Limit cycles of Quantum Heat Machines

Andrea Roberto Insinga
Peter Salamon
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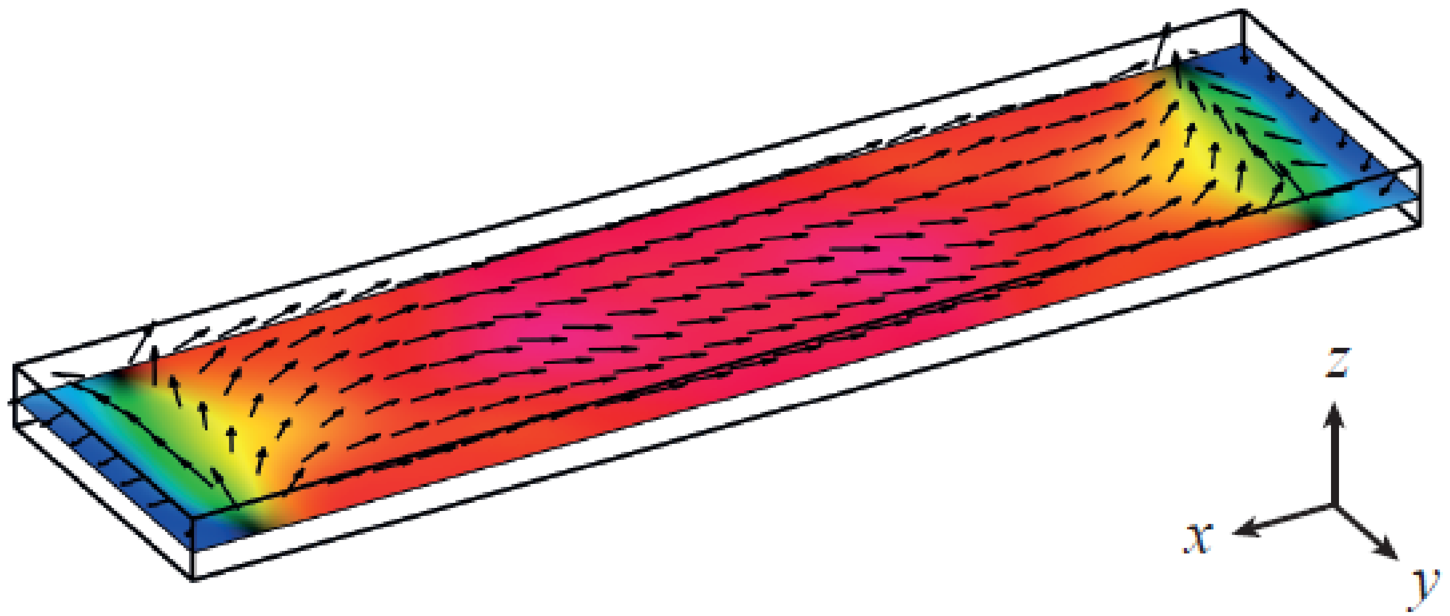
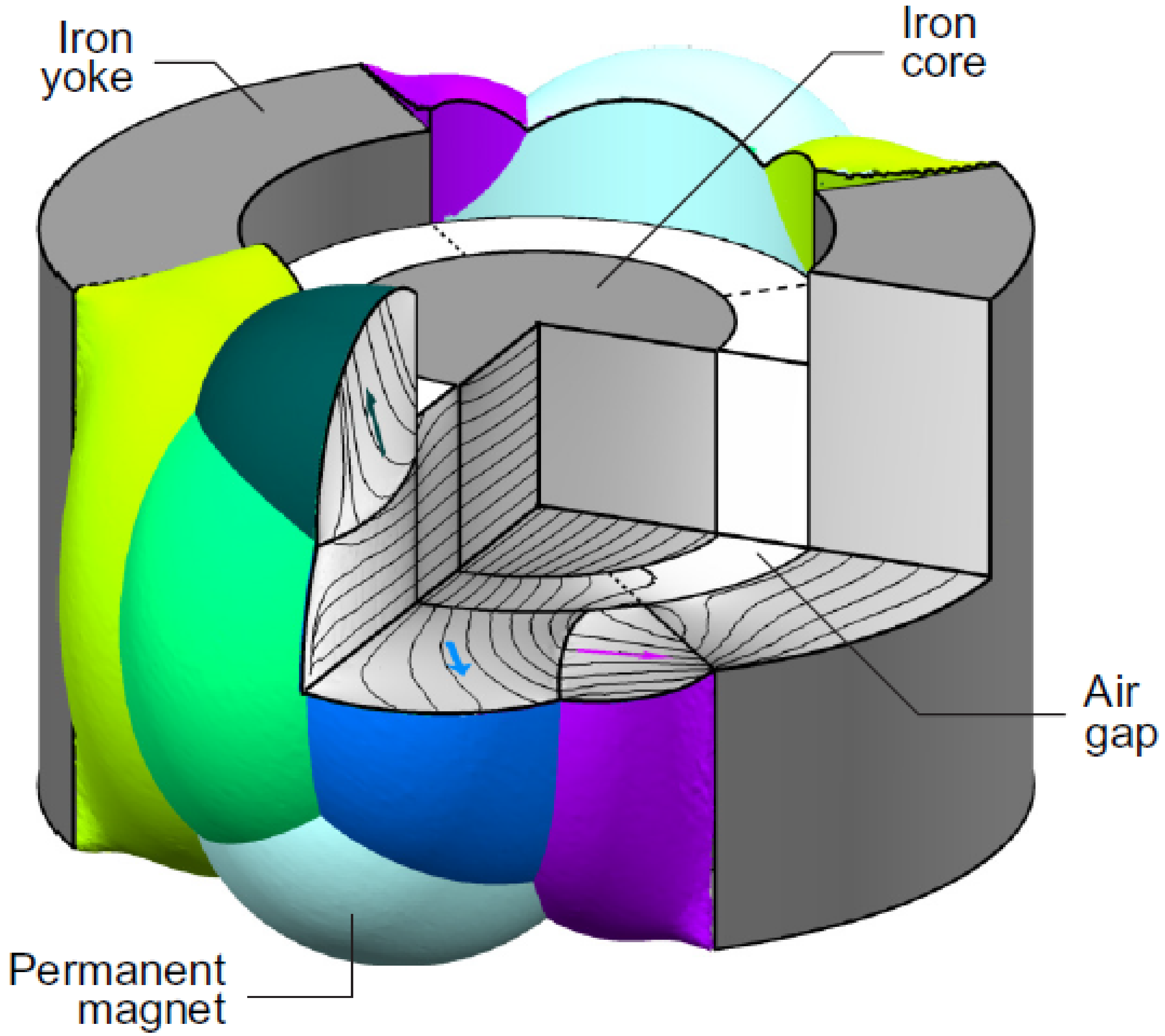
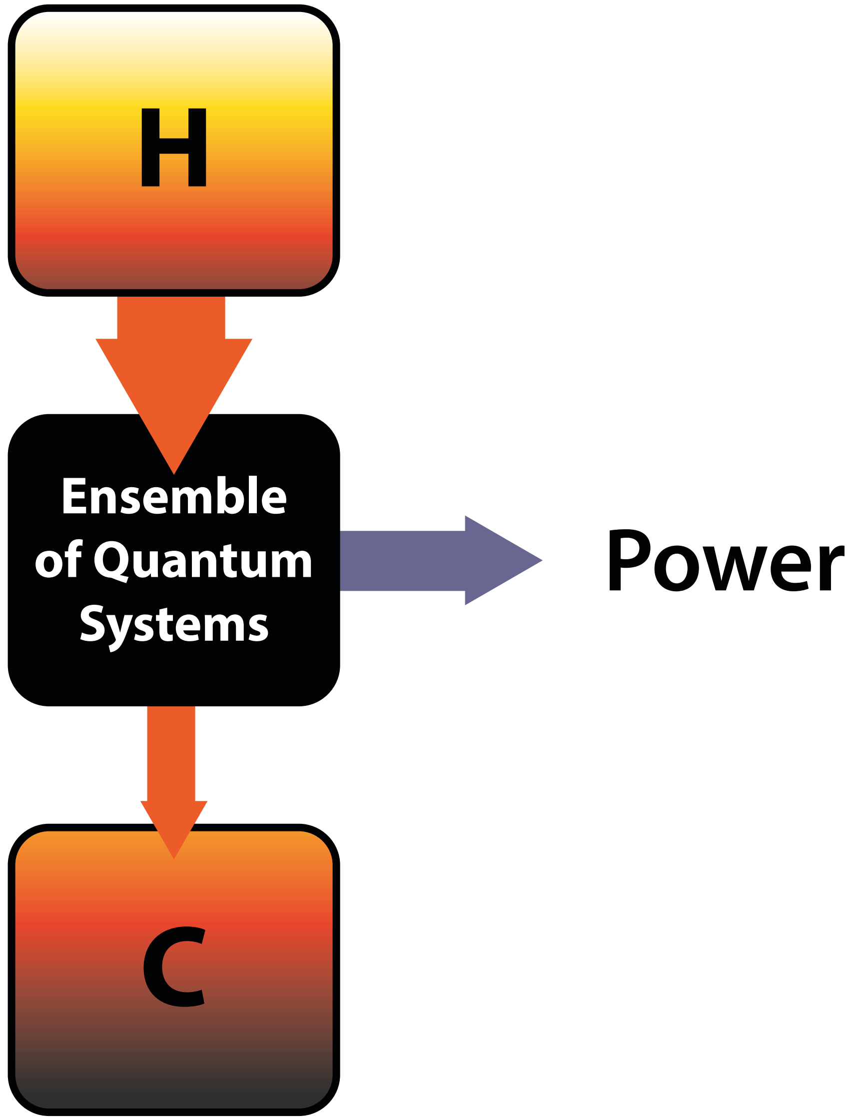
Micromagnetism simulations



