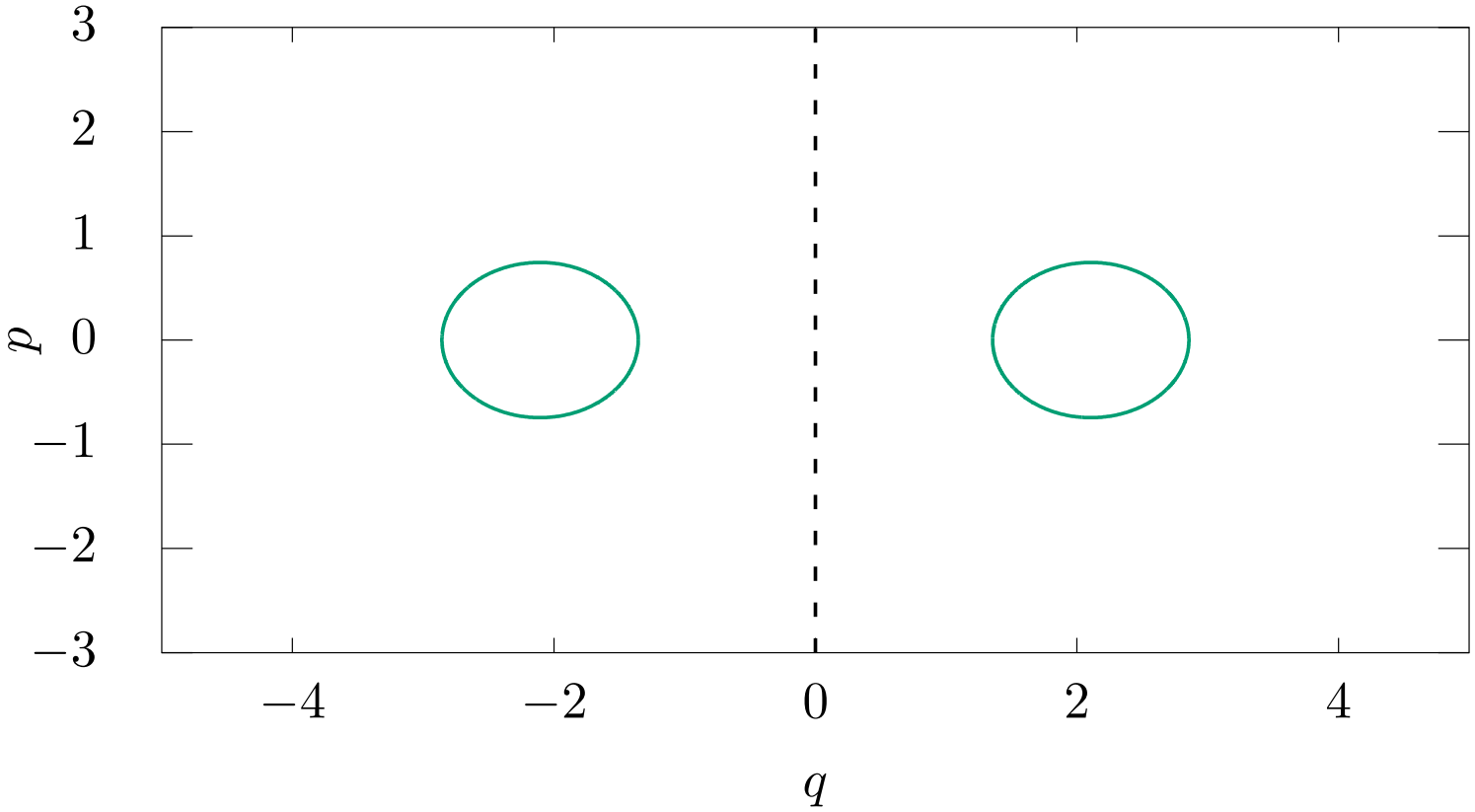
$$\nabla\mathcal{H}\left(\mathbf{p},\mathbf{q}\right)|_{(\mathbf{p}_c,\mathbf{q}_c)}=0,\ \ \mathcal{H}(\mathbf{p}_c,\mathbf{q}_c)=E_c.$$

- The classical Hamiltonian is reached in a certain limit:
  - Dicke model, $N\to\infty$.
  - Rabi model, $\dfrac{\omega_o}{\omega}\to\infty$.

Relying on the classical phase space

Curves with $E = \mathrm{cte}$ in the Rabi model:

$$2E/\omega_0 = -4$$



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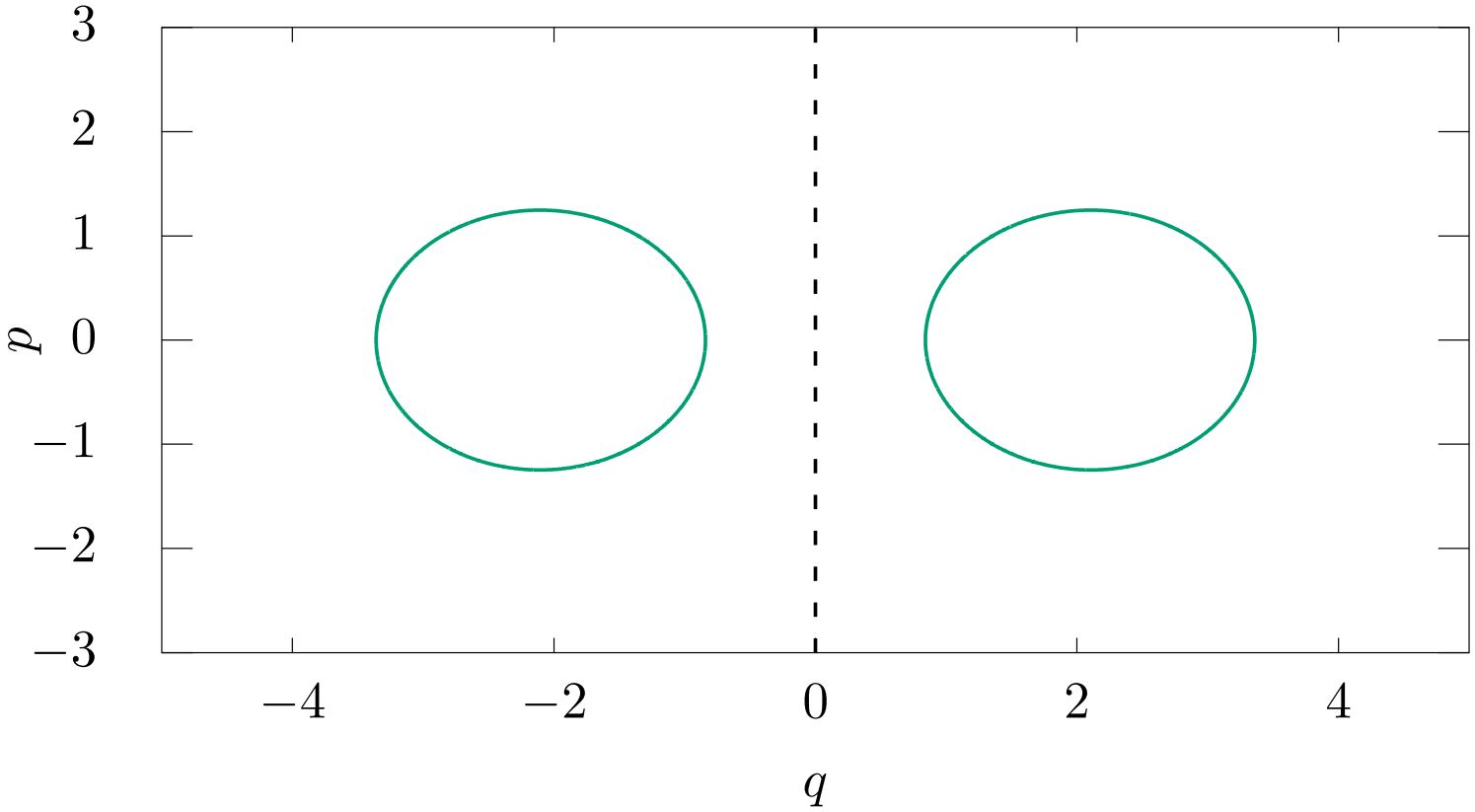

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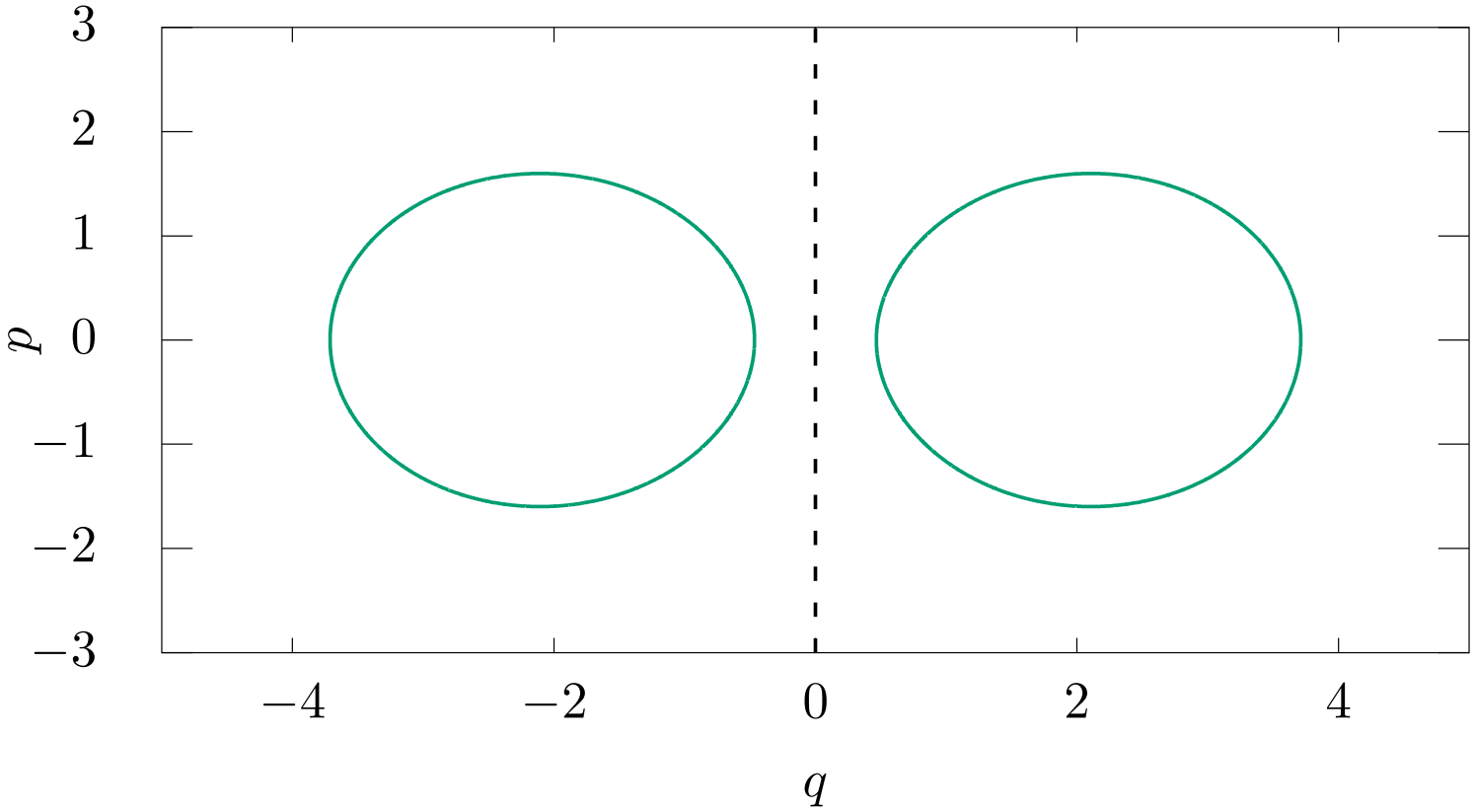

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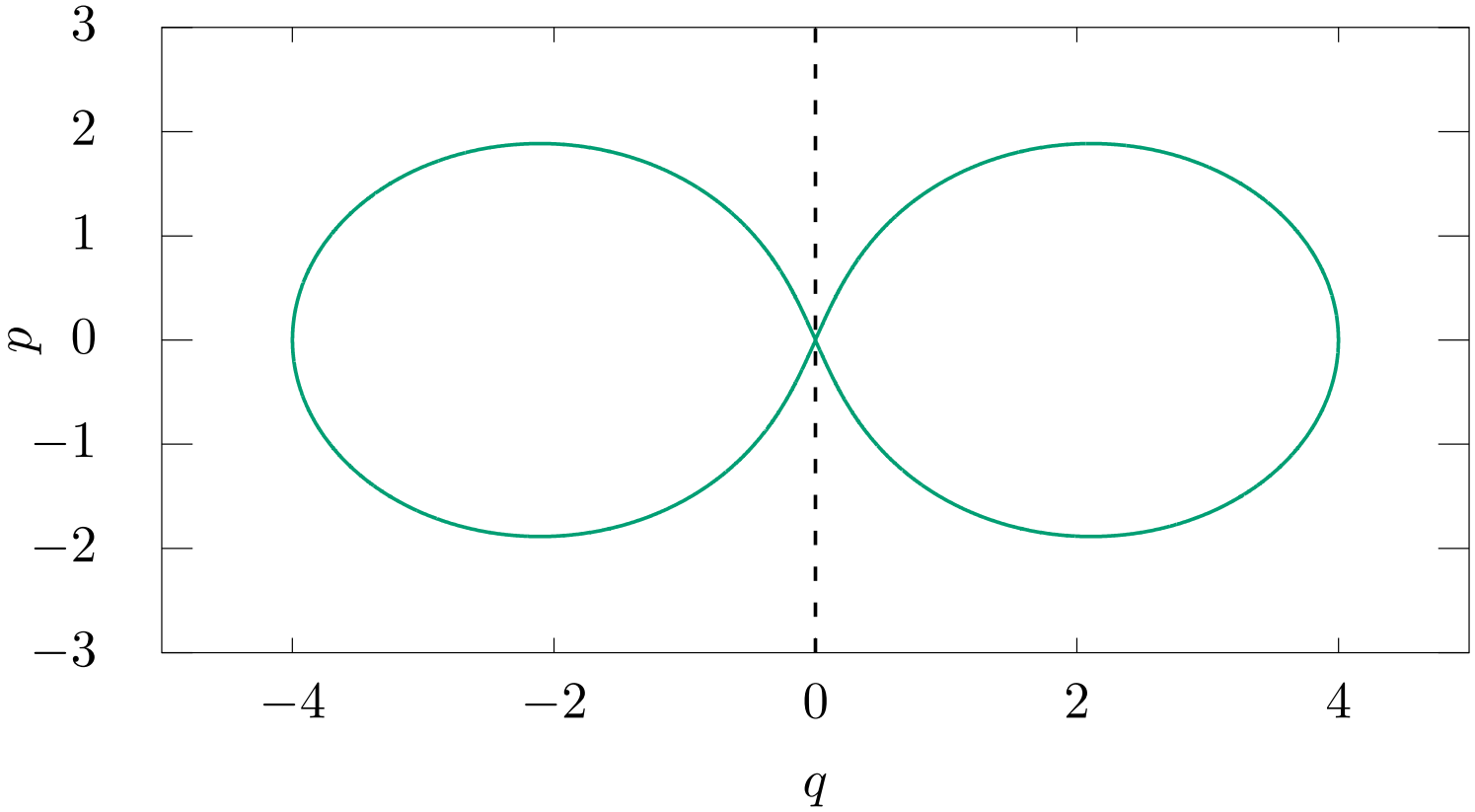

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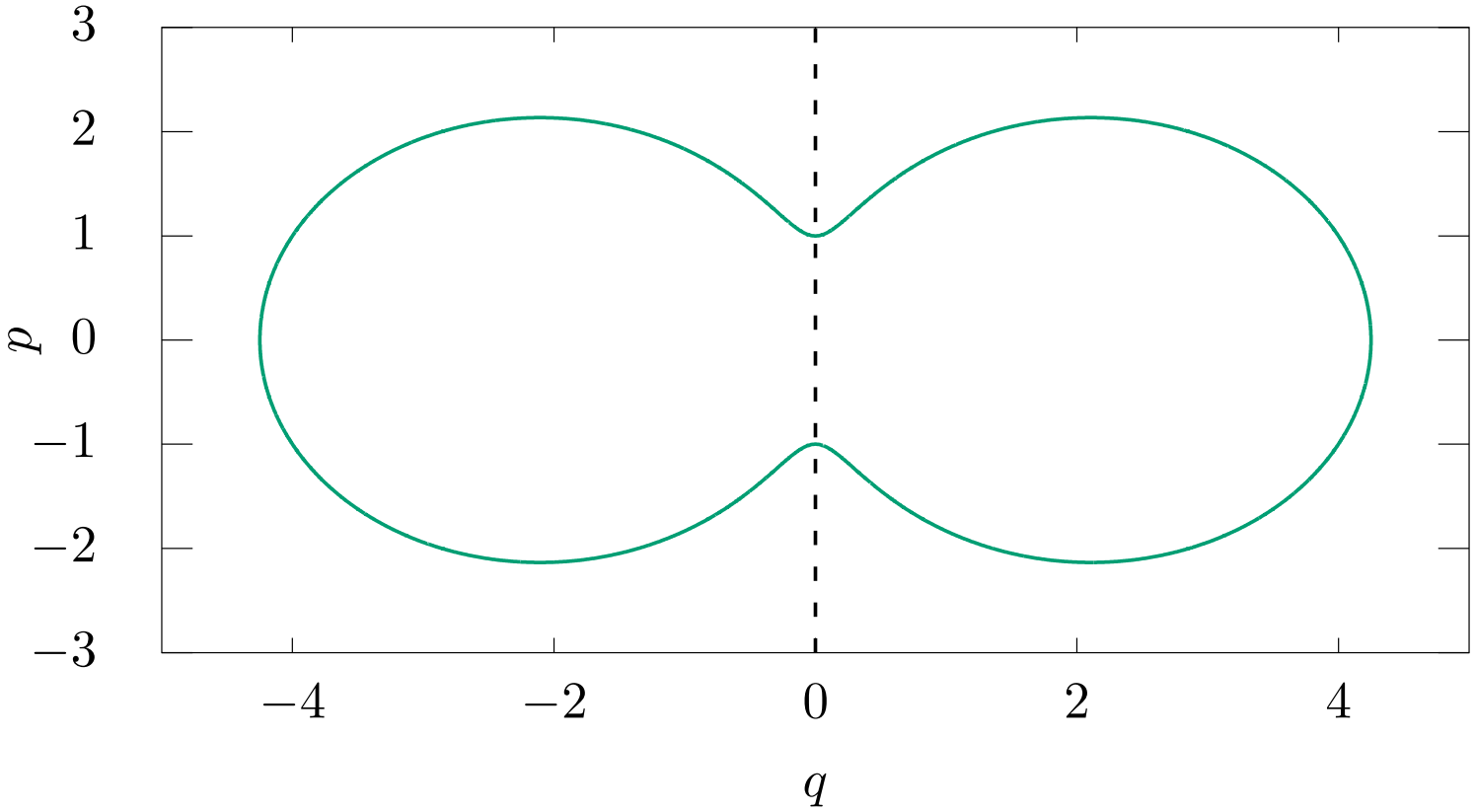

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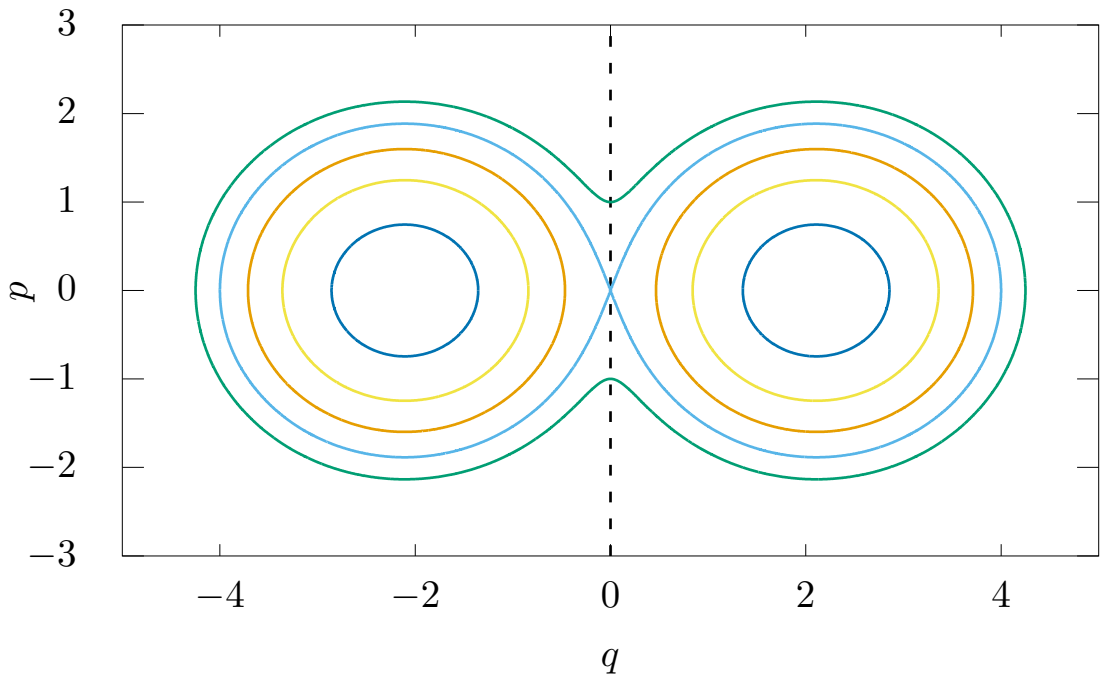
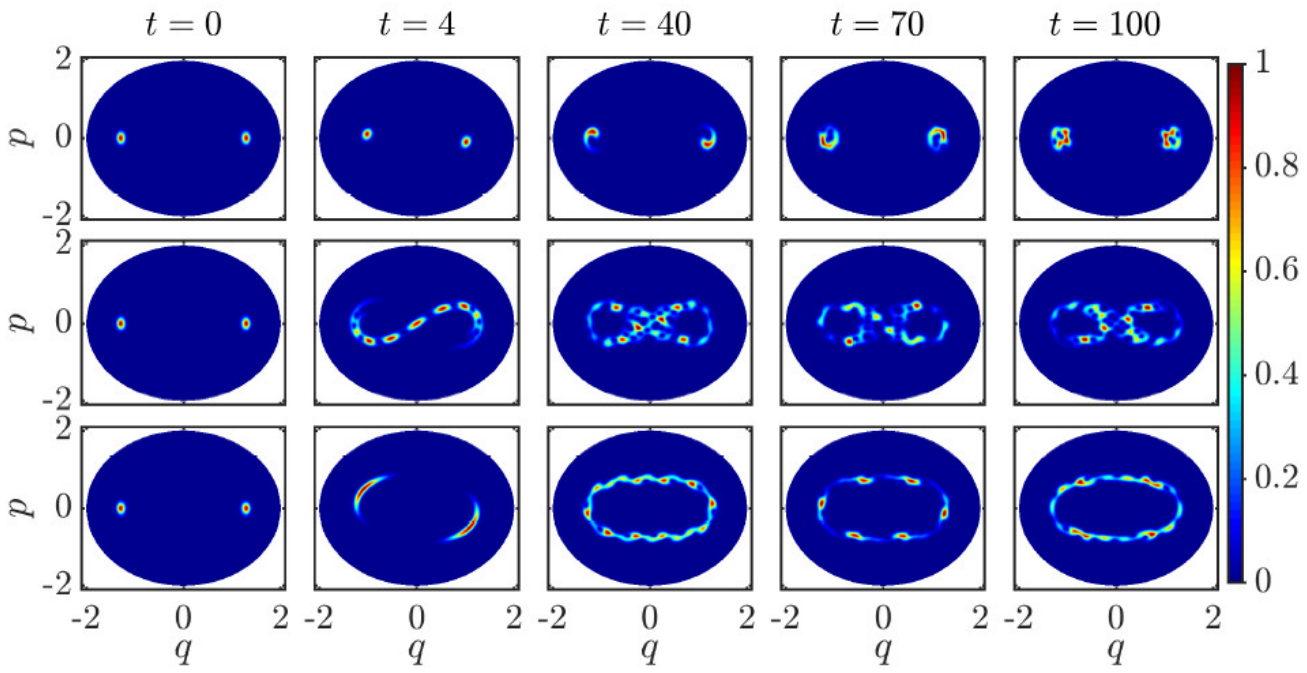


SUMMARY OF CLASSICAL RESULTS

- If $E < E_c$, trajectories are trapped either $q(t) < 0$ or $q(t) > 0$, $\forall t$.
- If $E > E_c$, trajectories pass through $q < 0$ and $q > 0$.