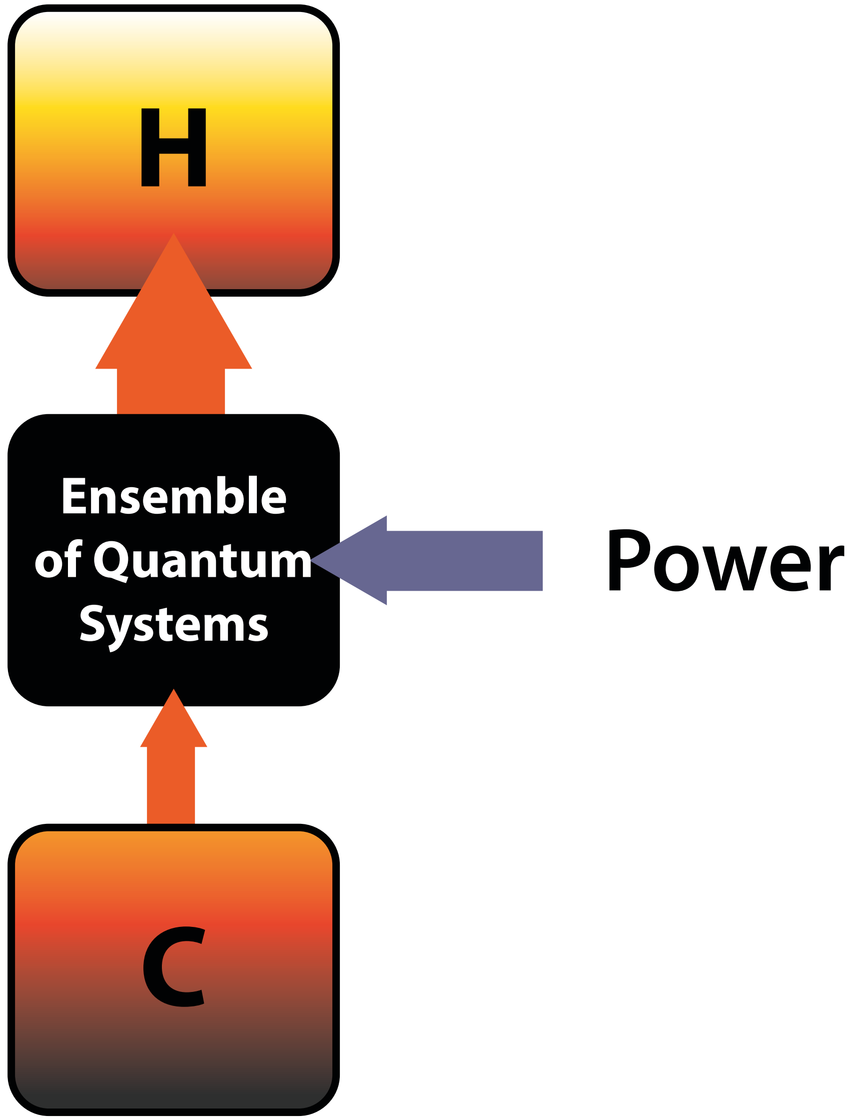
Permanent magnet optimization



Quantum heat machines

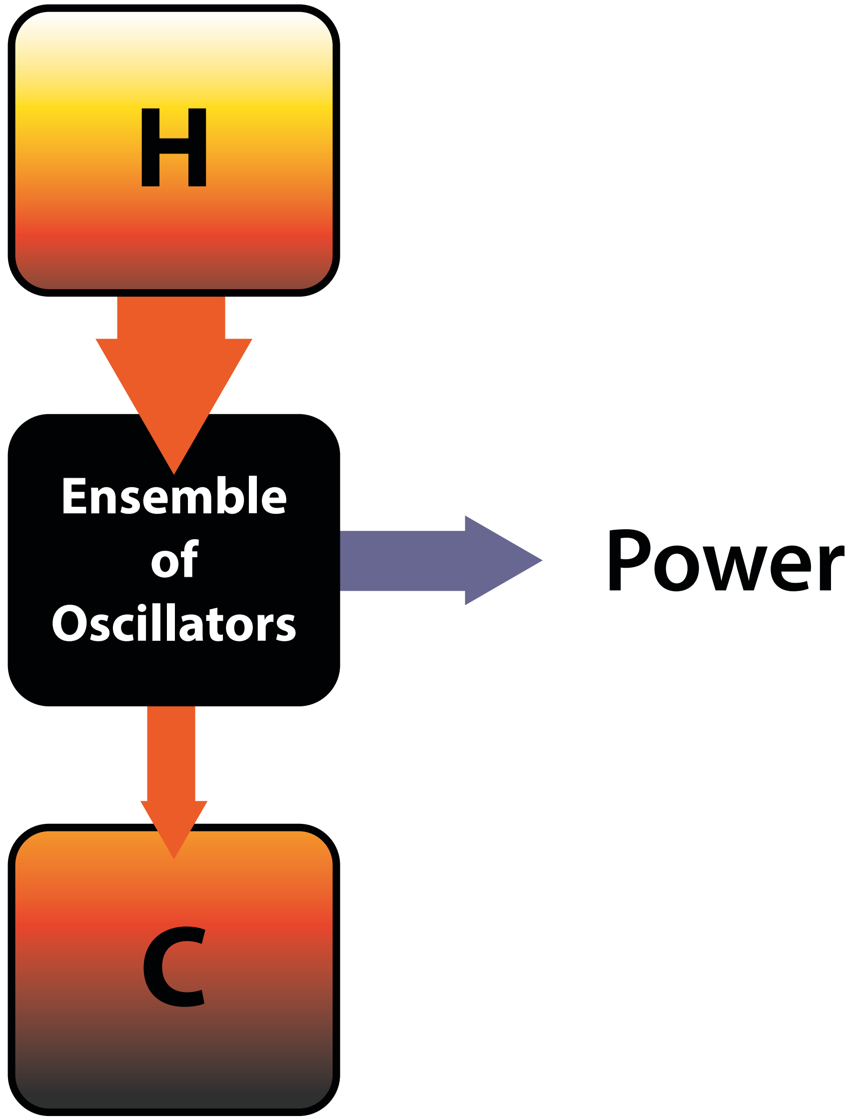


Heat engine

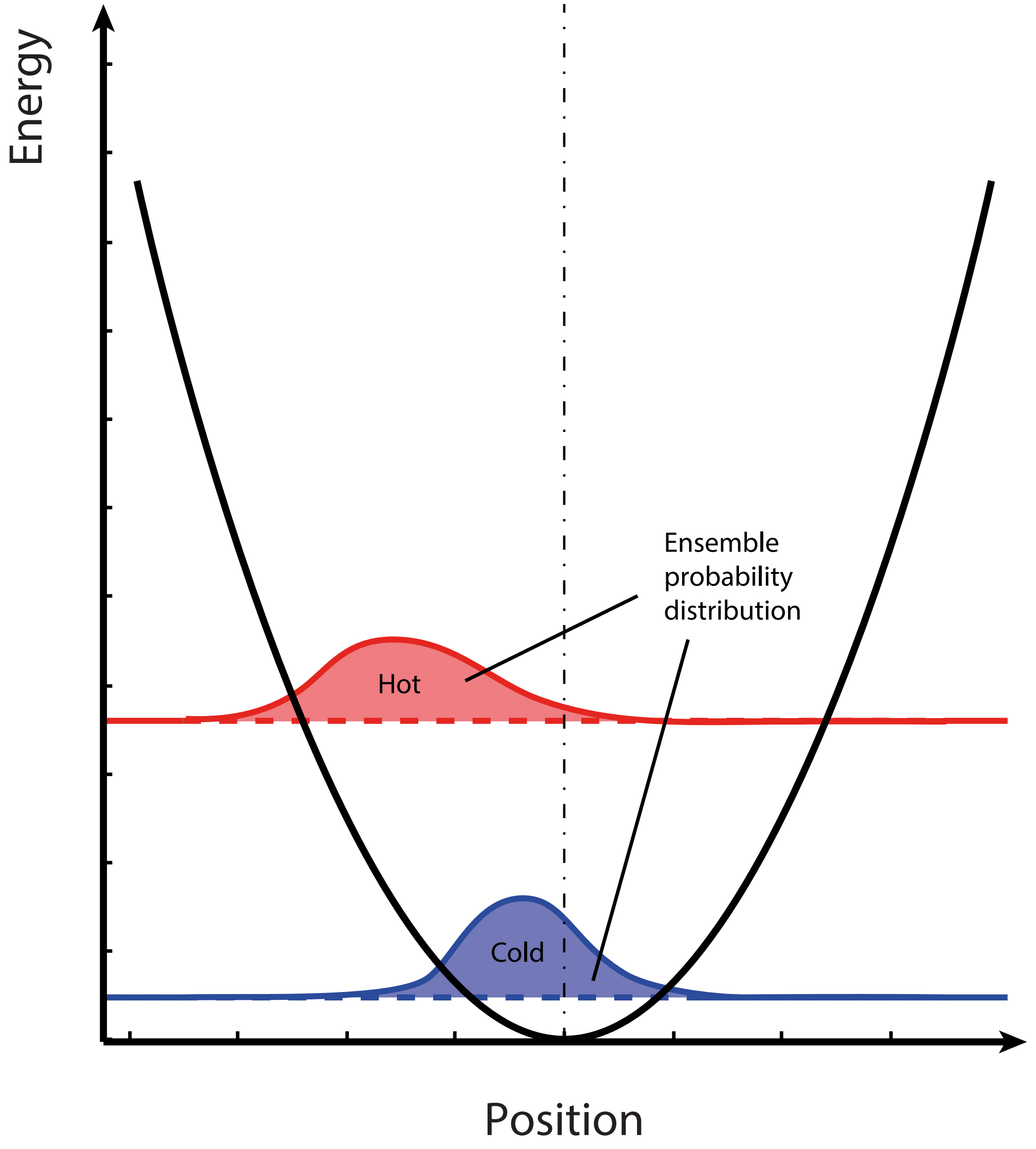


Refrigerator

Quantum harmonic heat engine

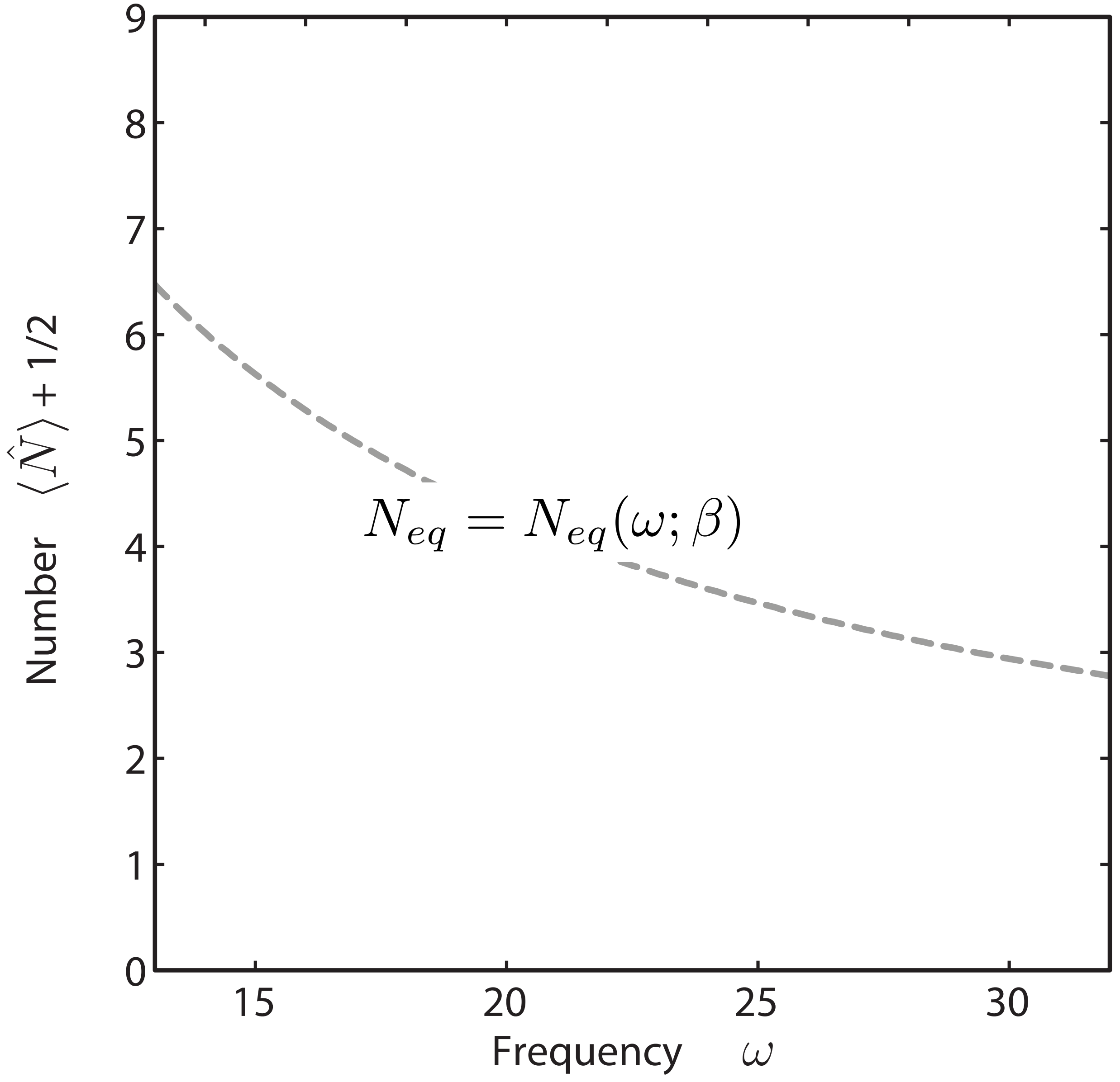


Heat engine

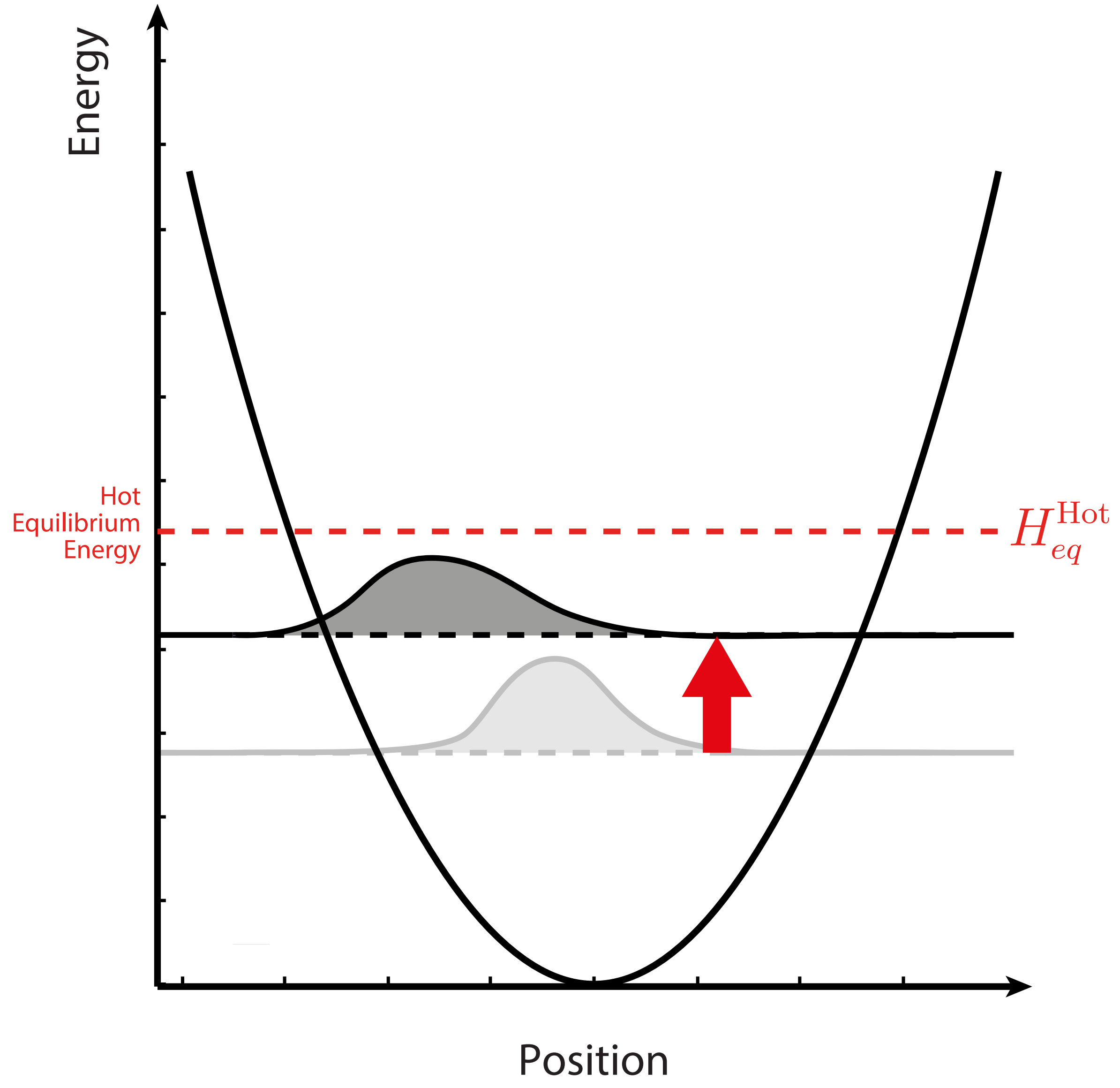


$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2$$

Thermal equilibrium



$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$



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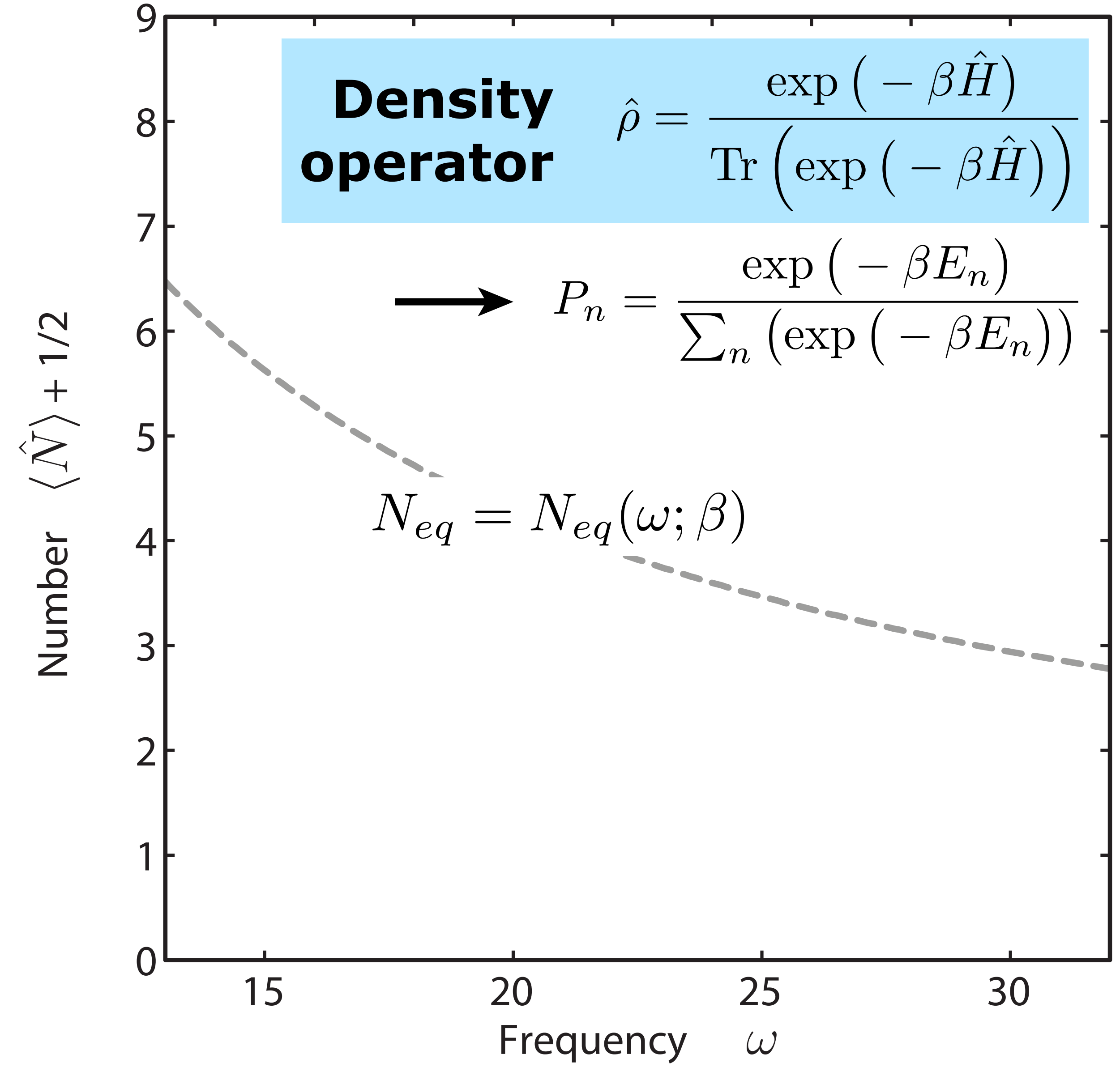
Thermal equilibrium