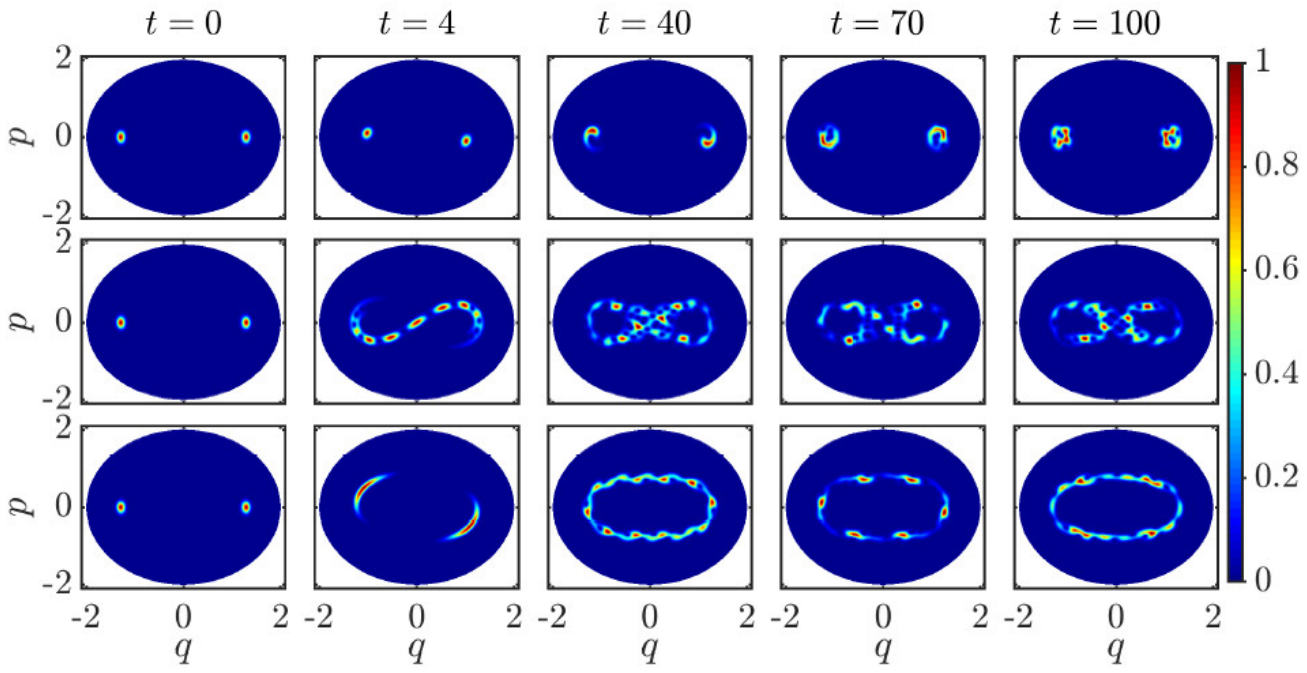
Relying on the classical phase space



What happens in quantum mechanics?

- Quantum and classical evolutions are different.
- We can find superpositions of both parts of the phase space.

Relying on the classical phase space



Our objective

Translate this features of classical dynamics into quantum thermodynamics.

From classical dynamics to quantum thermodynamics

Quantum system, $\mathcal{H}$, with a classical analogue, $\mathcal{H}(\mathbf{q}, \mathbf{p})$, and a dynamical function, $f(\mathbf{q}, \mathbf{p})$, so that

- If $E < E_c$, $f(t) \equiv f(\mathbf{q}[t], \mathbf{p}[t])$ is either $f(t) < 0$ or $f(t) > 0$, $\forall t$.
- If $E > E_c$, any trajectory passes through $f > 0$ and $f < 0$.

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Route to quantum thermodynamics

1. Quantum operator for f, $\hat{f} = \hat{f}\,(\hat{\mathbf{q}},\hat{\mathbf{p}})$.
2. **Definition:** $\mathcal{C} = \mathrm{sign}\left(\hat{f}\right)$.
   - $\mathcal{C} = M^{-1}\mathrm{sign}(\Lambda)M$, Λ diagonal matrix with eigenvalues of $\hat{f}$, and M matrix whose columns are the eigenvectors of $\hat{f}$.
   - $\mathcal{C} = \dfrac{2}{\pi}\displaystyle\int_0^\infty dx\,\hat{f}\left(x^2\mathbb{I} + \hat{f}^2\right)^{-1}$.
   - $\mathrm{Spec}(\mathcal{C}) = \pm 1$.

From classical dynamics to quantum thermodynamics

Let us write the Hamiltonian in terms of the prjectors onto the eigenstates, $\mathcal{H} = \sum_n E_n \hat{P}_n$.

CONJECTURE

- $[\mathcal{C}, \hat{P}_n] = 0, \forall E_n < E_c$.
- $[\mathcal{C}, \hat{P}_n] \neq 0, \forall E_n > E_c$.

COROLLARY

Let us consider an initial condition, $|\psi(0)\rangle$. $\mathcal{C}$ is a constant of motion for the corresponding time evolution, $|\psi(t)\rangle$, iff $\langle\psi(0)|\,\mathcal{H}\,|\psi(0)\rangle < E_c$.

$\mathcal{C}$ acts like a discrete $\mathbb{Z}_2$ symmetry if $E < E_c$.

Thermodynamics consequences of the new constant of motion

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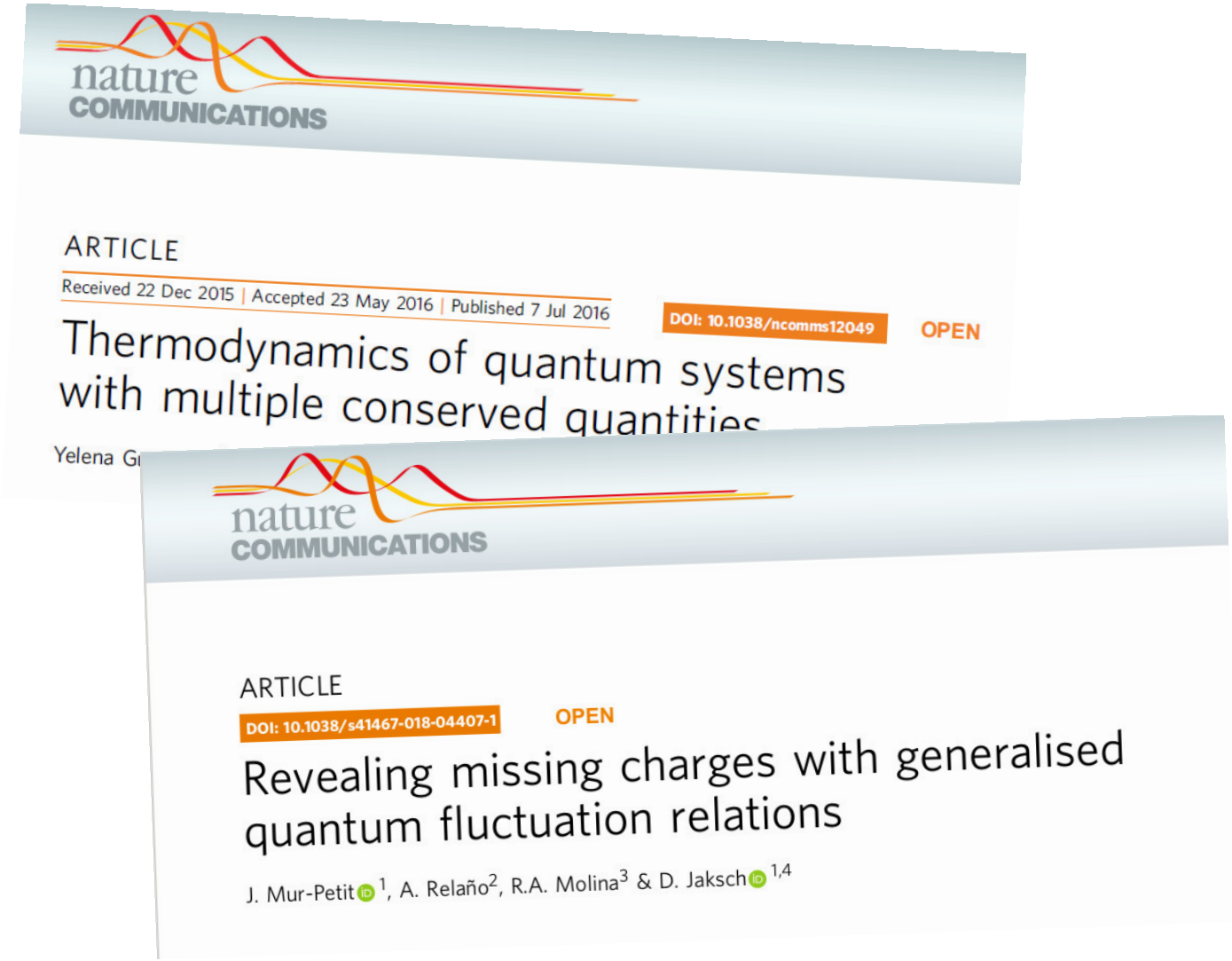
Thermodynamics of quantum systems with multiple conserved quantities

Yelena Guryanova[1], Sandu Popescu[1], Anthony J. Short[1], Ralph Silva[1,2] & Paul Skrzypczyk[1]

Thermodynamics consequences of the new constant of motion



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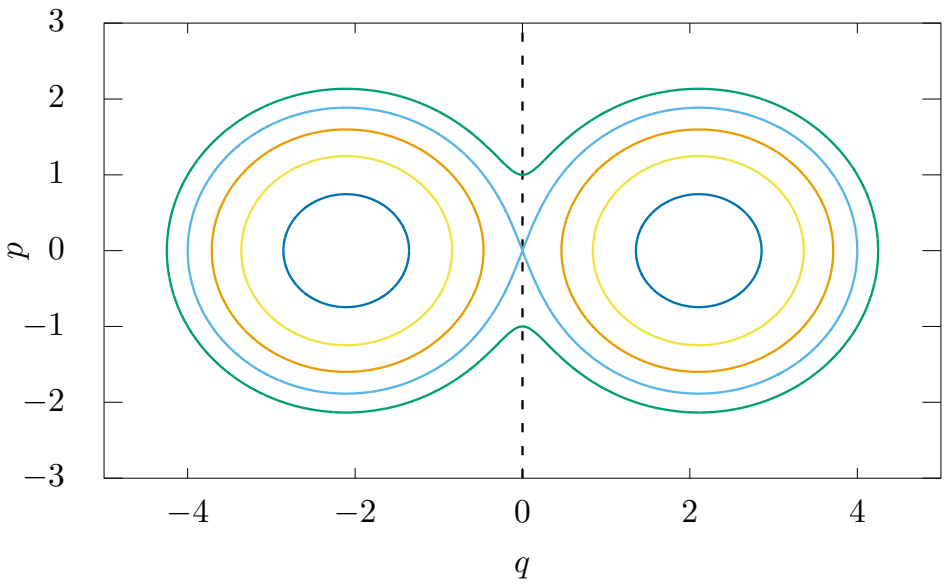
Revealing missing charges with generalised quantum fluctuation relations

J. Mur-Petit[1], A. Relaño[2], R.A. Molina[3] & D. Jaksch[1,4]

Studying the behavior of $\mathcal{C}$

Rabi and Dicke models



CONSTANT OF MOTION FOR THE RABI AND DICKE MODELS

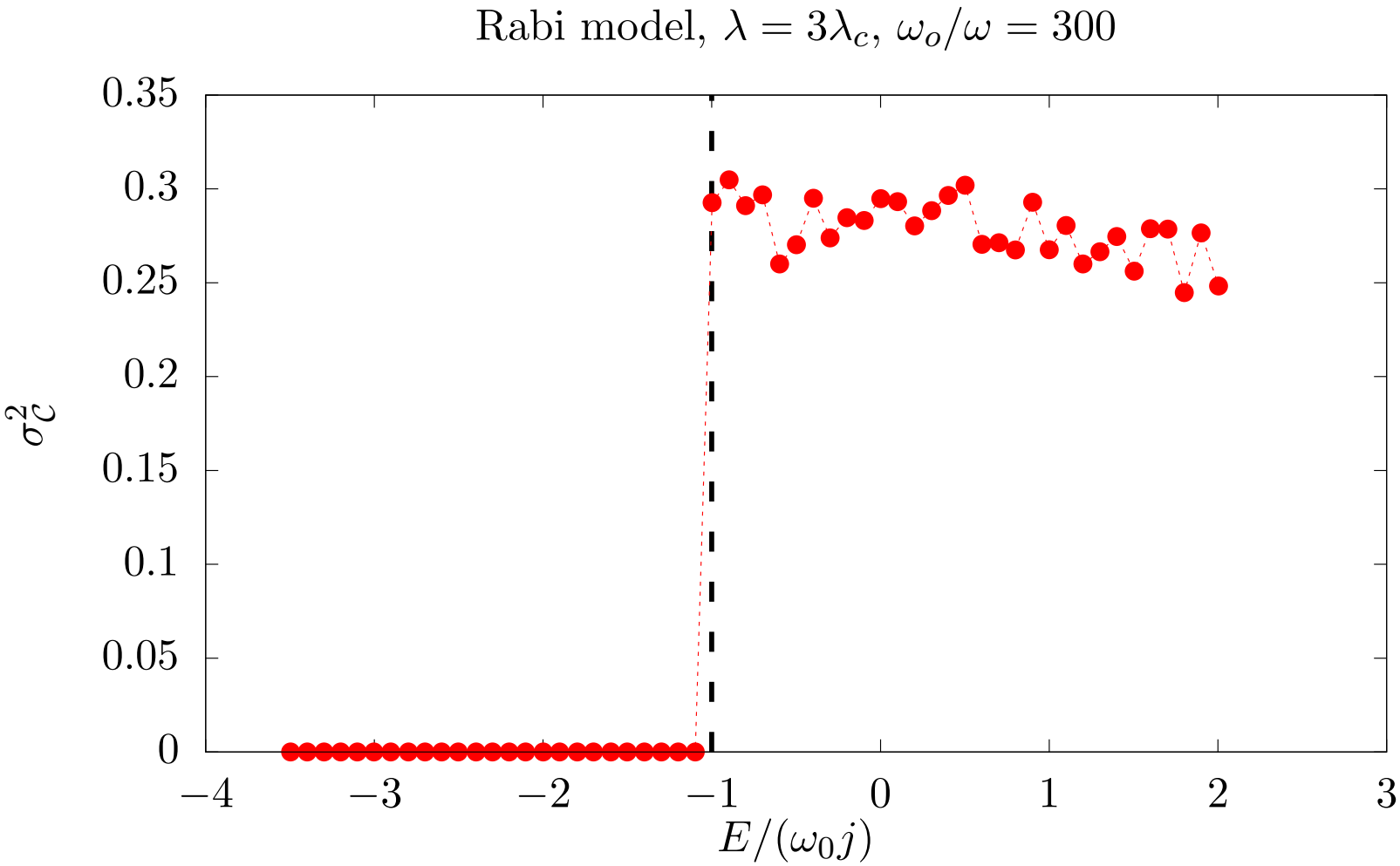
- If $E < E_c$, classical trajectories have either $q > 0$ or $q < 0$.
- If $E > E_c$, classical trajectories pass through $q > 0$ and $q < 0$.

We propose that $\mathcal{C} = \mathbf{sign}\left(\hat{a}^\dagger + \hat{a}\right)$ is a constant of motion if $E < E_c$

Numerical experiment I

- Initial condition, $|\psi(0)\rangle = \frac{1}{\sqrt{10}} \sum_{i=M}^{M+9} |E_i\rangle$, different values for M
- Time evolution, $\mathcal{C}(t) = \langle\psi(t)| \mathcal{C} |\psi(t)\rangle$.
- Dispersion, $\sigma_{\mathcal{C}}^2 = \frac{1}{N} \sum_{i=1}^{N} \left(\mathcal{C}(t_i) - \overline{\mathcal{C}}\right)^2$.

Numerical experiment I



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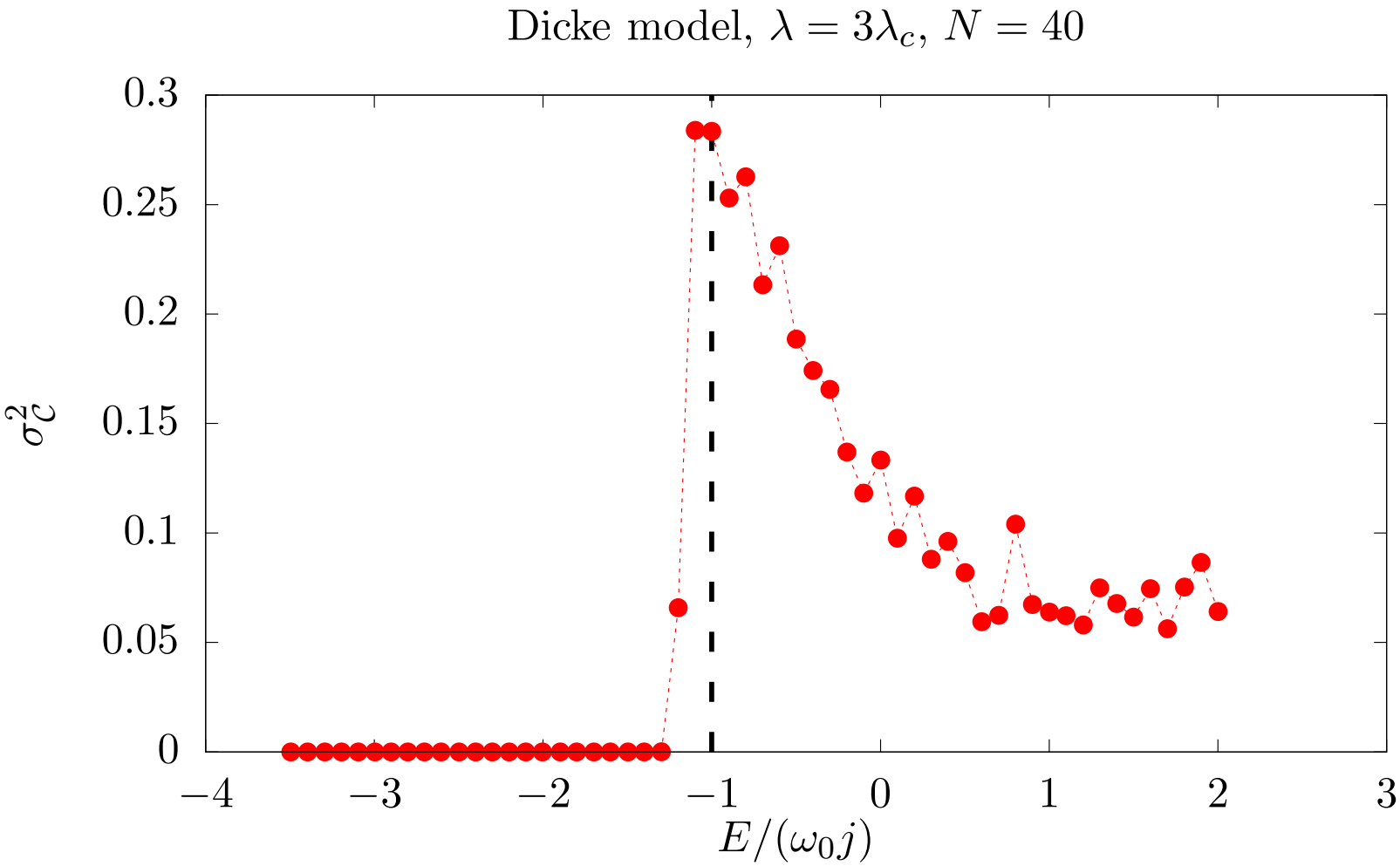

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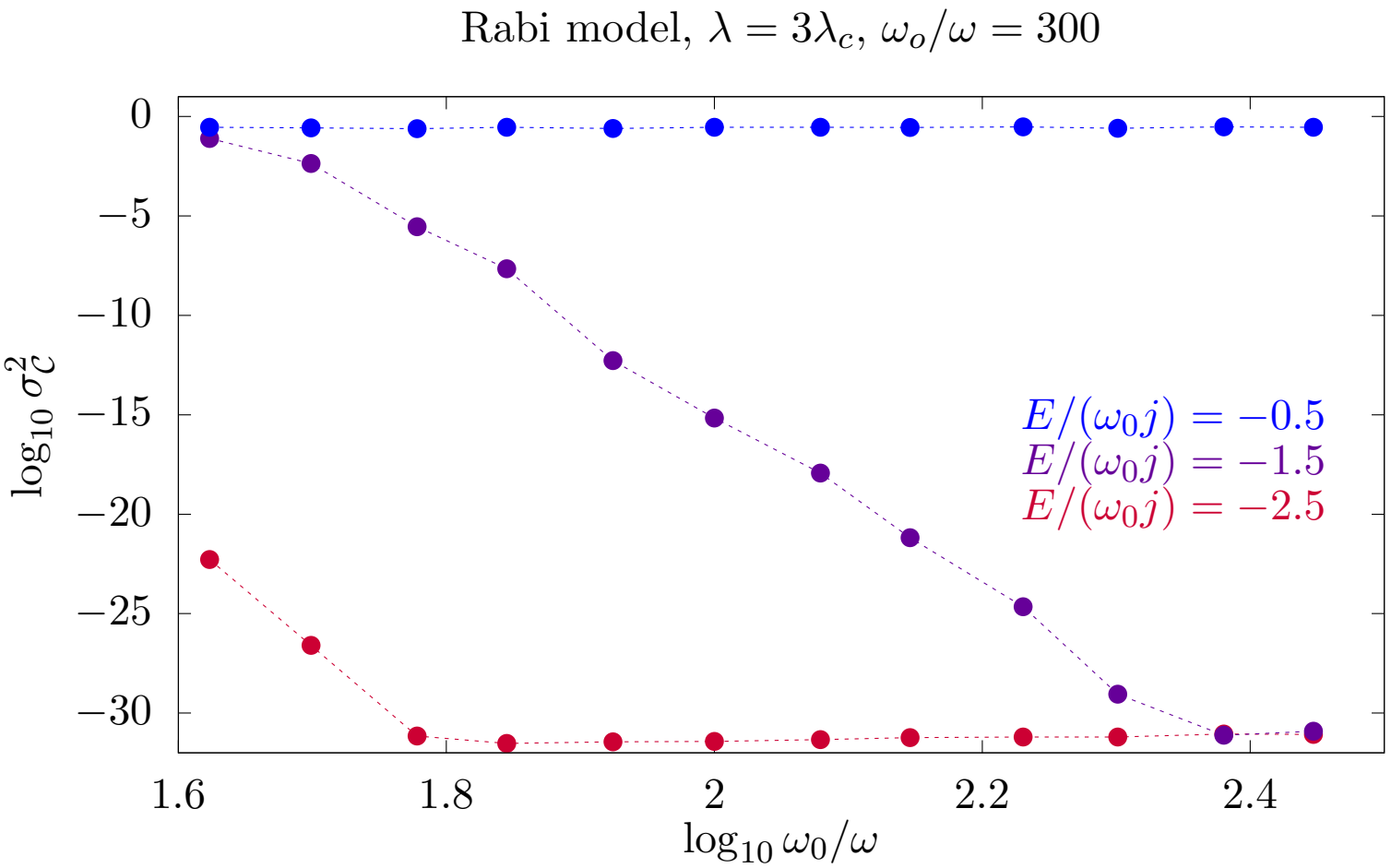
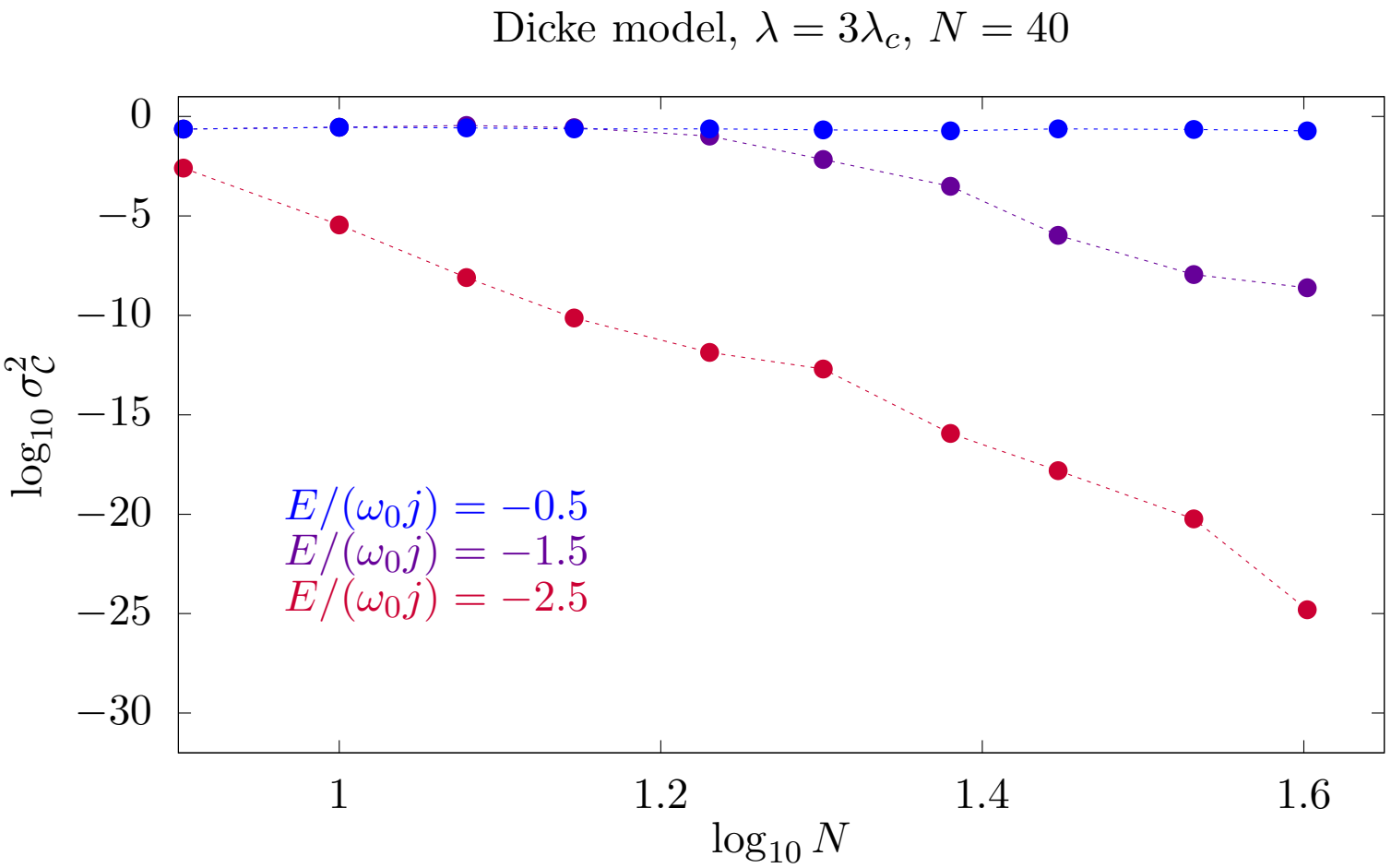