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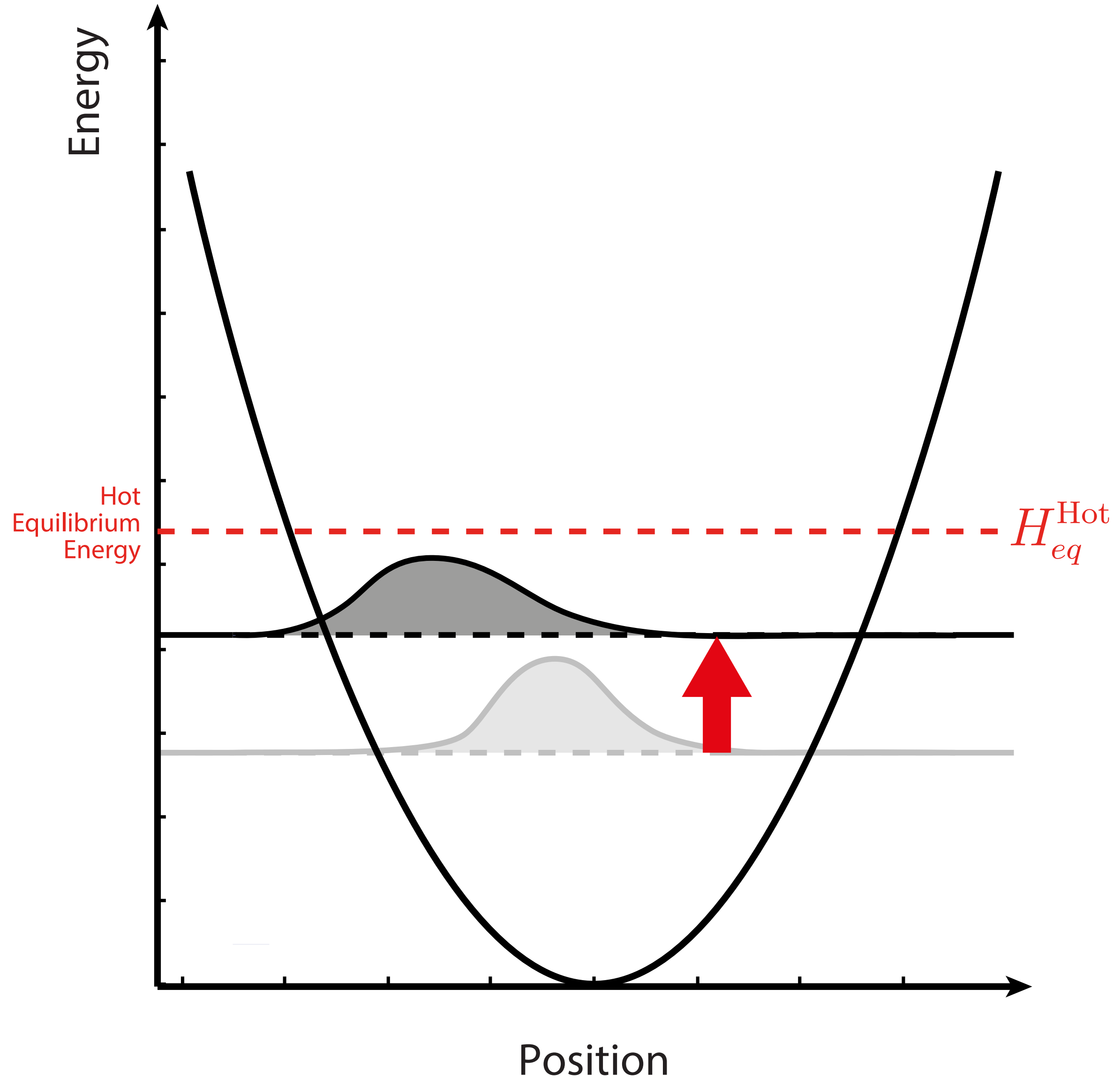
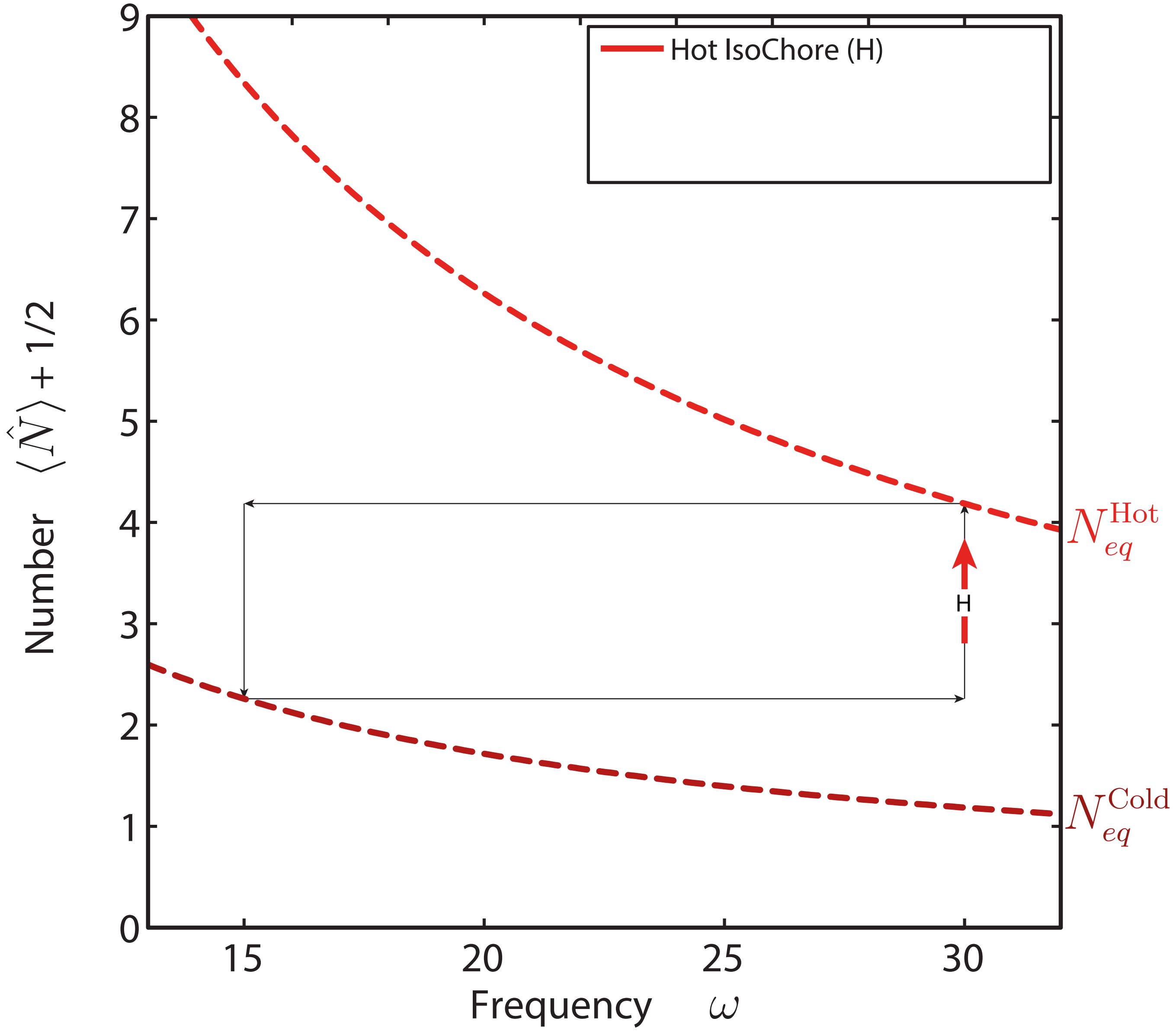


$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2$$

The Otto cycle - Hot IsoChore



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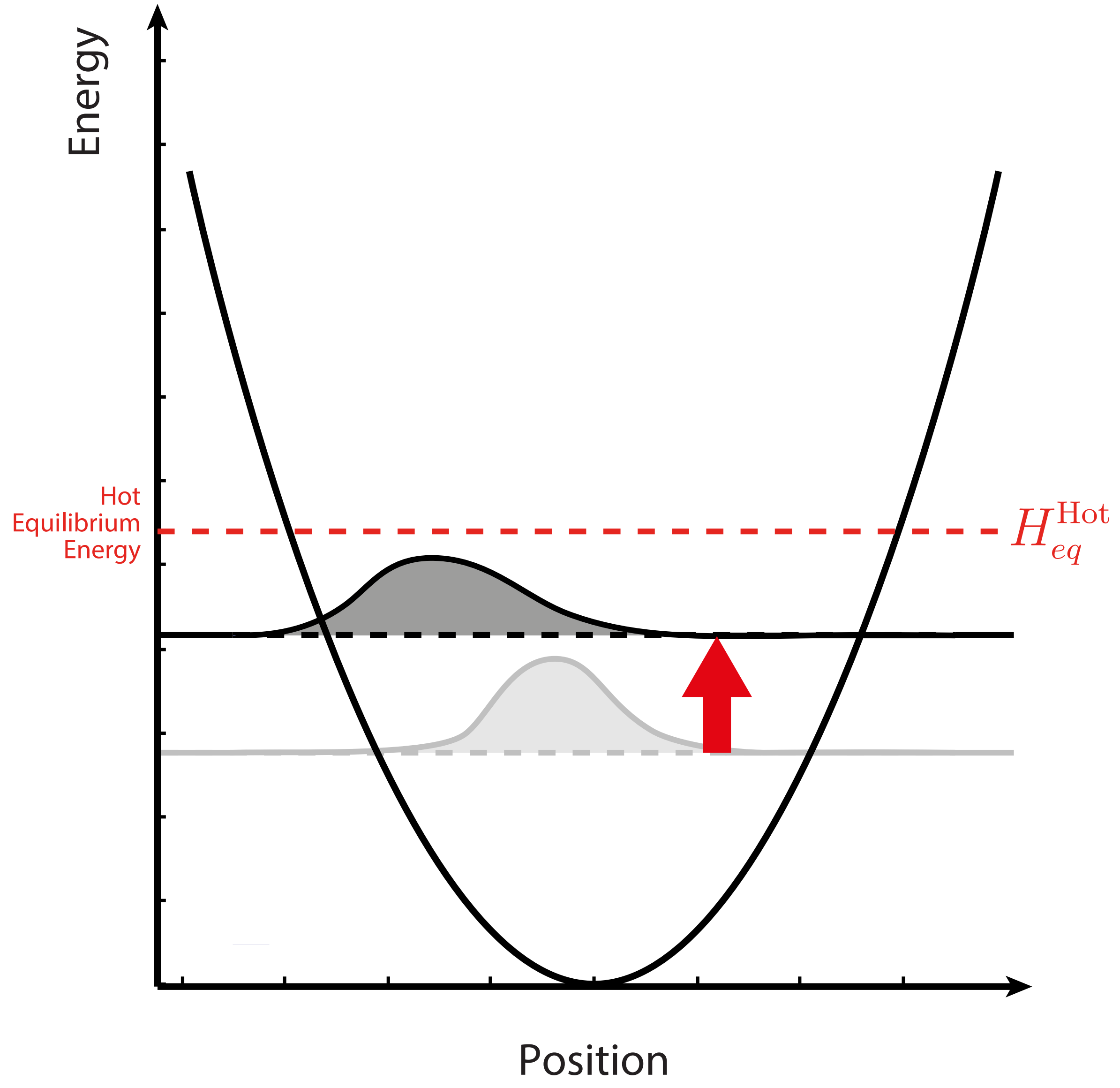
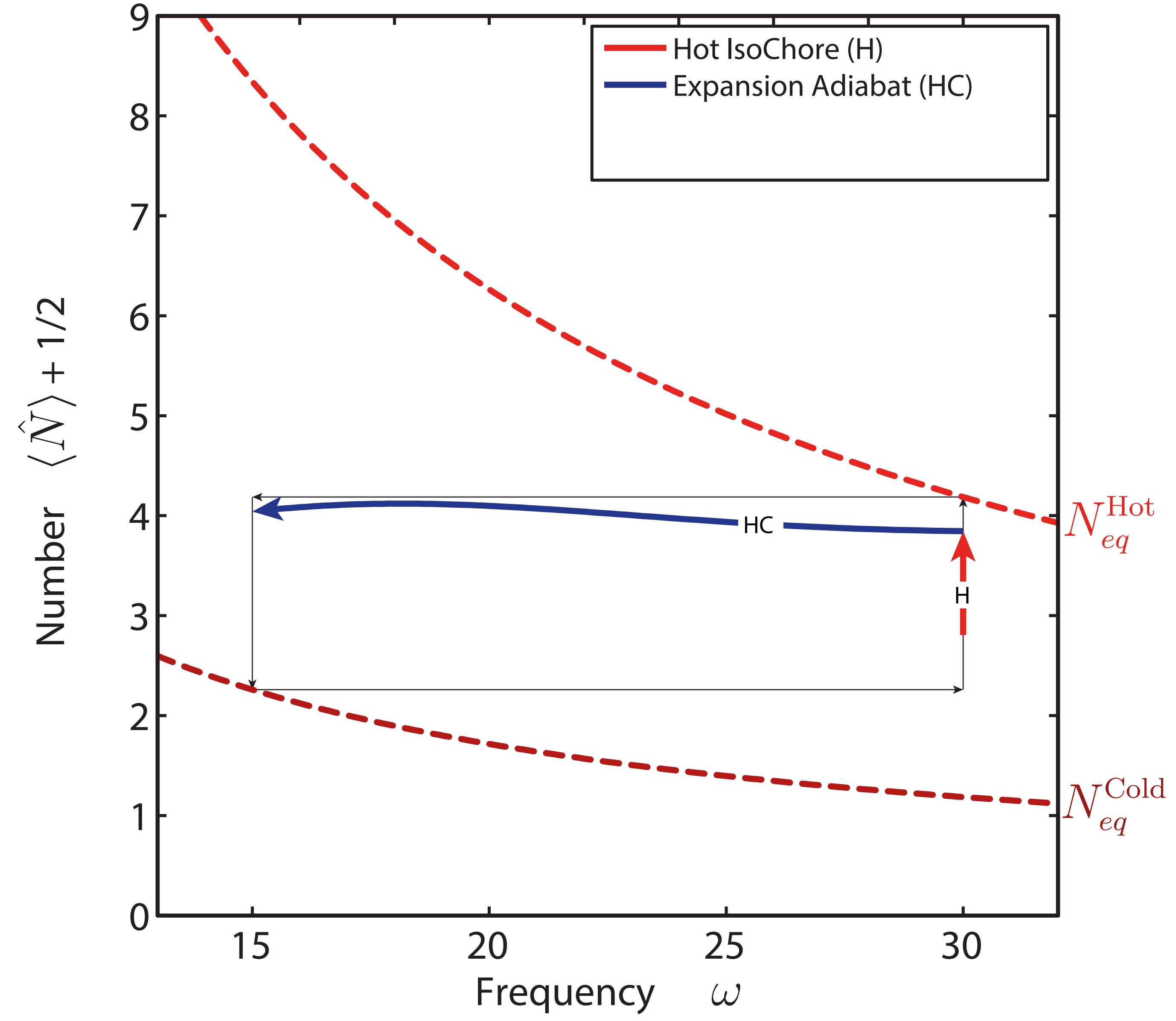
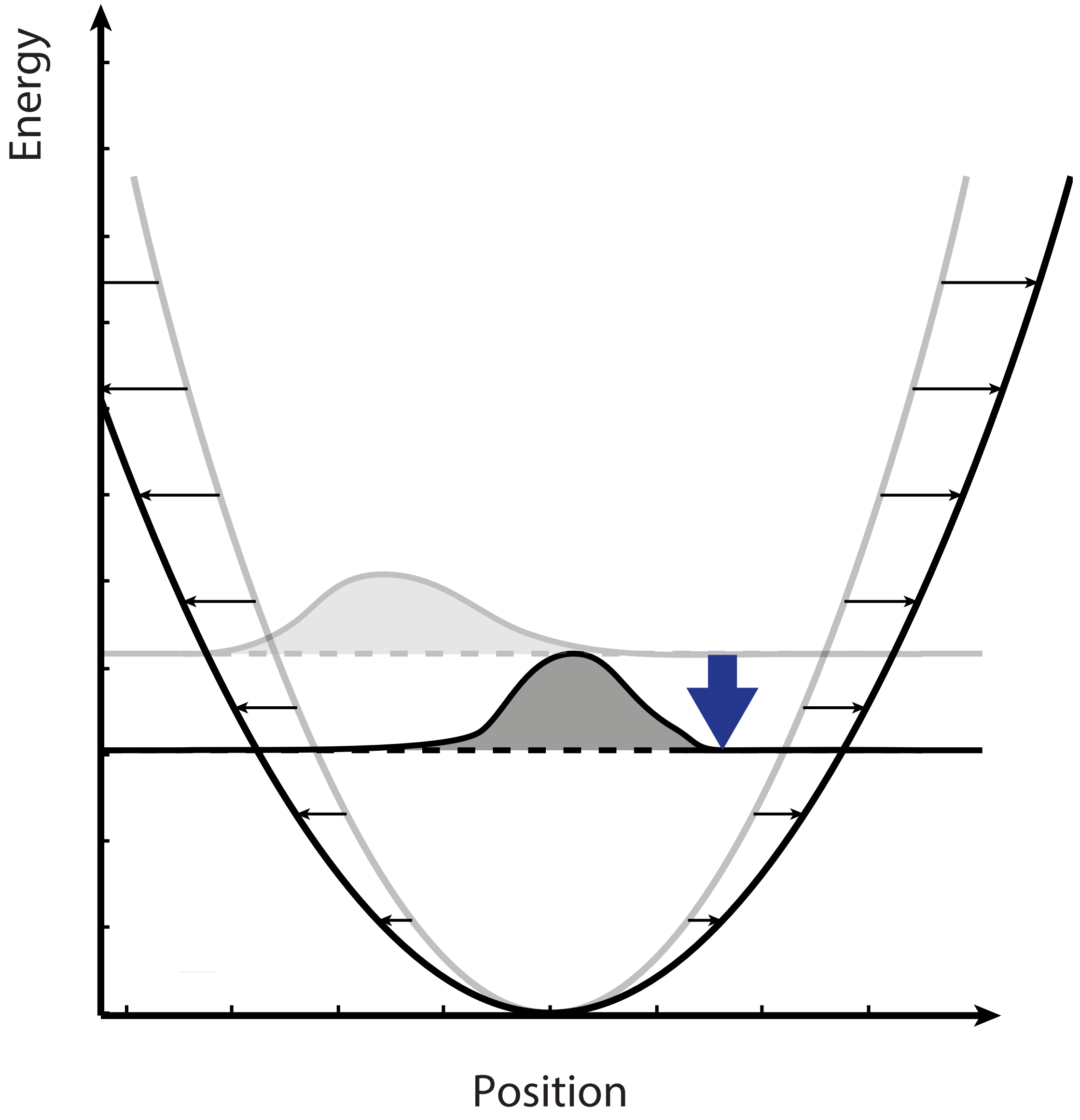


$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2$$

The Otto cycle - Expansion Adiabat

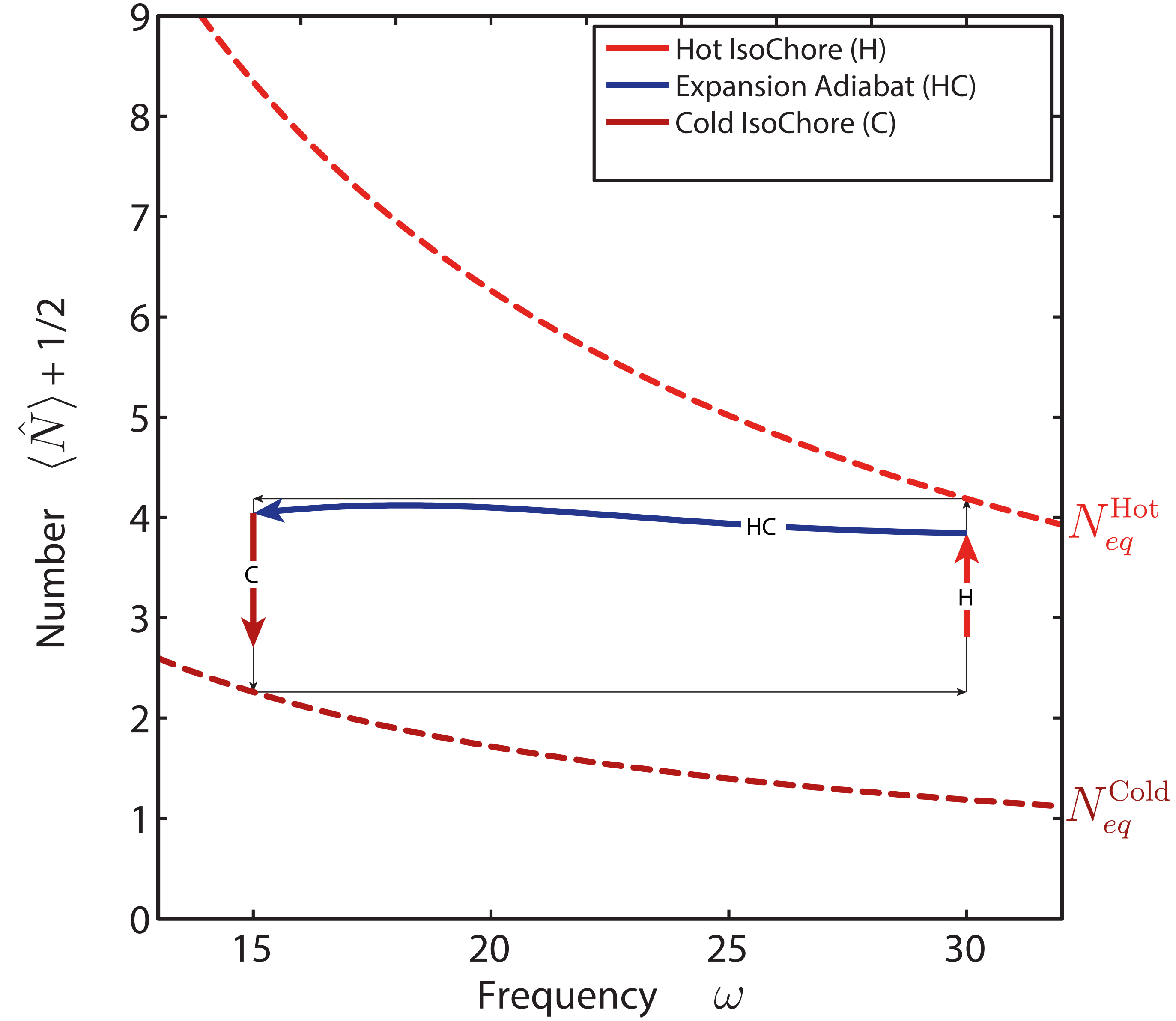




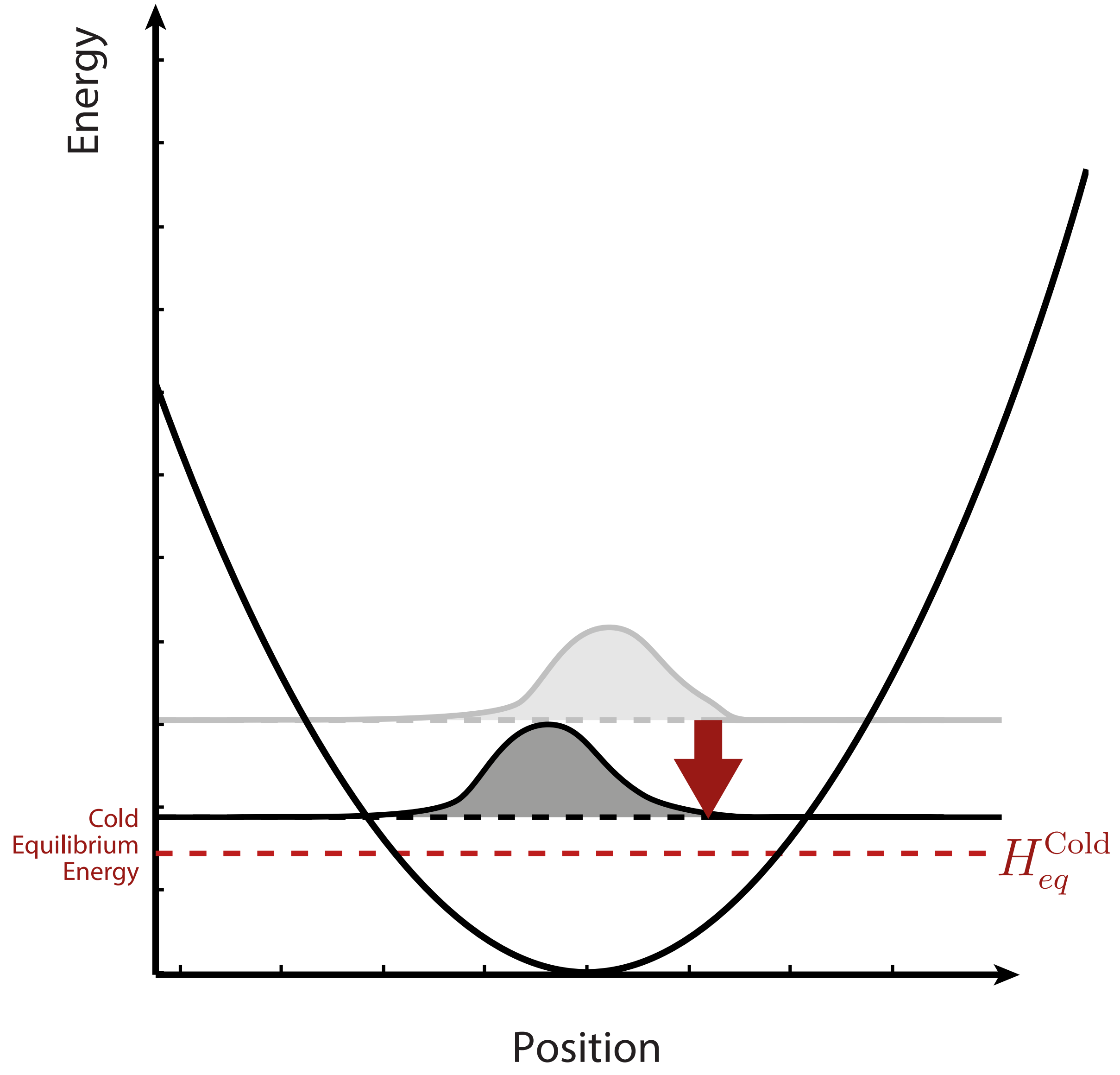
$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2$$

The Otto cycle - Cold IsoChore

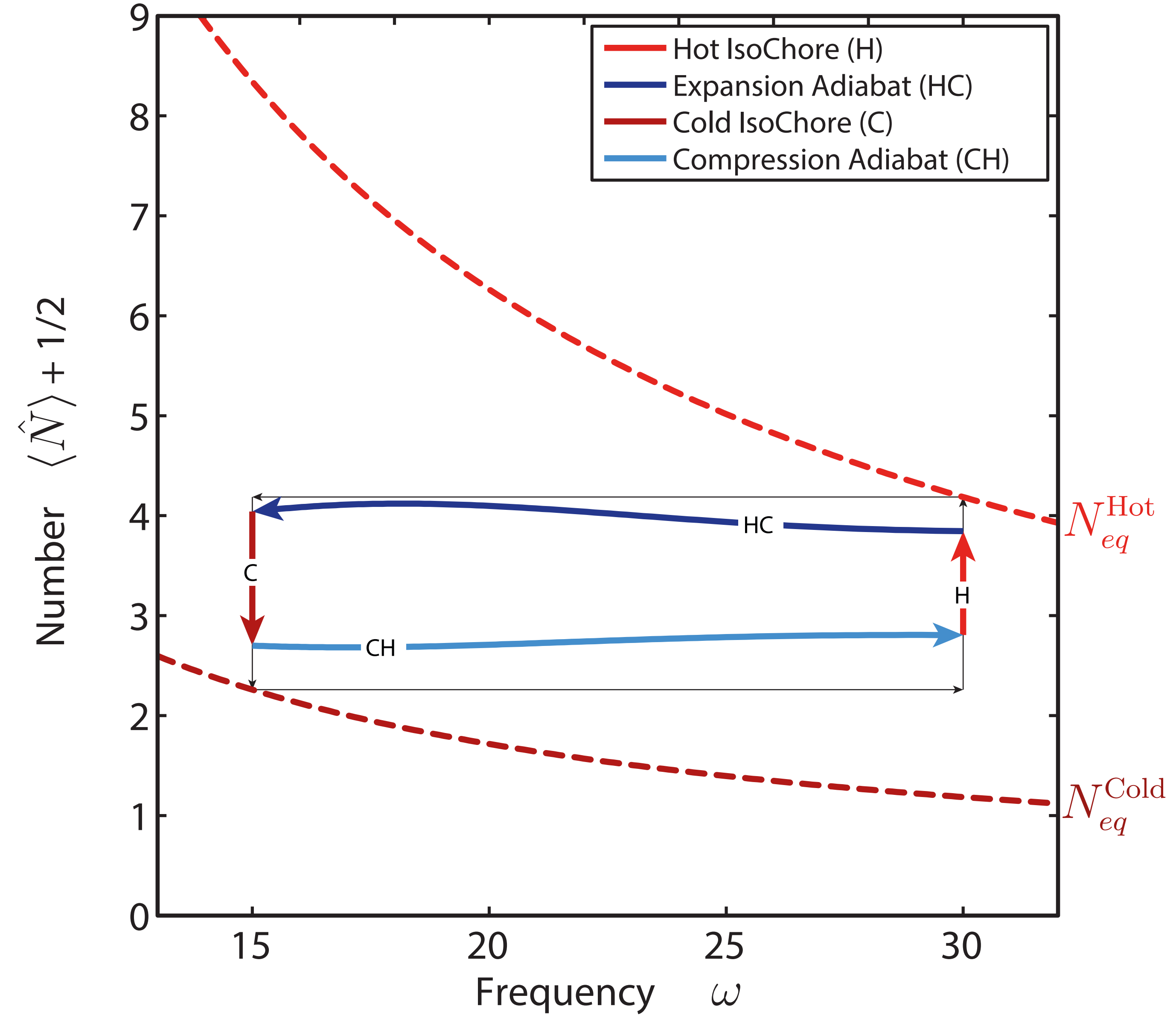


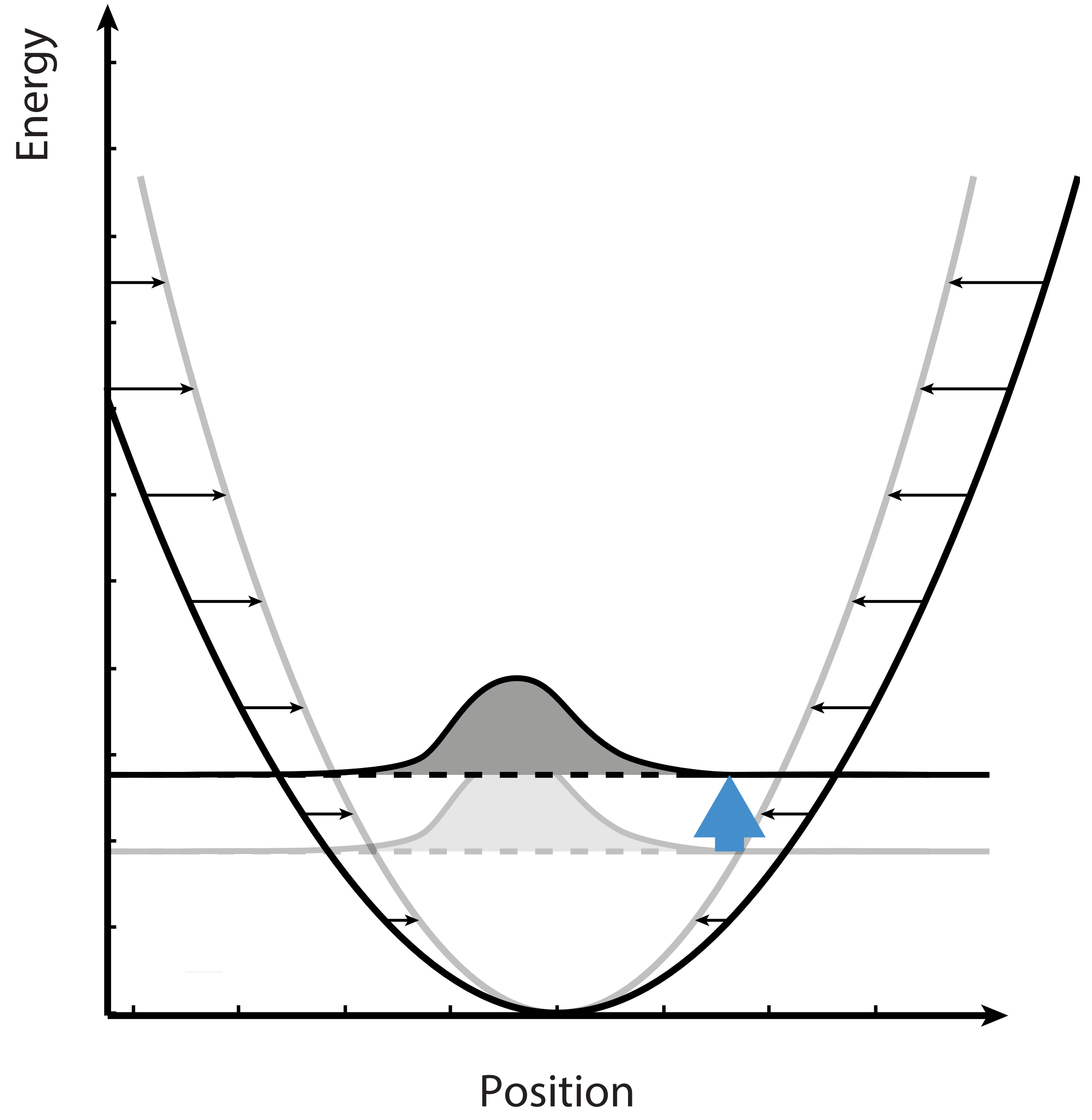
$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$