Calculations done in quadruple precision!

Numerical experiment I



Calculations done in quadruple precision!

Thermodynamics of the Rabi and Dicke models

- Both the Rabi and Dicke models have a $\mathbb{Z}_2$ symmetry, $[\mathcal{H}, \hat{\Pi}] = 0$,

$$\hat{\Pi} = \exp\left(i\pi\left[j + \hat{J}_z + \hat{a}^\dagger \hat{a}\right]\right).$$

- In both cases,

$$\begin{aligned} \mathcal{H}\left|E_{n,\pm}\right\rangle &= E_{n,\pm}\left|E_n, \pm\right\rangle, \\ \hat{\Pi}\left|E_{n,\pm}\right\rangle &= \pm\left|E_n, \pm\right\rangle. \end{aligned}$$

THERMODYNAMICS OF THE RABI AND DICKE MODELS

- If $E < E_c$, any statistical ensemble must depend on $\mathcal{H}$, $\hat{\Pi}$, and $\mathcal{C}$.
- If $E > E_c$, any statistical ensemble must depend on $\mathcal{H}$ and $\hat{\Pi}$.

Mathematical properties of $\mathcal{C}$

Let us consider the definition of $\mathcal{C}$:

$$\mathcal{C} = \frac{2}{\pi}\int_0^\infty dx\, \hat{f}\left(x^2\mathbb{I} + \hat{f}^2\right)^{-1}, \quad \hat{f} = \hat{a}^\dagger + \hat{a}.$$

- $\hat{f}$ changes the parity of any state.
- $\hat{f}^2$ commutes with parity.
- $x^2\mathbb{I} + \hat{f}^2$ commutes with parity $\forall x$.
- $\left(x^2\mathbb{I} + \hat{f}^2\right)^{-1}$ commutes with parity $\forall x$.
- $\hat{f}\left(x^2\mathbb{I} + \hat{f}^2\right)^{-1}$ changes the parity $\forall x$.

Therefore, $\mathcal{C}$ changes the parity of any state.

Main consequence

From previous results we know:

- $\hat{\Pi} : \mathcal{E}_n \to \mathcal{E}_n$, where the $\mathcal{E}_n$ is the subspace with energy E_n, $\forall\ \mathcal{E}_n$.
- $\mathcal{C} : \mathcal{E}_n \to \mathcal{E}_n$, if $E_n < E_c$.
- *But $\mathcal{C}$ changes parity:* $\mathcal{C} : \pm \to \mp$.

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- *But $\mathcal{C}$ changes parity:* $\mathcal{C} : \pm \to \mp$.

Degeneracies if $E < E_c$

The spectrum must be pairwise degenerate if $E < E_c$. We have two different eigenbasis:

$$\mathcal{H}\,|E_{n,\pm}\rangle = E_n\,|E_{n,\pm}\rangle \quad \mathcal{H}\,|\varepsilon_{n,\pm}\rangle = E_n\,|\varepsilon_{n,\pm}\rangle$$
$$\hat{\Pi}\,|E_{n,\pm}\rangle = \pm\,|E_{n,\pm}\rangle \quad \mathcal{C}\,|\varepsilon_{n,\pm}\rangle = \pm\,|\varepsilon_{n,\pm}\rangle$$

Mathematical properties of $\mathcal{C}$

- Property I:

$$\begin{aligned} \mathcal{C}\,|E_n,+\rangle &= \alpha\,|E_n,-\rangle\,,\ \text{if } E_n < E_c, \\ \mathcal{C}\,|E_n,-\rangle &= \beta\,|E_n,+\rangle\,,\ \text{if } E_n < E_c. \end{aligned}$$

- Property II:

$$\begin{aligned} \mathcal{C}\left(\gamma\,|E_n,+\rangle + \delta\,|E_n,-\rangle\right) &= \left(\gamma\,|E_n,+\rangle + \delta\,|E_n,-\rangle\right),\ \text{if } E_n < E_c \\ \mathcal{C}\left(\delta\,|E_n,+\rangle - \gamma\,|E_n,-\rangle\right) &= -\left(\delta\,|E_n,+\rangle - \gamma\,|E_n,-\rangle\right),\ \text{if } E_n < E_c. \end{aligned}$$

$$\text{With } |\gamma|^2 + |\delta|^2 = 1.$$

There are just two solutions for these equations:

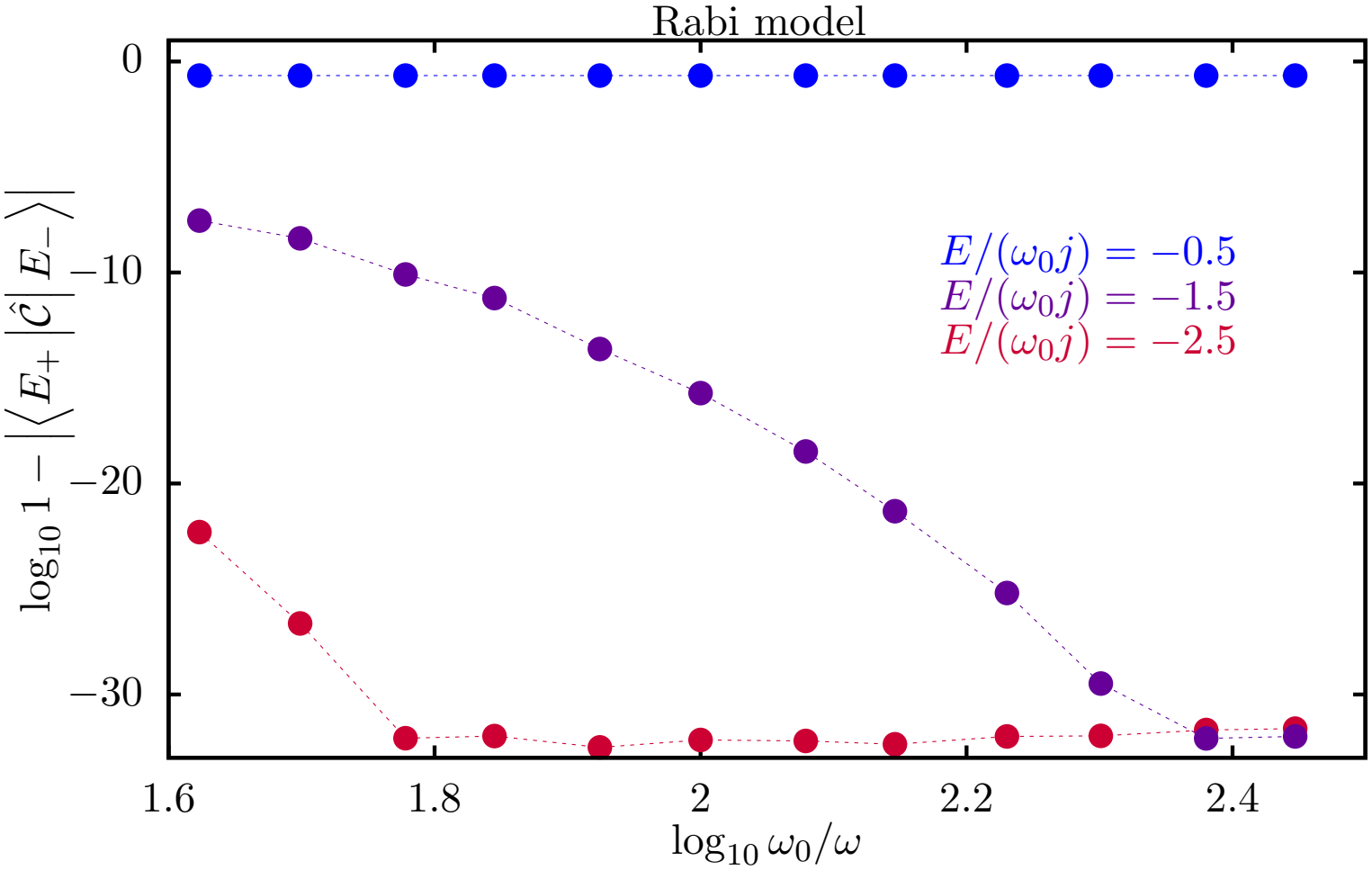
$$\text{Solution I:} \qquad \alpha = \beta = 1,\ \gamma = \delta = \frac{1}{\sqrt{2}},$$

$$\text{Solution II:} \qquad \alpha = \beta = -1,\ \gamma = -\frac{1}{\sqrt{2}},\ \delta = \frac{1}{\sqrt{2}}.$$

Numerical experiment II

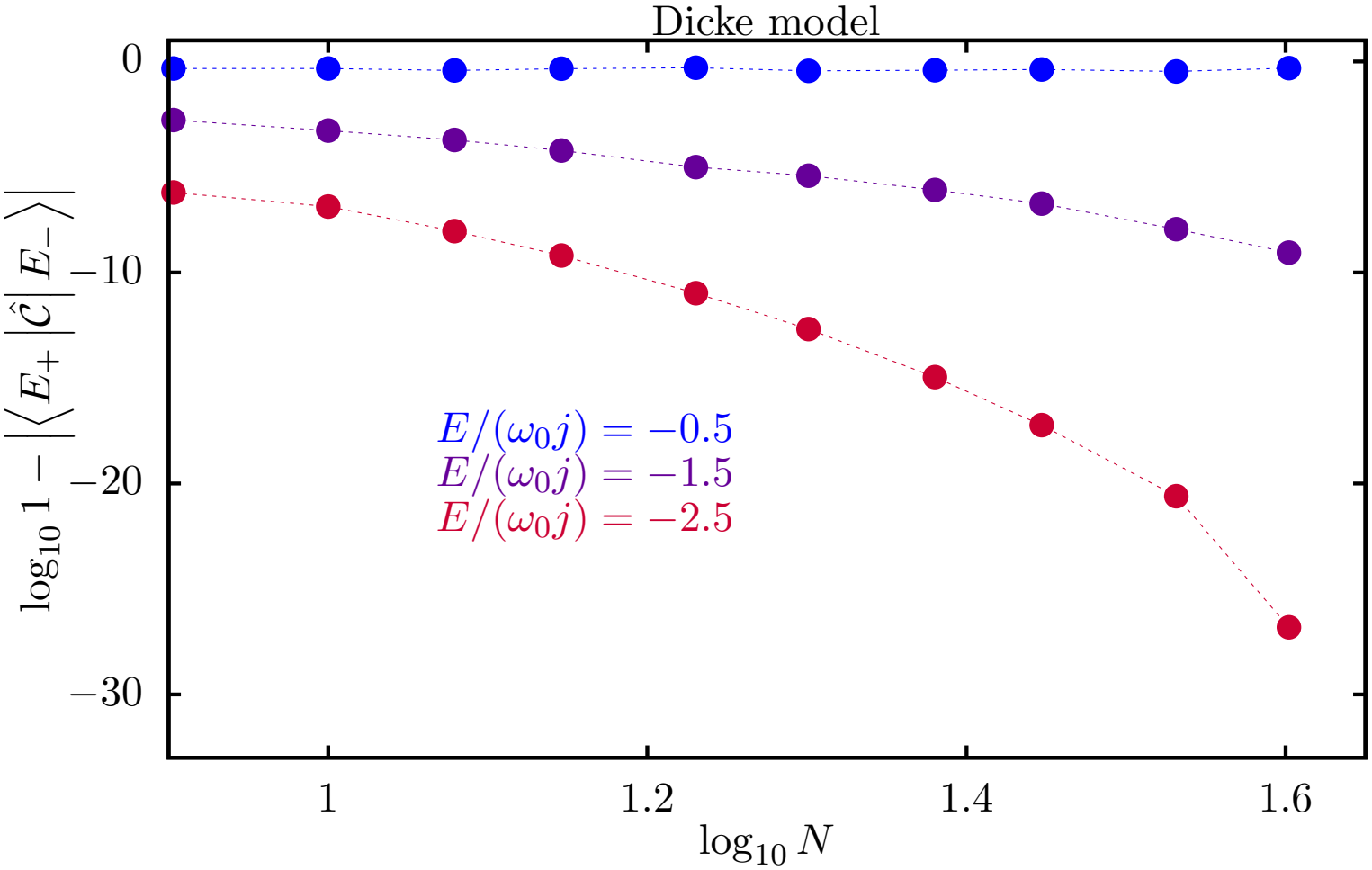
- Given a certain eigenstate with positive parity, $|E_{n,+}\rangle$, and energy $E_{n,+}$, we seek the eigenstate with negative parity, $|E_{n,-}\rangle$, and the closest energy, $E_{n,-}$.
- We study the evolution of the gap, $d = |E_{n,+} - E_{n,-}|$ as a function of the energy.
- We study the evolution of $D = 1 - |\langle E_{n,+}| \mathcal{C} |E_{n,-}\rangle|$ as a function of the energy.

Numerical experiment II



Calculations in quadruple precision!

Numerical experiment II



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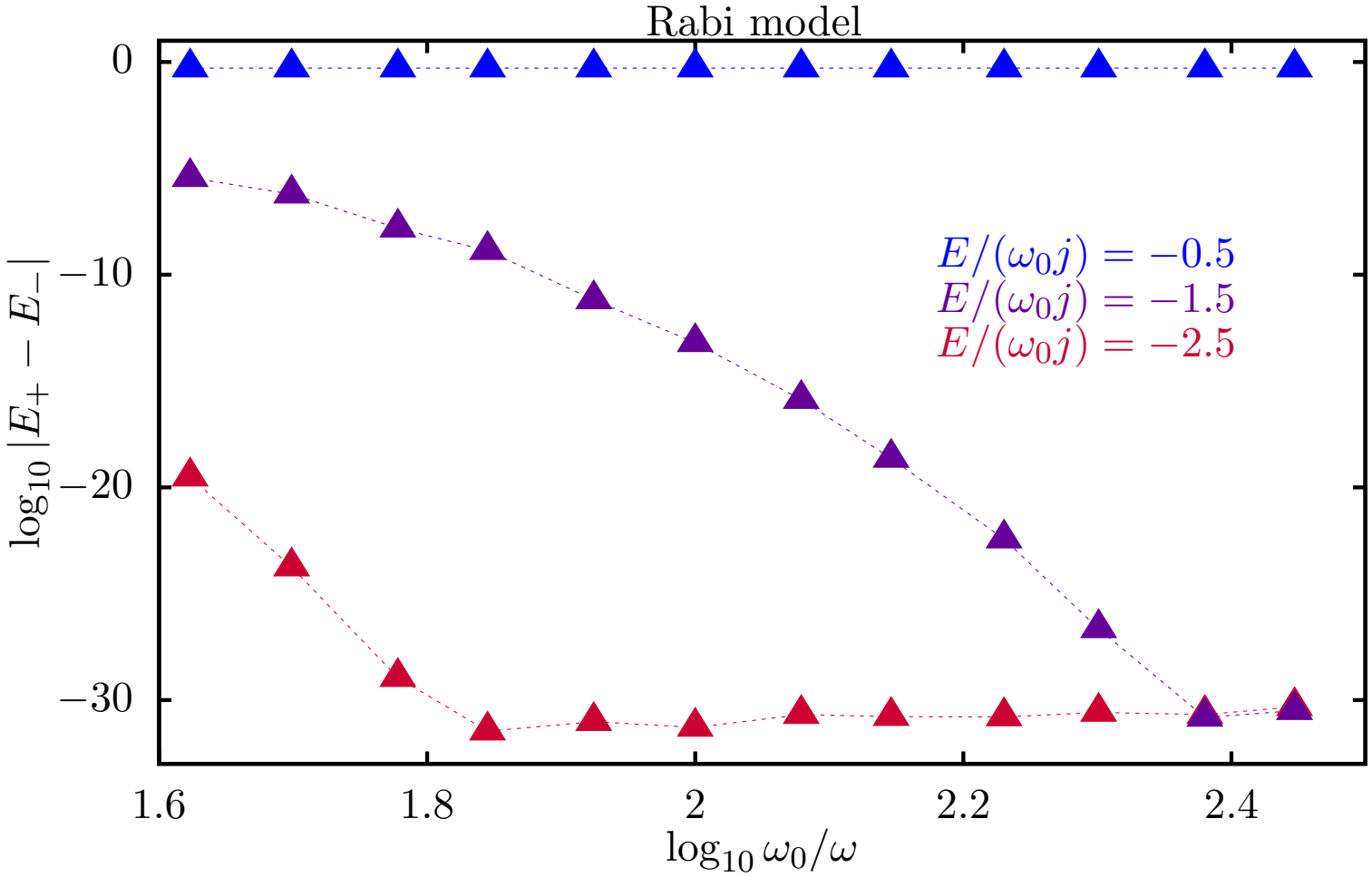

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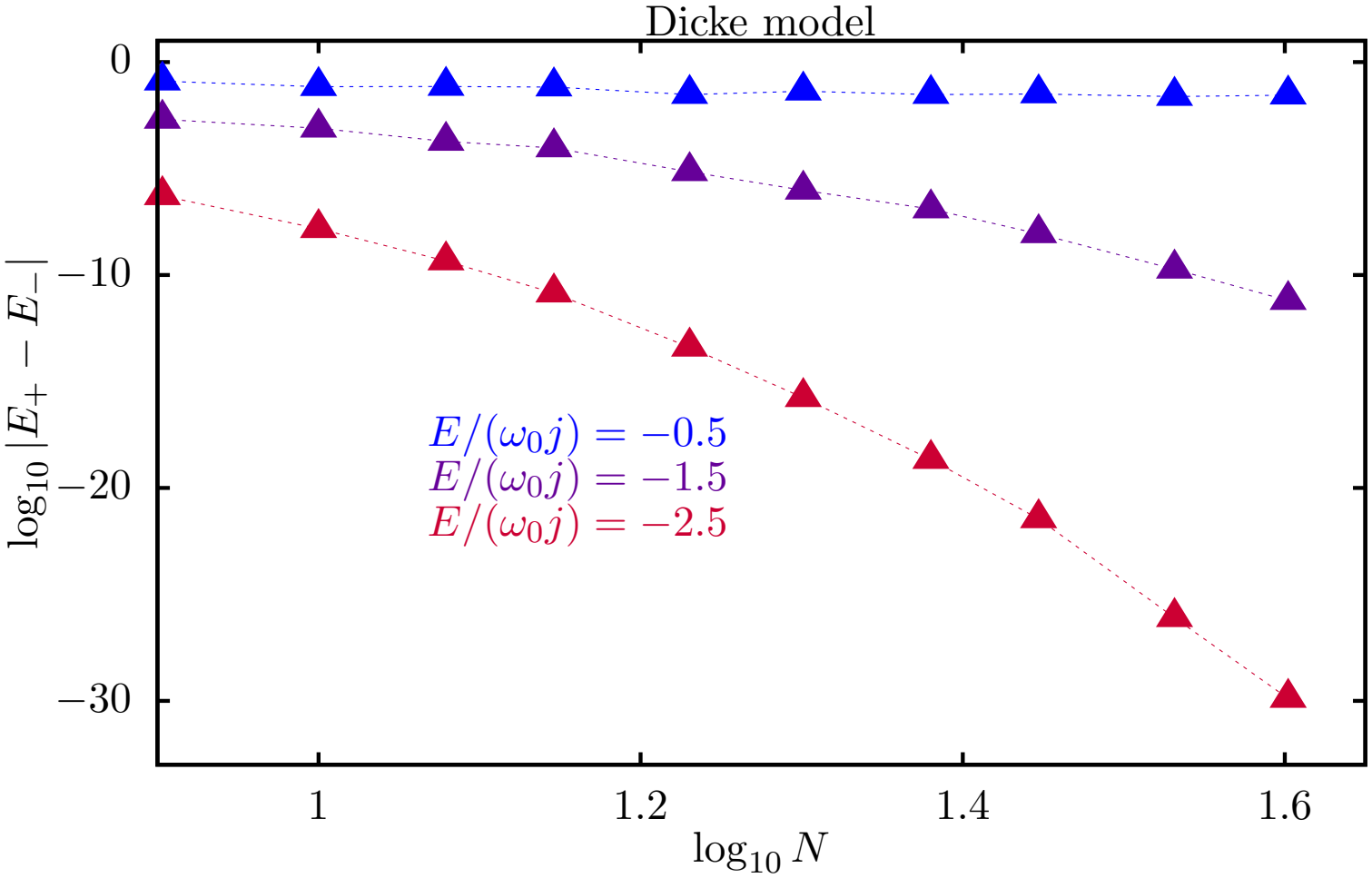


Calculations in quadruple precision!