$$\hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2$$

The Otto cycle - Compression Adiabat





$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$

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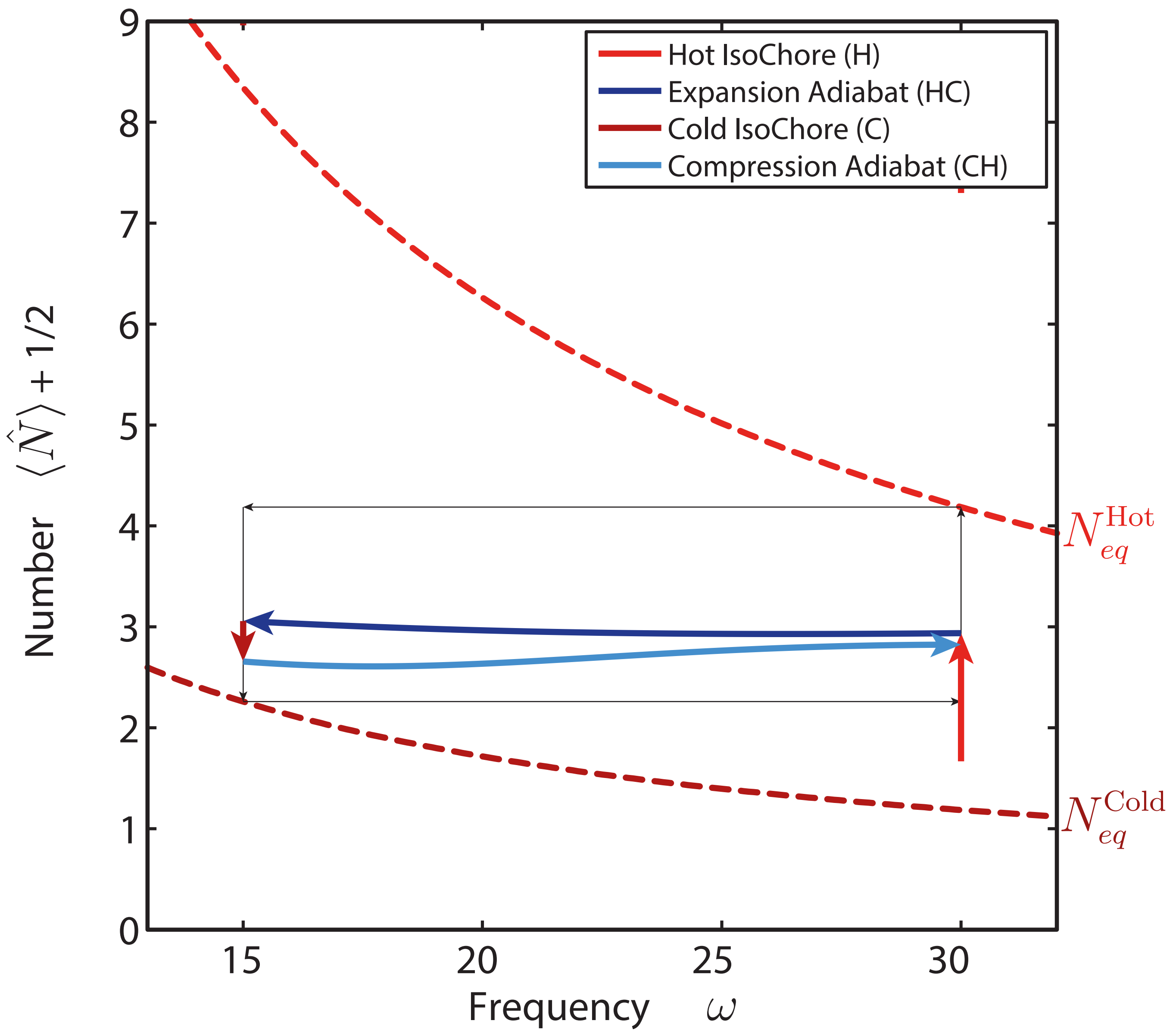
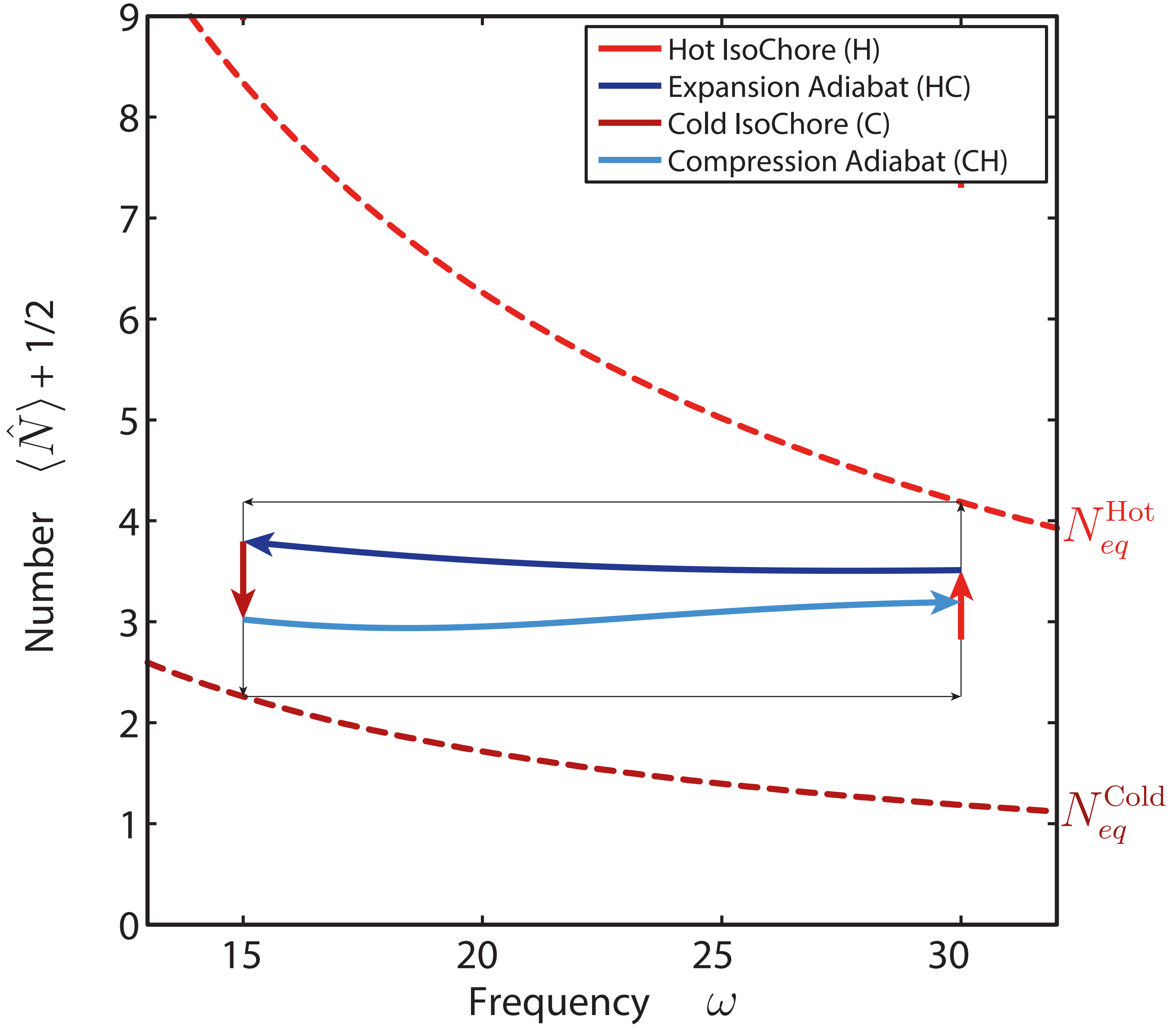
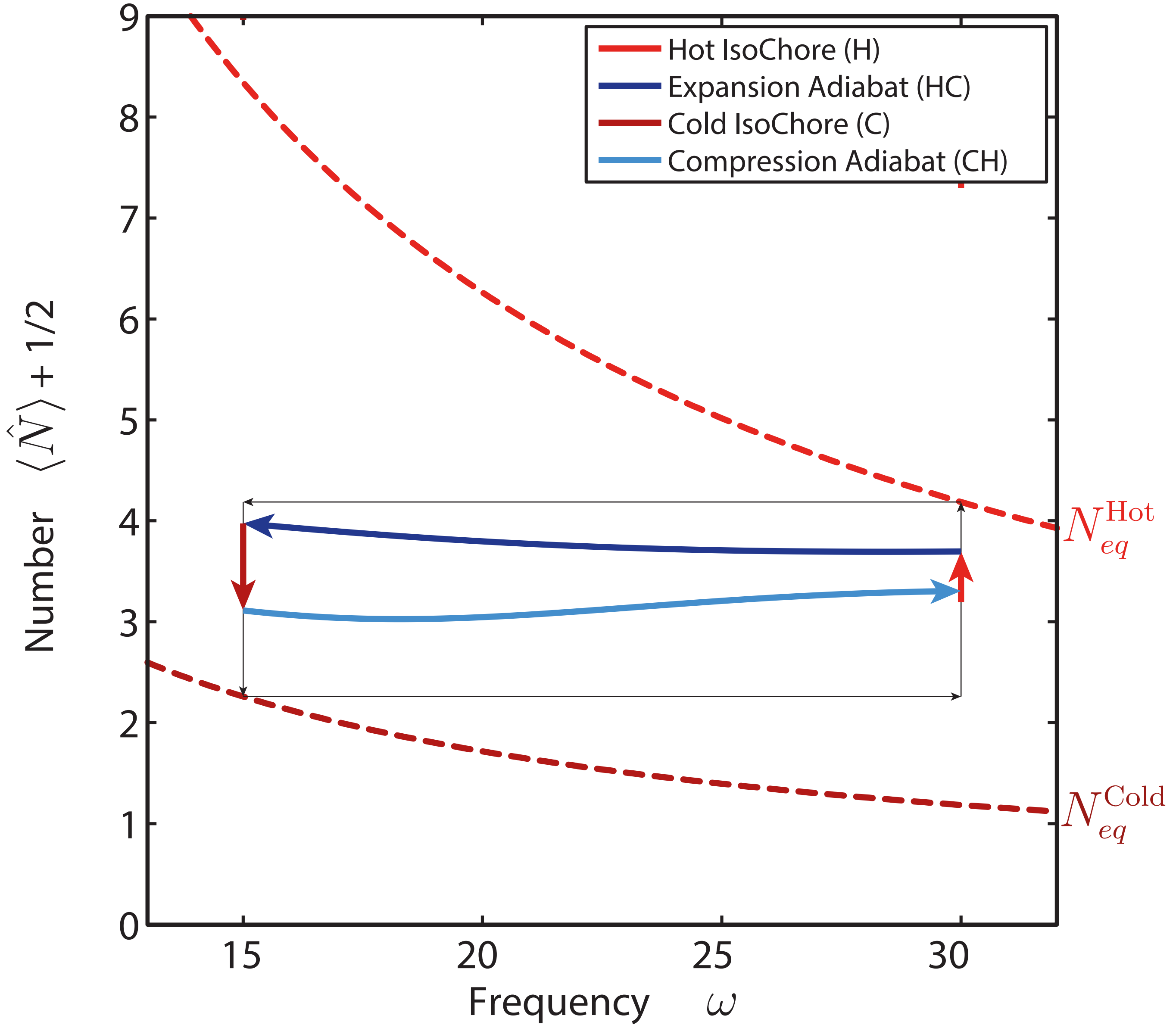
Convergence to the limit cycle



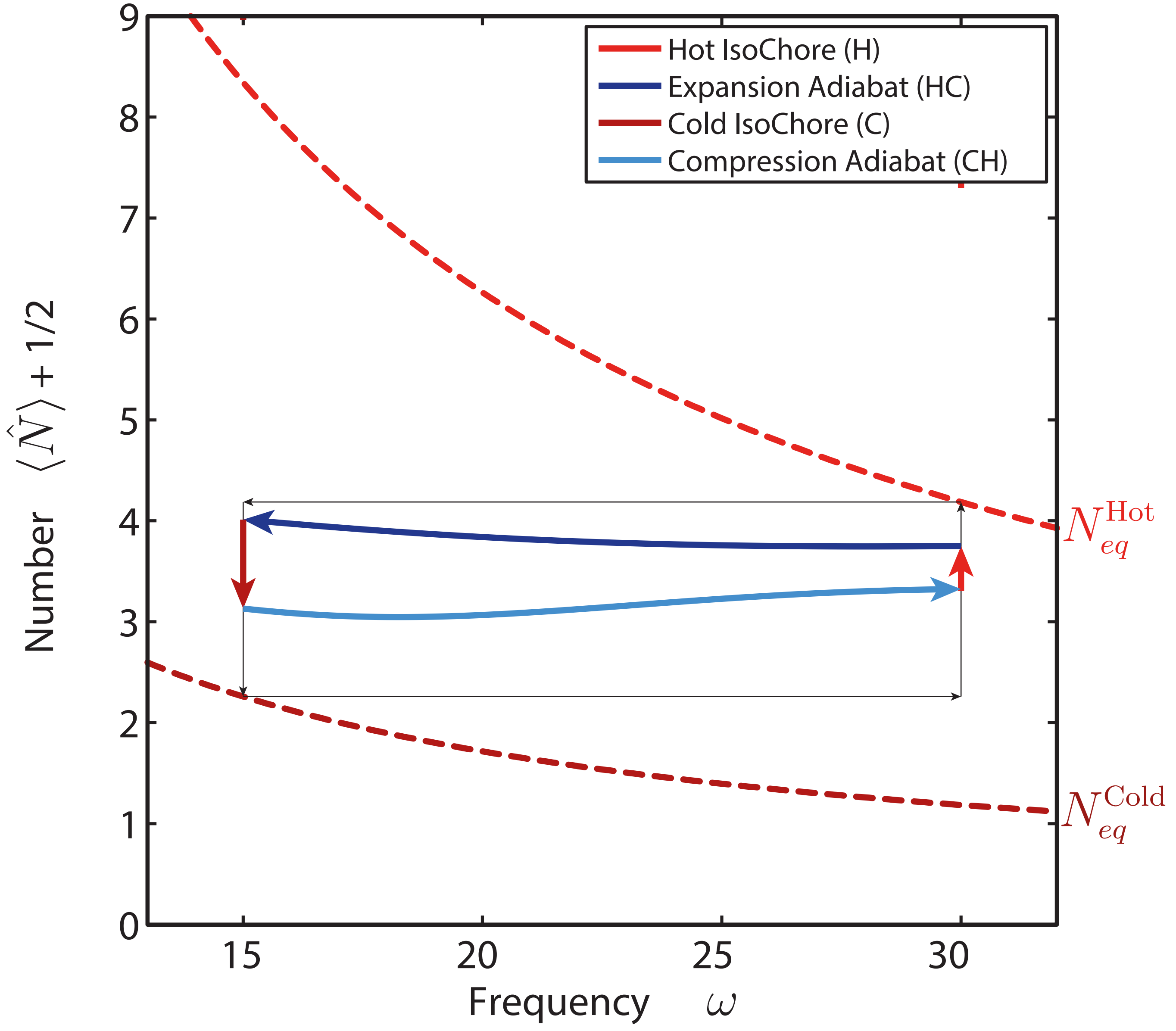
Convergence to the limit cycle



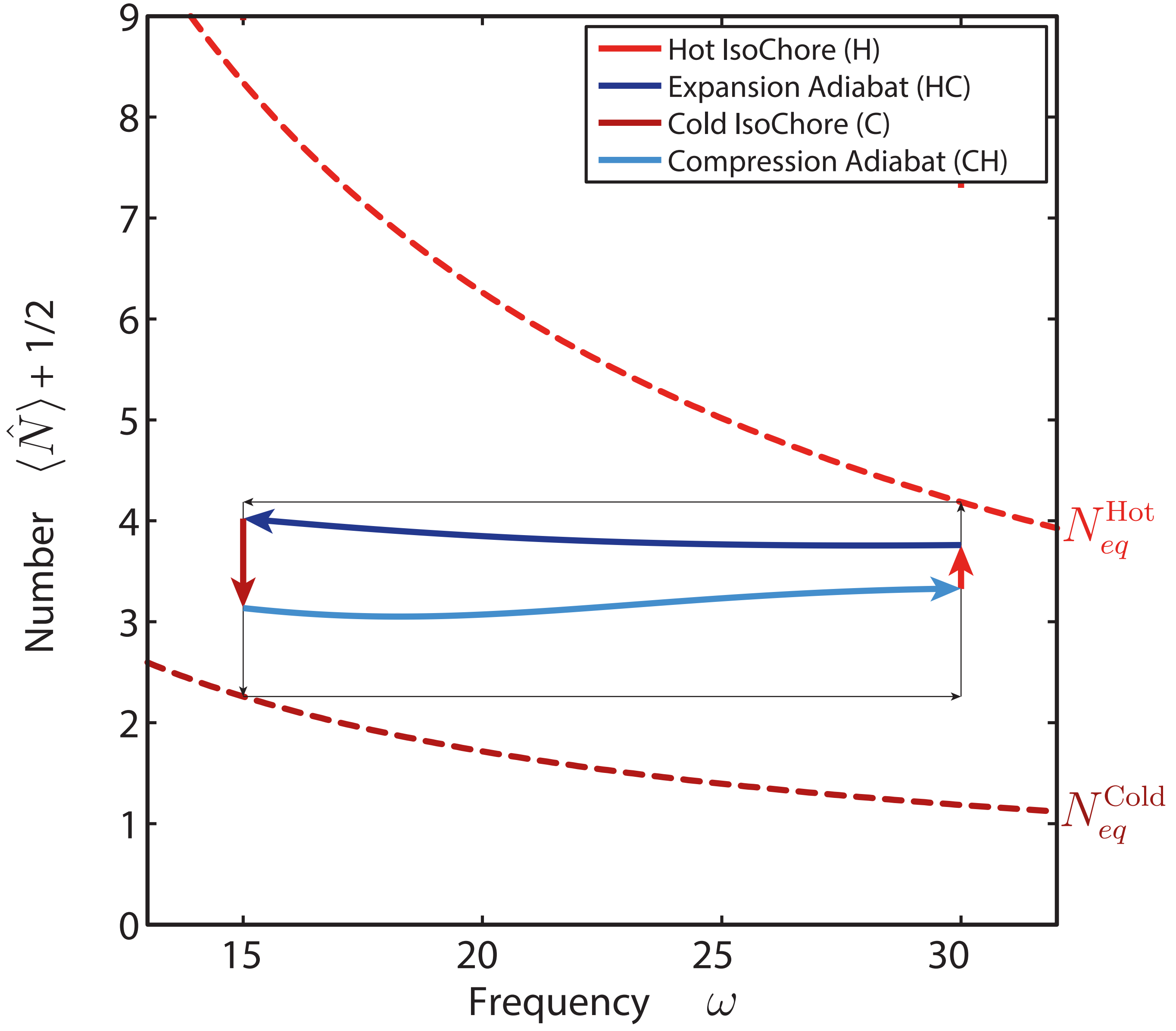
Convergence to the limit cycle



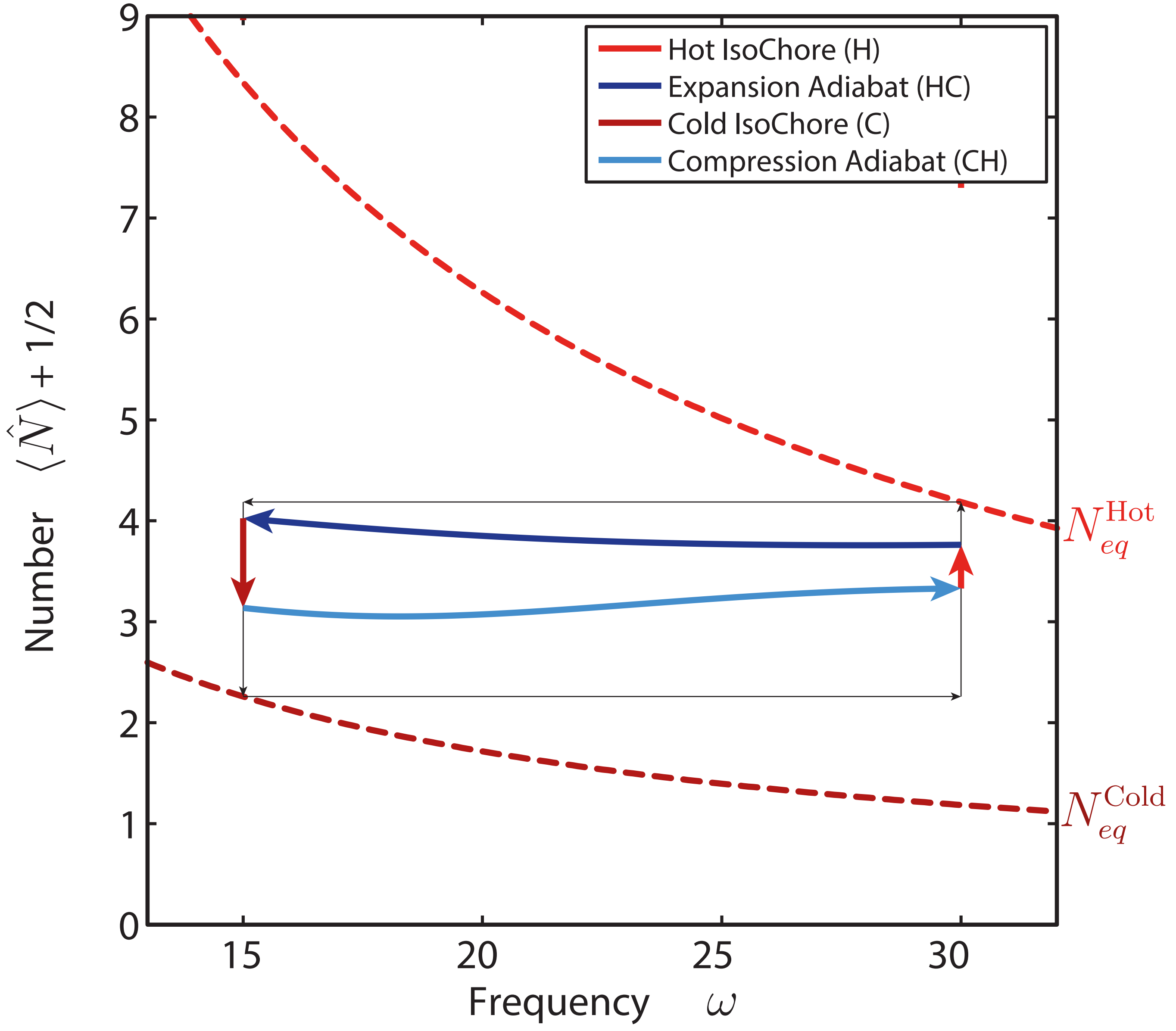
Convergence to the limit cycle



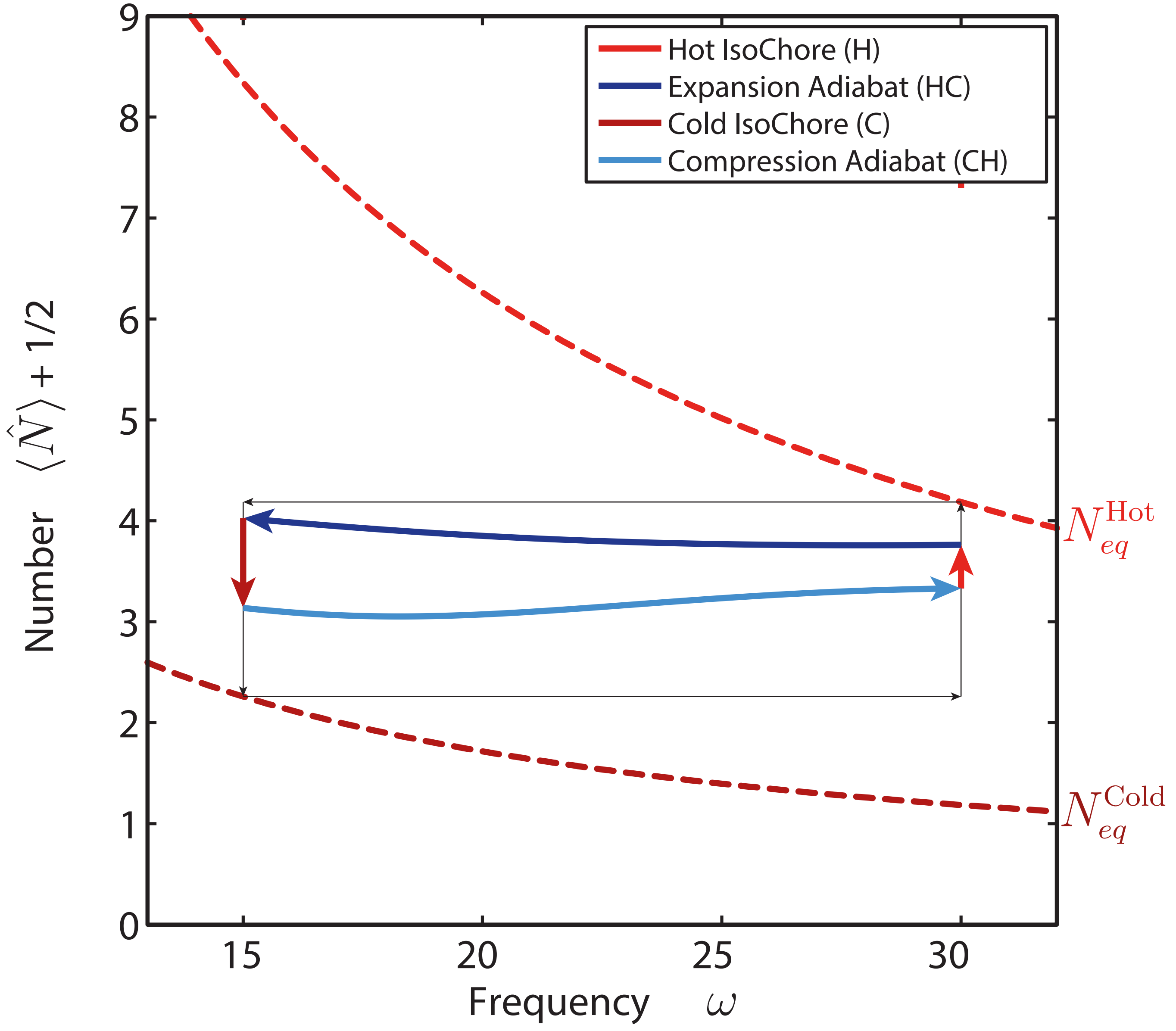
Convergence to the limit cycle

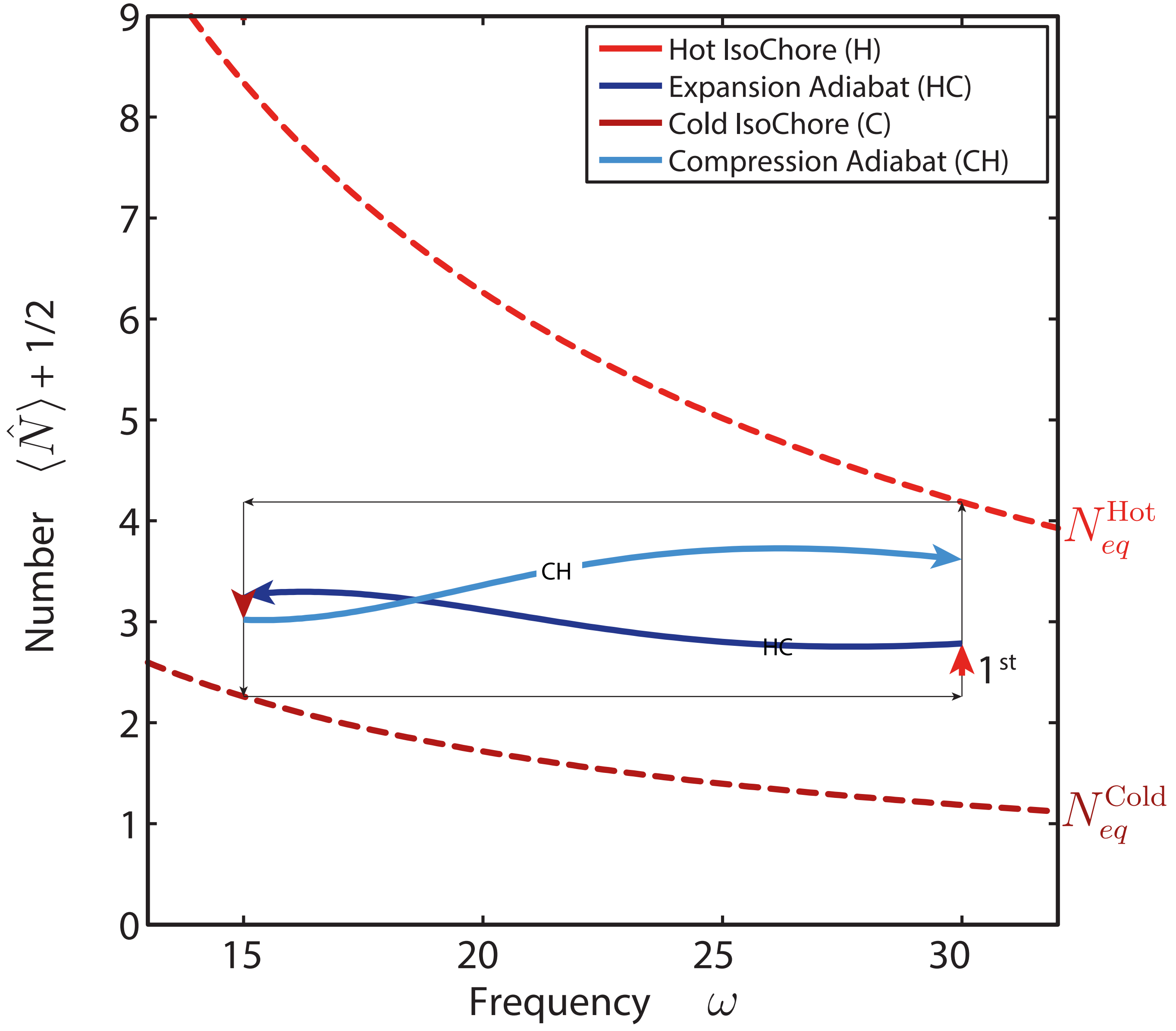


Convergence to the limit cycle