Expected values in equilibrium and $\mathcal{C}$

Let us consider a closed system following an unitary evolution. Does it reach an equilibrium state? Not rigurously... but we can define an effective equilibrium state, near which the time-evolved wavefunction stays mostly of the time.

$$|\psi(0)\rangle = \sum_n \left[C_{n,+}\,|E_{n,+}\rangle + C_{n,-}\,|E_{n,-}\rangle\right] \longrightarrow$$

$$\longrightarrow |\psi(t)\rangle\langle\psi(t)| = \sum_{n,m}\sum_{i,j} C^*_{n,i}C_{m,j}\mathrm{e}^{-i\left(E_{n,i}-E_{m,j}\right)t/\hbar}\left|E_{n,i}\right\rangle\left\langle E_{m,j}\right|$$

$$\text{If } E < E_c,\ \ \rho_{\mathrm{eq}} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau dt\ |\psi(t)\rangle\langle\psi(t)| =$$

$$= \sum_n \Big\{|C_{n,+}|^2\,|E_{n,+}\rangle\langle E_{n,+}| + |C_{n,-}|^2\,|E_{n,-}\rangle\langle E_{n,-}| +$$

$$+\ C^*_{n,-}C_{n,+}\,|E_{n,+}\rangle\langle E_{n,-}| + C^*_{n,+}C_{n,-}\,|E_{n,-}\rangle\langle E_{n,+}|\Big\}$$

P. Reimann, Phys. Rev. Lett. **101**, 190403 (2008).

Numerical experiment III

Analysis of equilibrium expected values of physical observables:

$$\langle \mathcal{O} \rangle_{\rm eq} = {\rm Tr}\left[\rho_{\rm eq}\mathcal{O}\right]$$

- Initial state: ground state of the Dicke model with $\lambda = 1.5\lambda_c$.

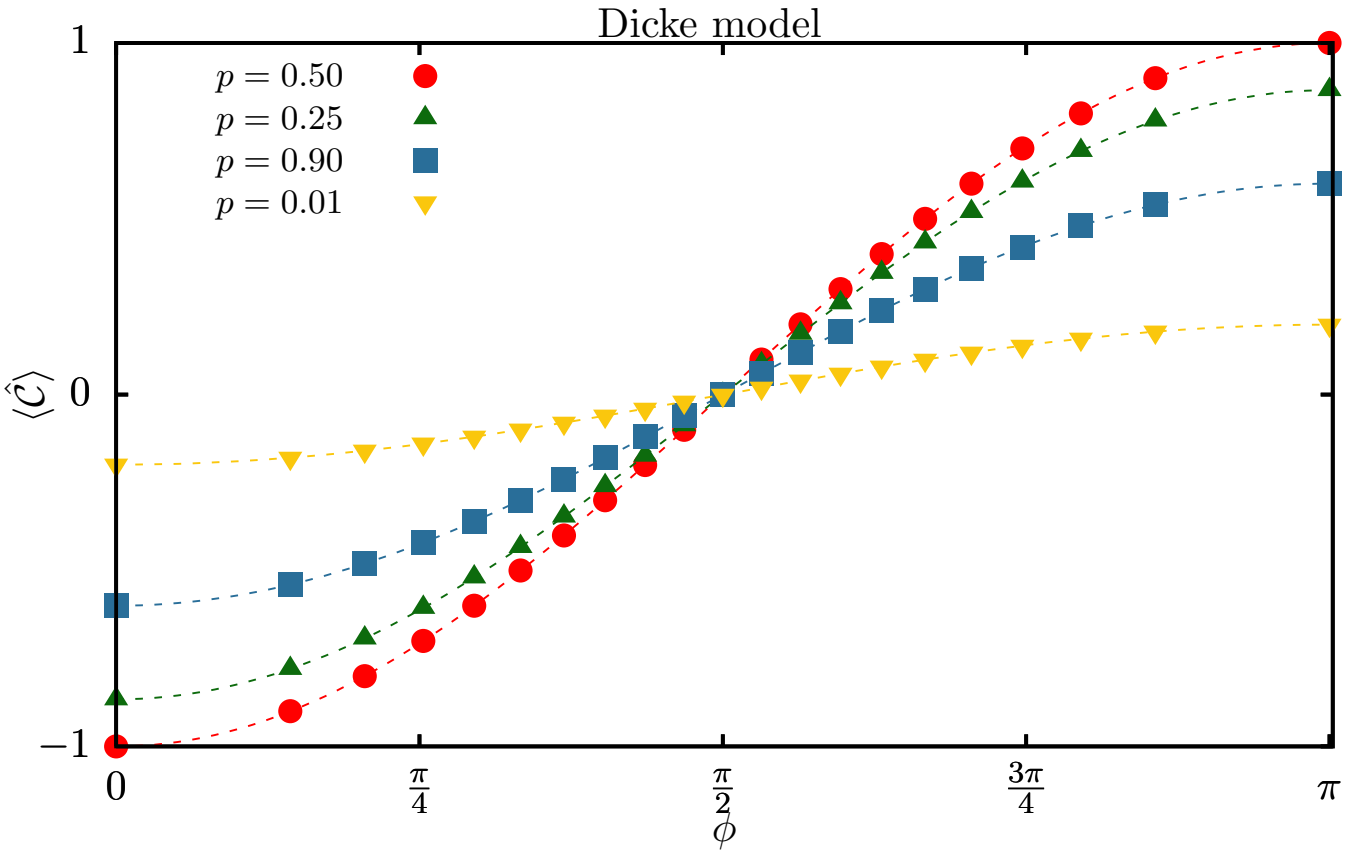
$$|\psi(0)\rangle = \sqrt{p}\left|E_{0,+}\right\rangle + {\rm e}^{i\phi}\sqrt{1-p}\left|E_{0,-}\right\rangle .$$

- Quench the system up to $\lambda = 3\lambda_c$.
- Calculate long-time averages of physical observables.
- Relevant initial values:

$$\begin{aligned} \langle\psi(0)|\,\hat{\Pi}\,|\psi(0)\rangle &= 2p-1, \\ \langle\psi(0)|\,\mathcal{C}\,|\psi(0)\rangle &= -2\sqrt{p(1-p)}\cos\phi. \end{aligned}$$

Numerical experiment III

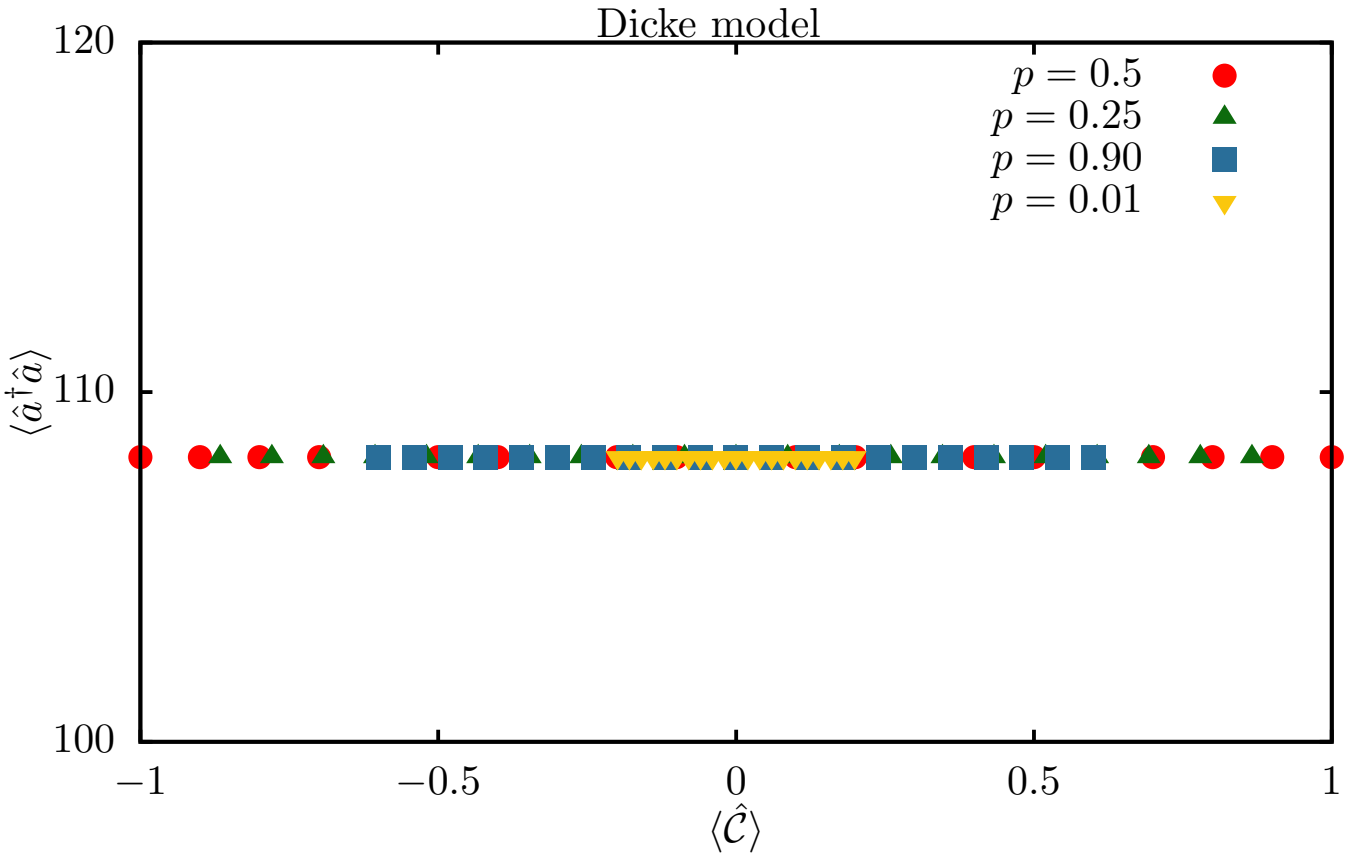
Testing the final value of $\mathcal{C}$:



$\mathcal{C}$ is conserved, as expected.

Numerical experiment III

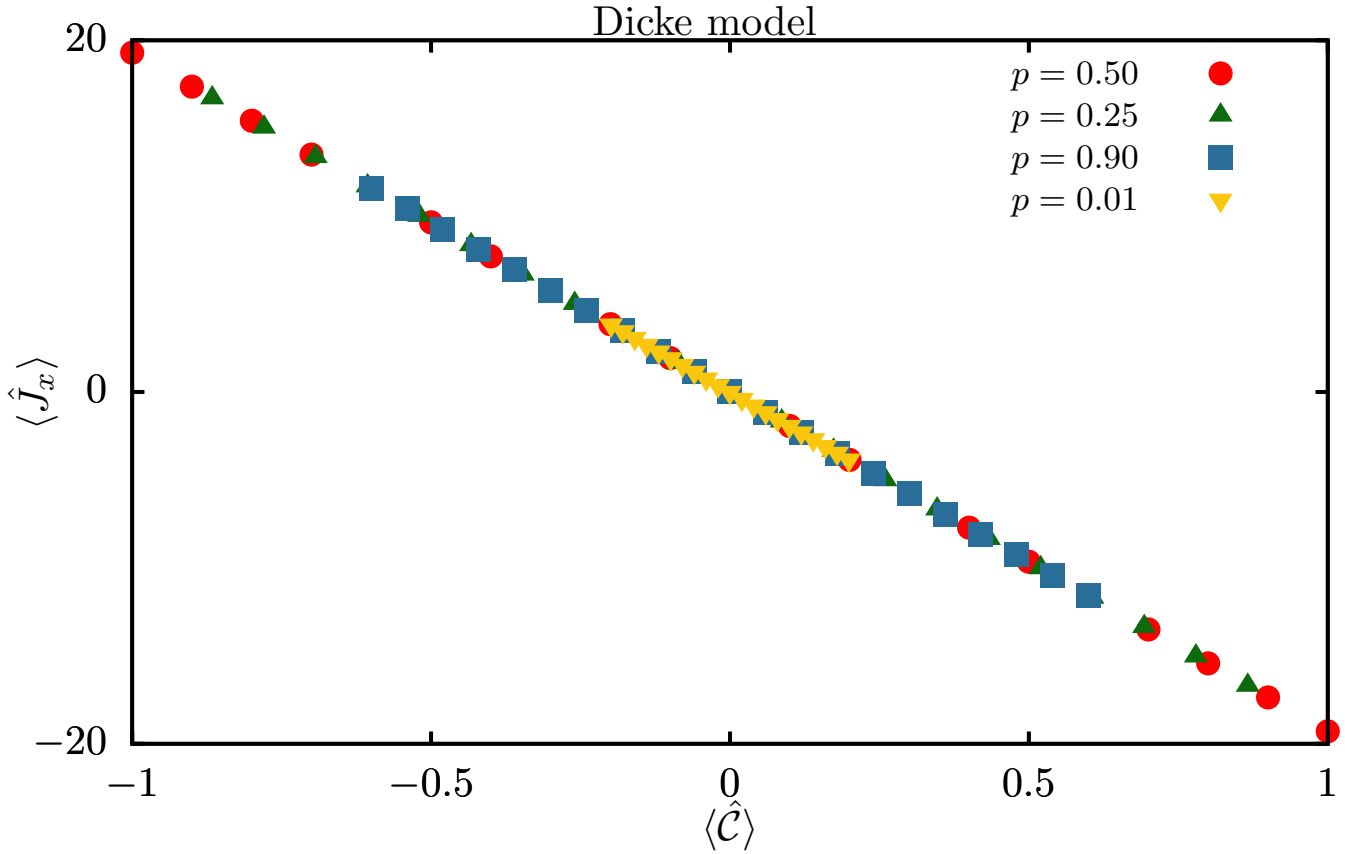
Number of photons, $\langle a^\dagger a \rangle_{\rm eq}$:



Same results $\forall$ p & ϕ. Equilibrium only depending on E . . . boring!