Divergent behavior





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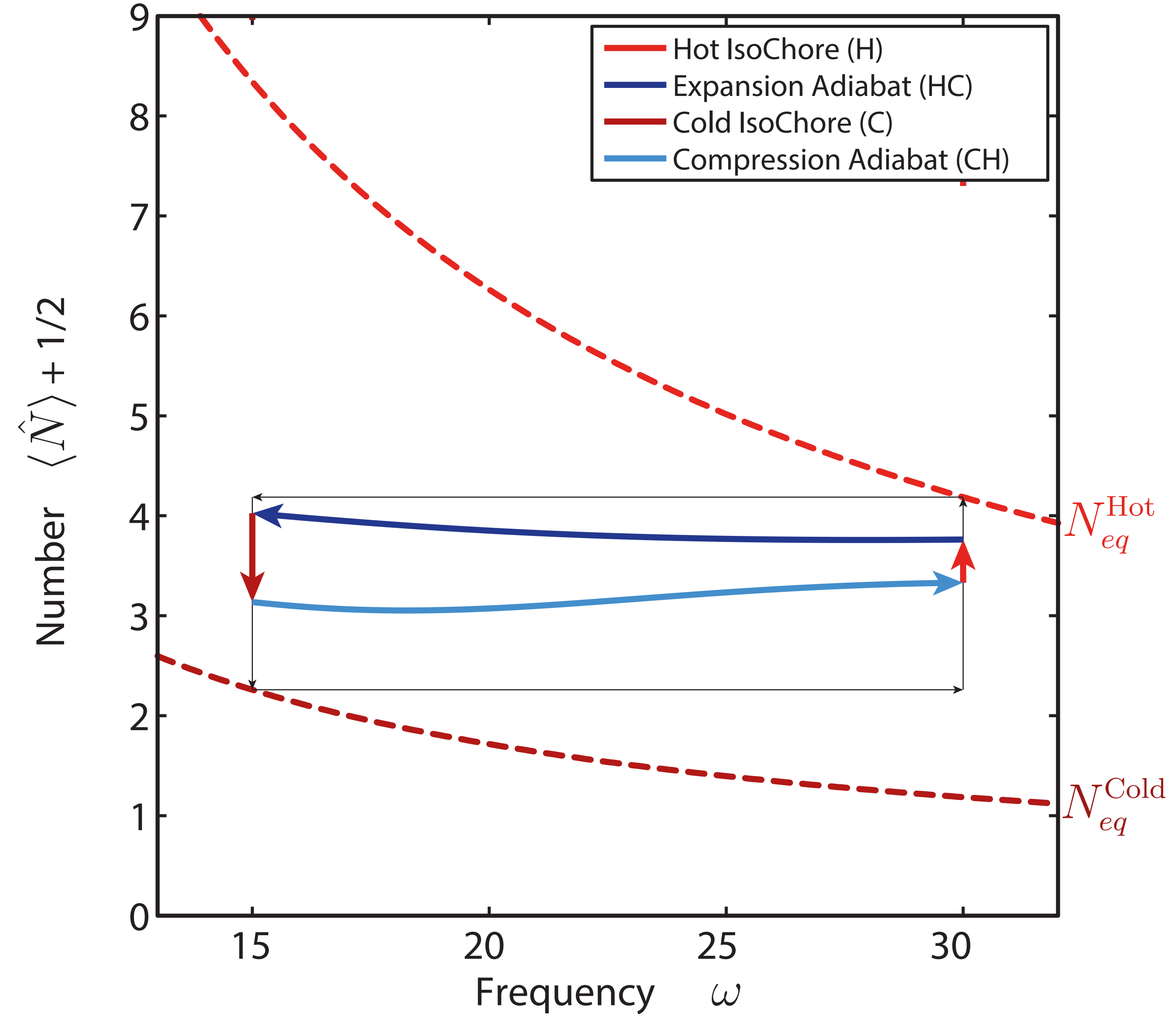

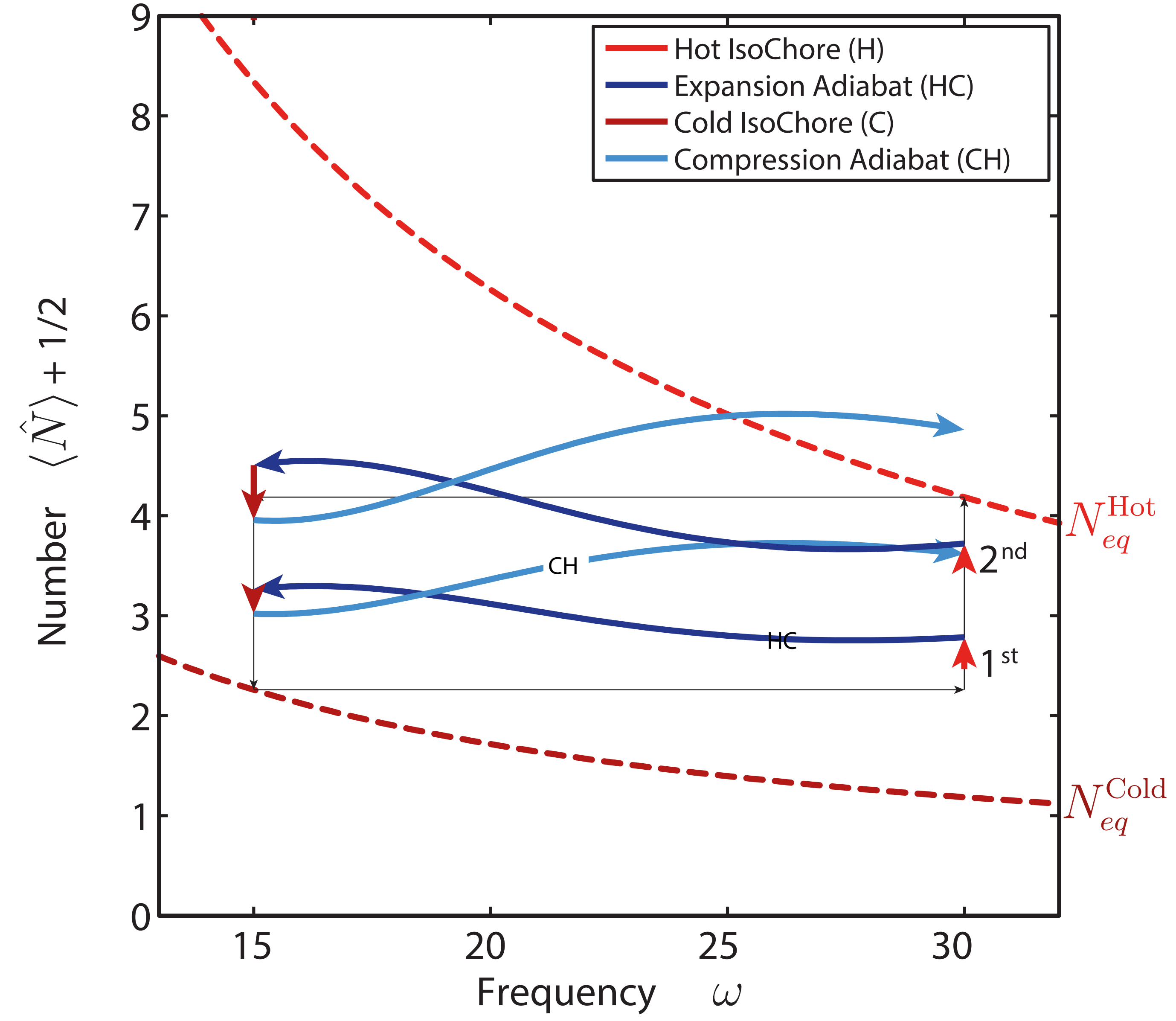

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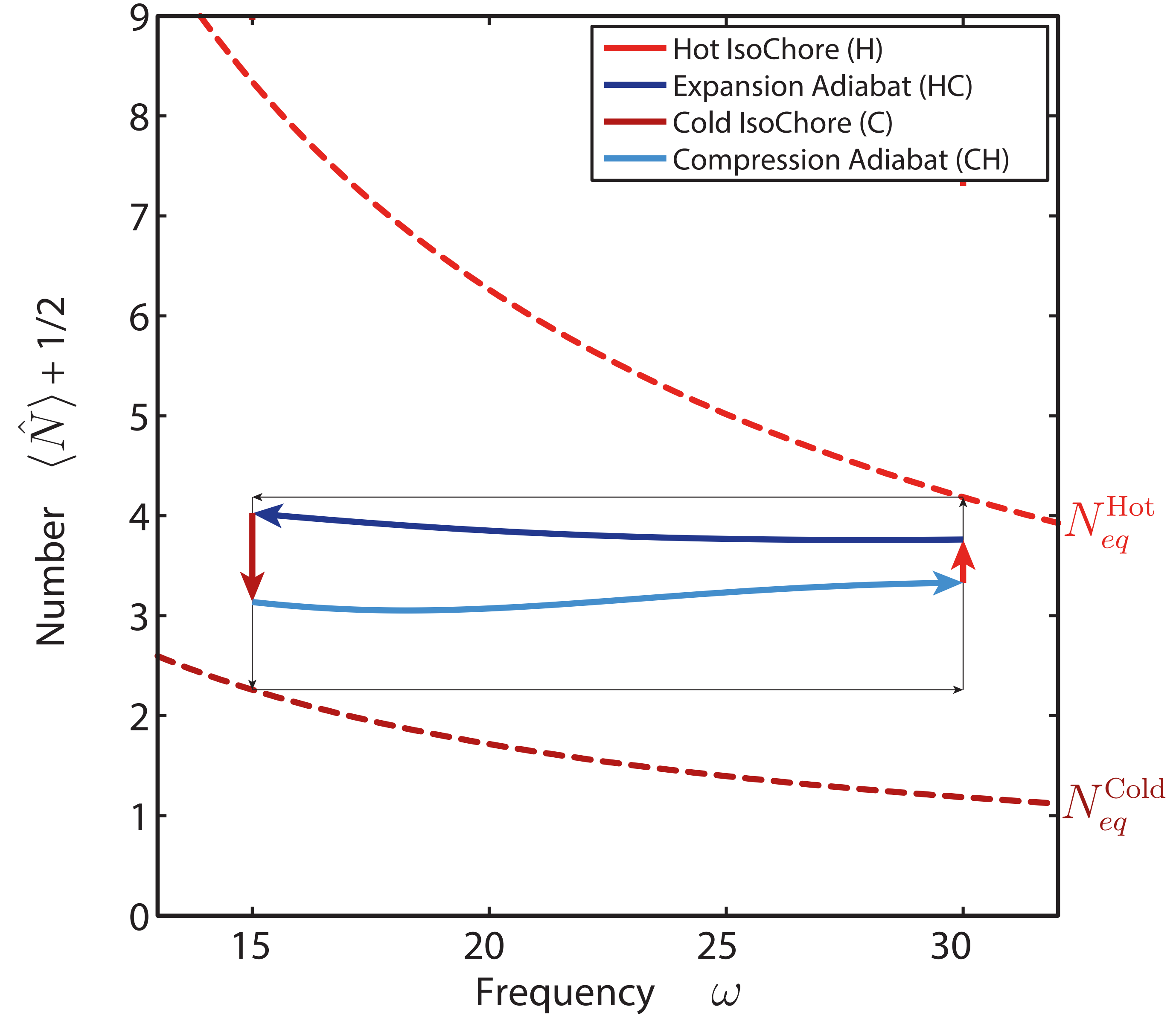

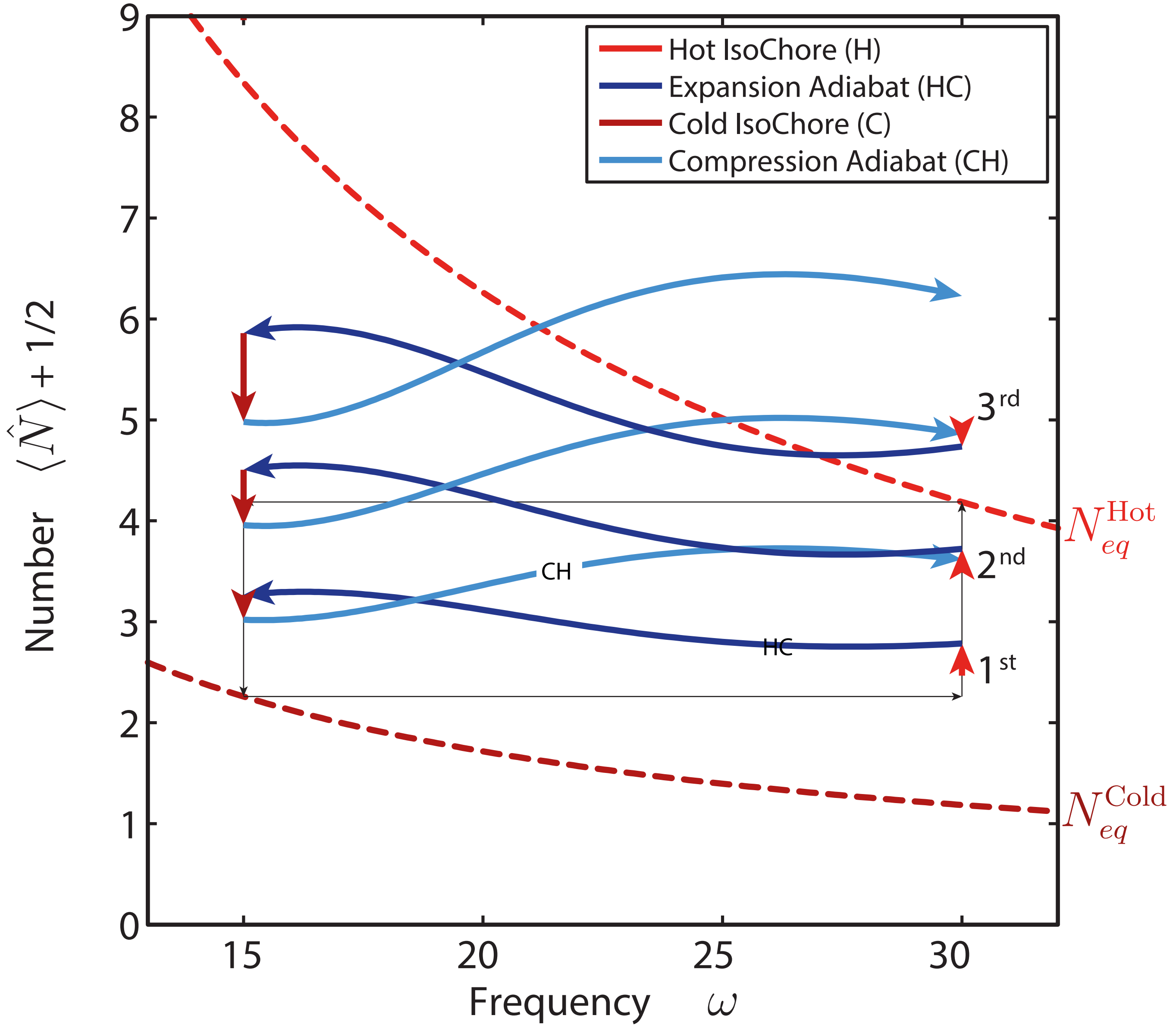

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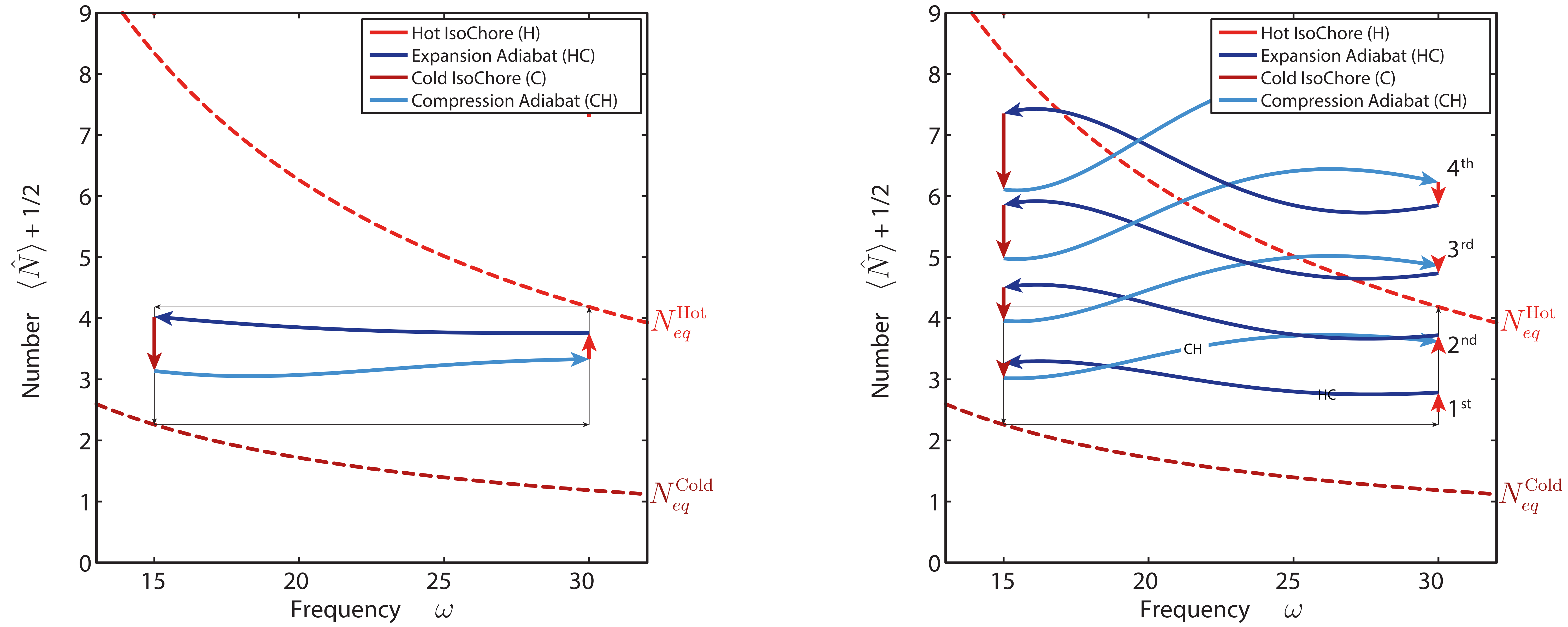