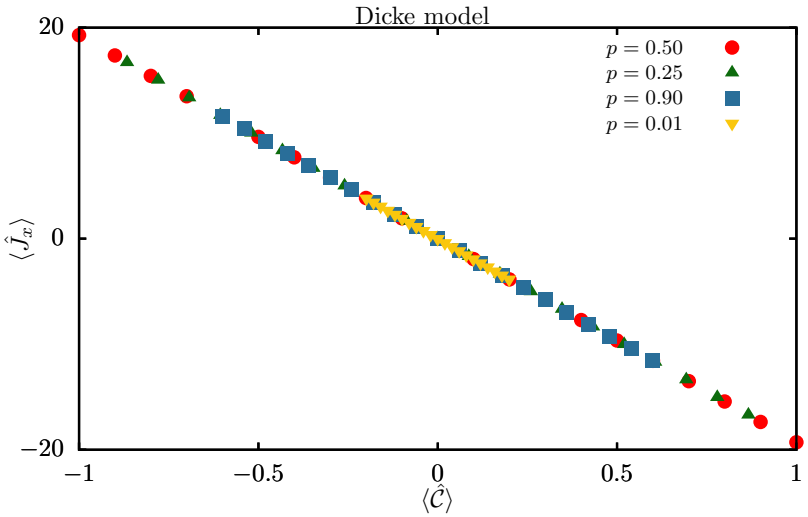
Numerical experiment III

Parity-breaking observable, $\langle J_x \rangle_{\rm eq}$:



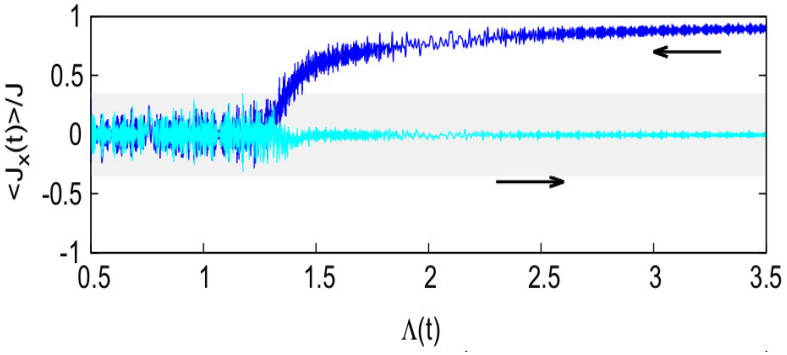
Equilibrium values depend on $\mathcal{C}$!

Numerical experiment III



Explains this result

$\longrightarrow$

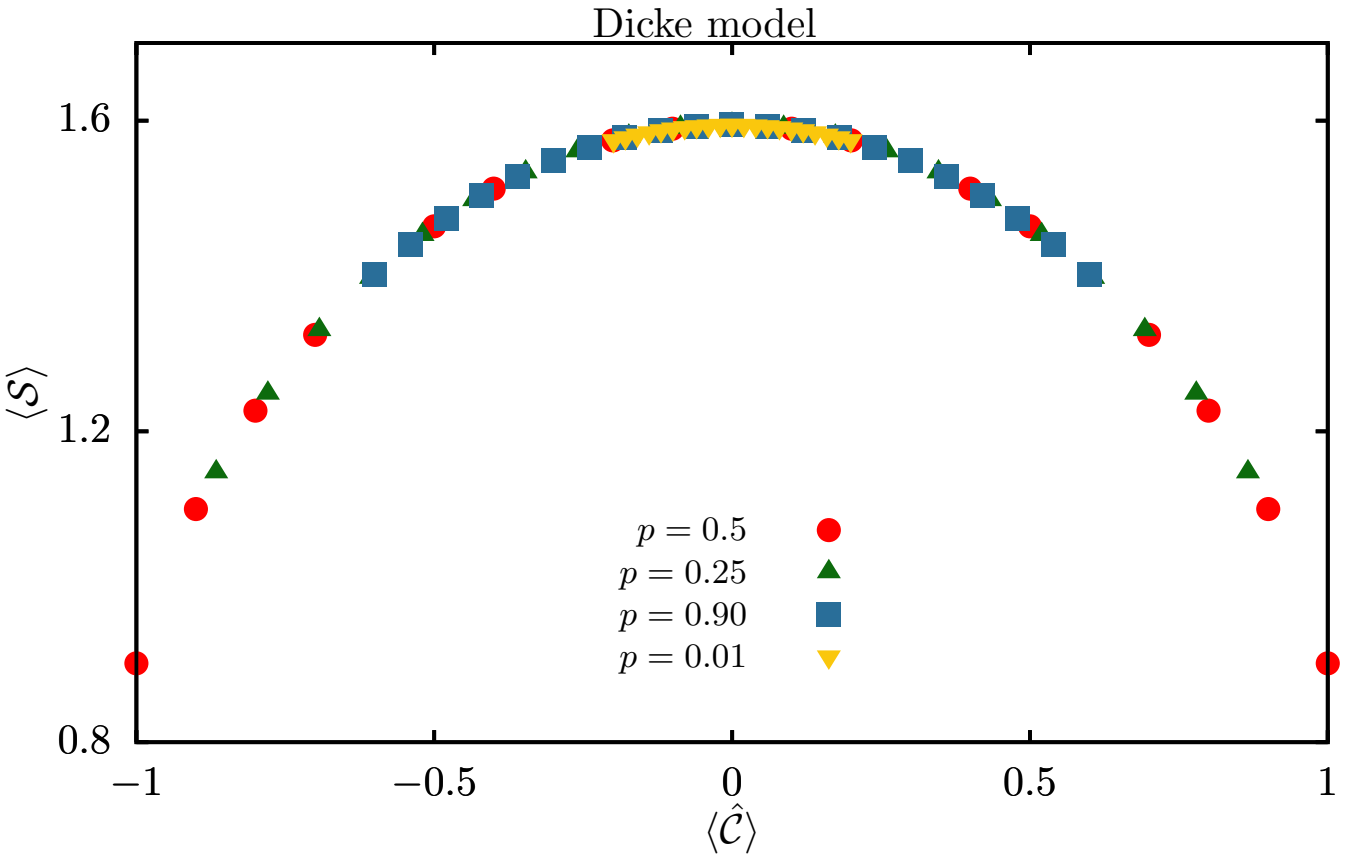


R. Puebla and A. R., Phys. Rev. E **92**, 012101 (2015)

Expected values in equilibrium and $\mathcal{C}$

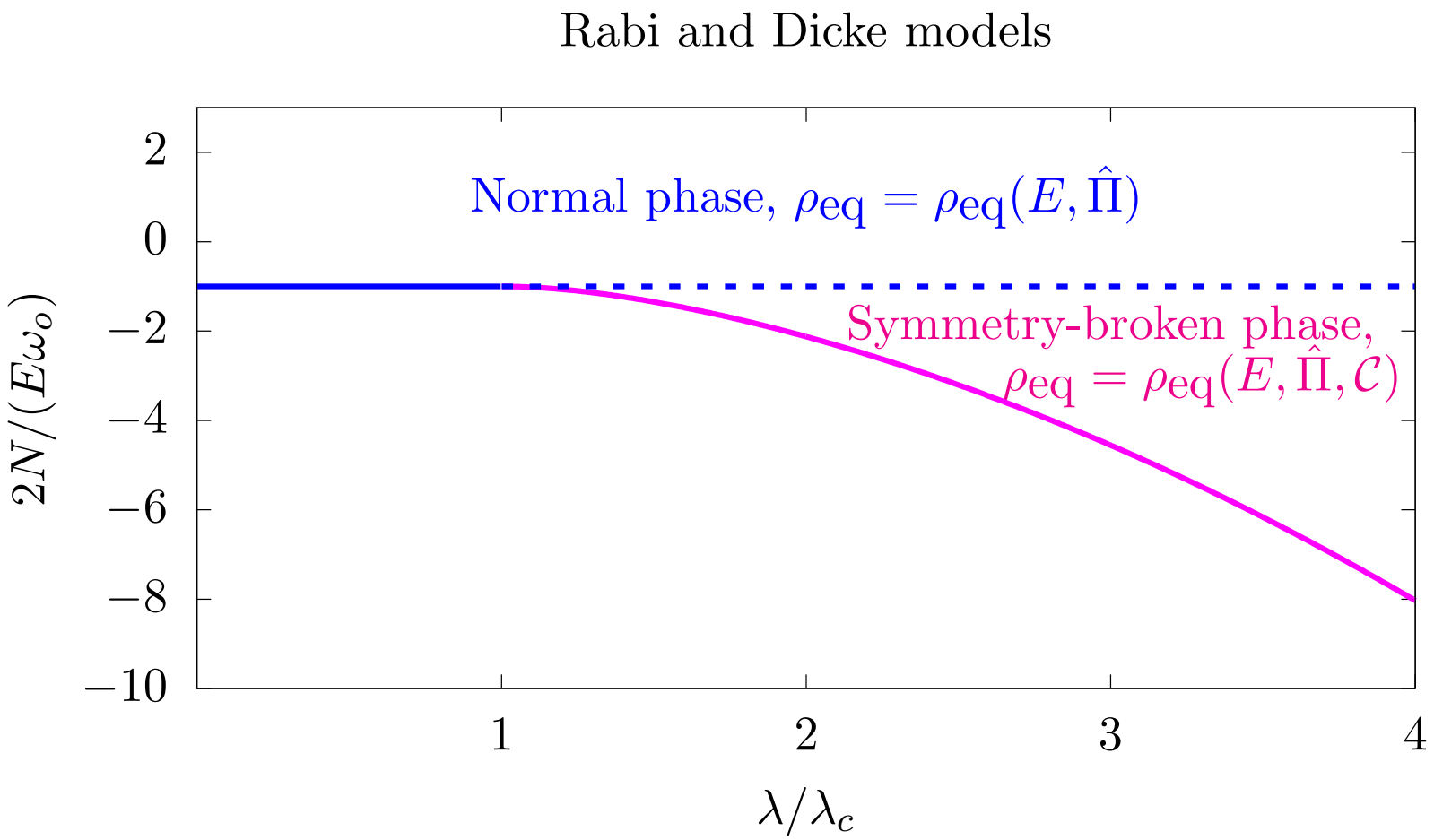
Numerical experiment III

Atoms-photons entanglement entropy, S_{ent}:



Equilibrium values also depend on $\mathcal{C}$!

Excited-state phase diagram



Normal phase —$\rho_{\rm eq}$, mixture of states with well-defined $\hat{\Pi}$.
Symmetry-broken phase —$\rho_{\rm eq}$, mixture of states with not well-defined $\hat{\Pi}$, $\mathcal{C}$ or both.

Main result

- We find two phases separated by the critical energy of an ESQPT, with different thermodynamics.
  - In the normal phase, equilibrium values depend on E maybe other global conserved charges.
  - In the symmetry-broken phase, equilibrium values depend also on $\mathcal{C}$.

A. L. Corps and A. R., arXiv:2103.10762 (2021)

Future work

- Statistical ensembles to account for the role played by $\mathcal{C}$.
- Consequences of the existence of two non-commuting $\mathbb{Z}_2$ symmetries in non-equilibrium processes.