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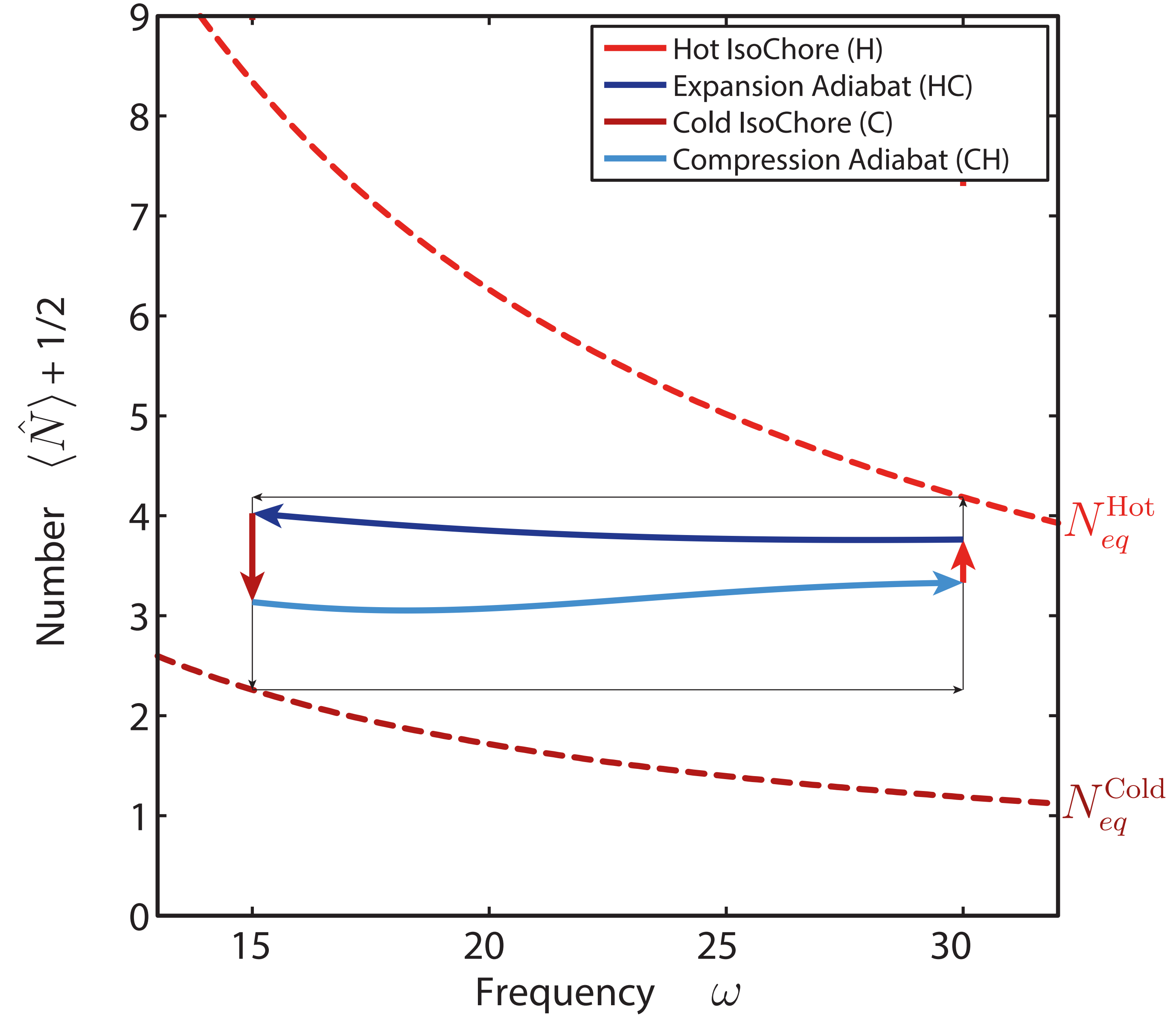

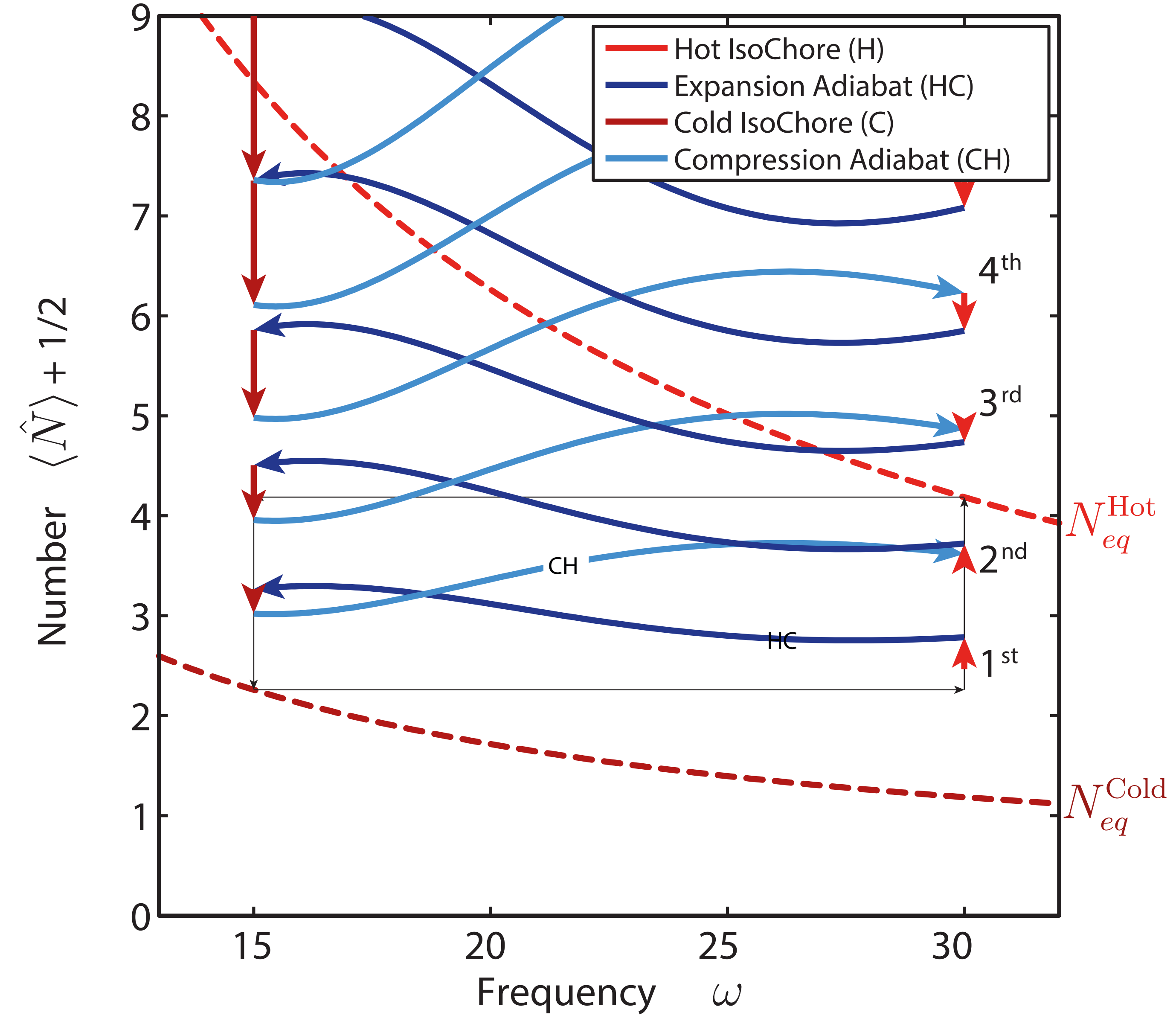

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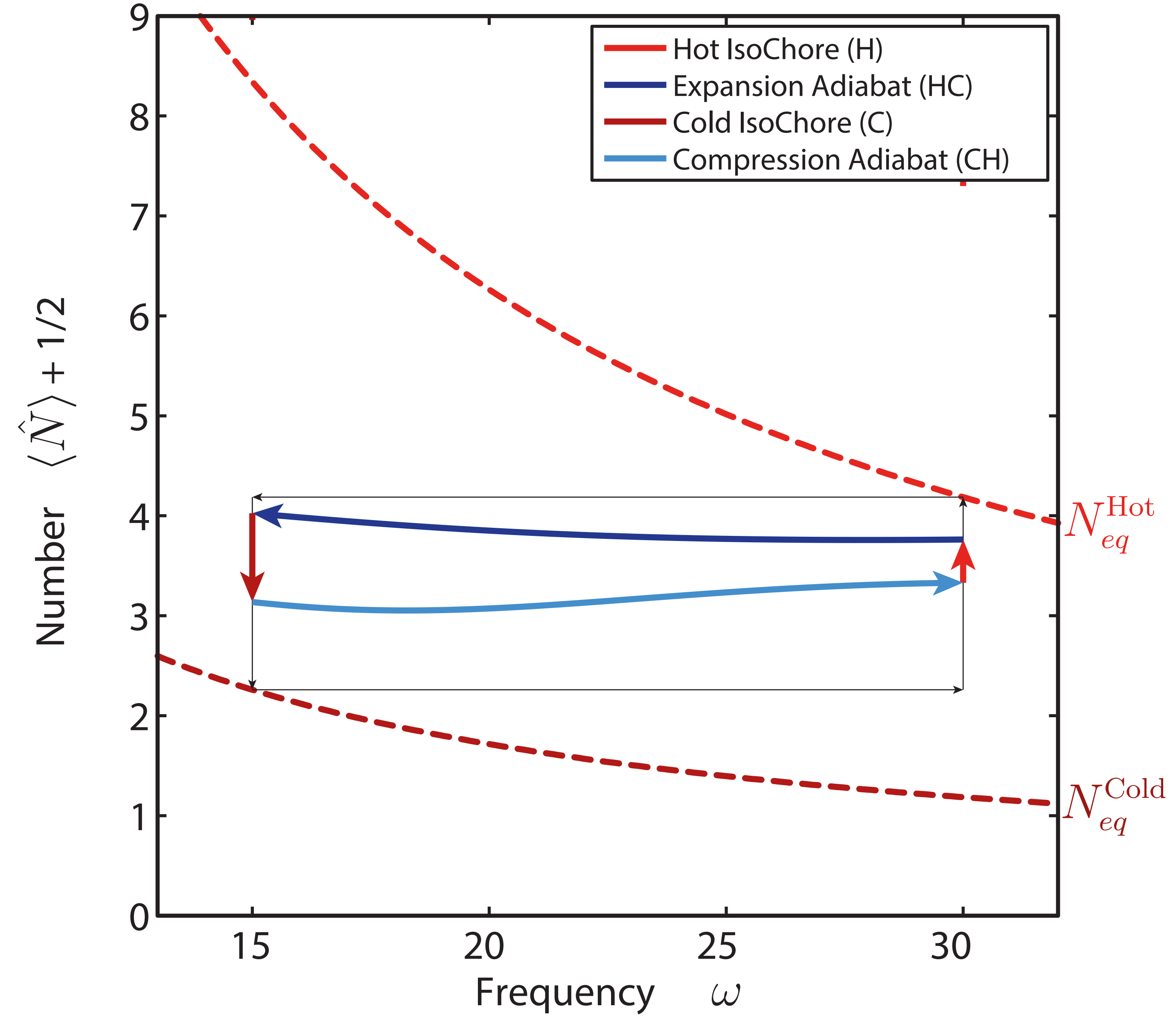

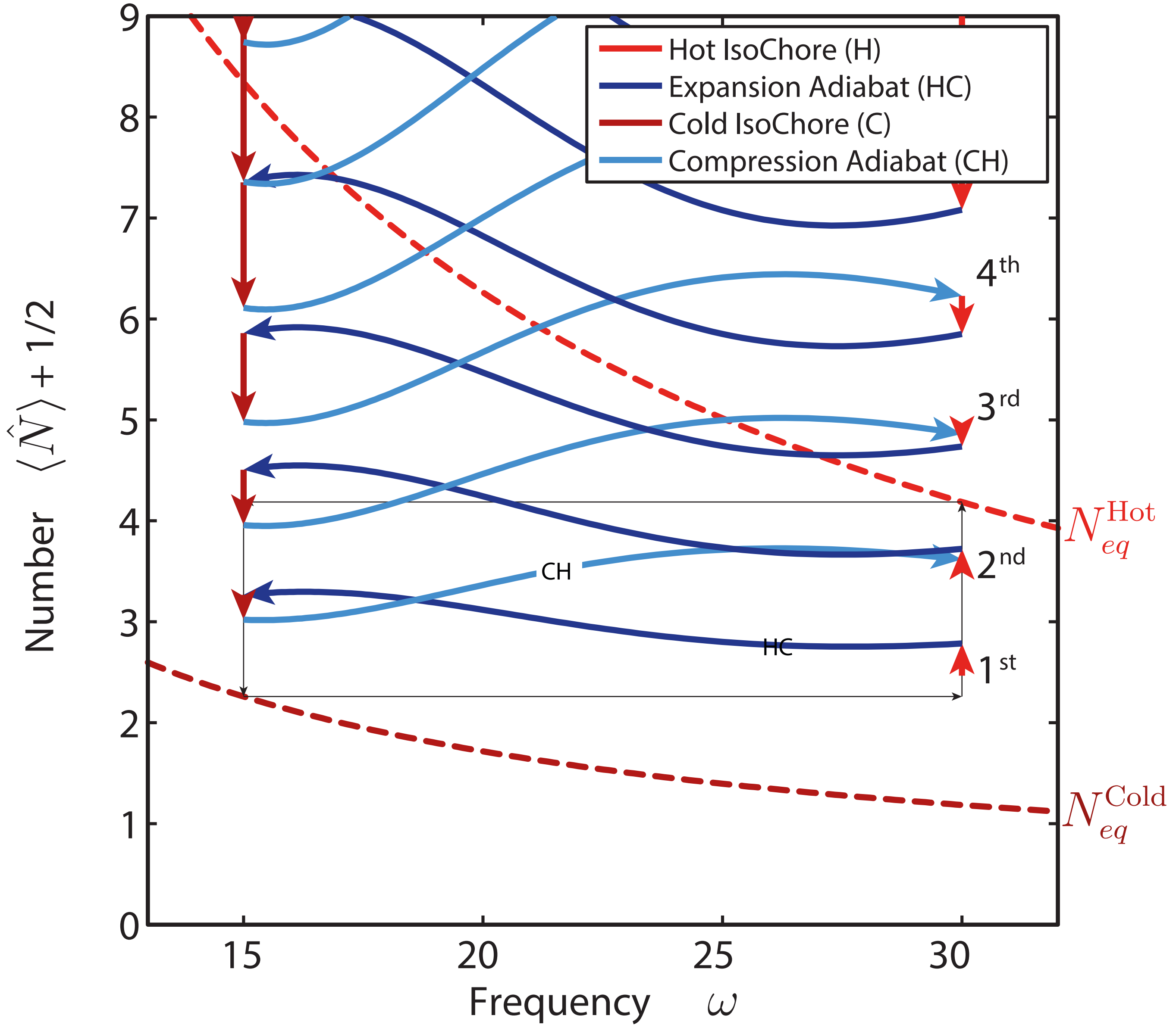

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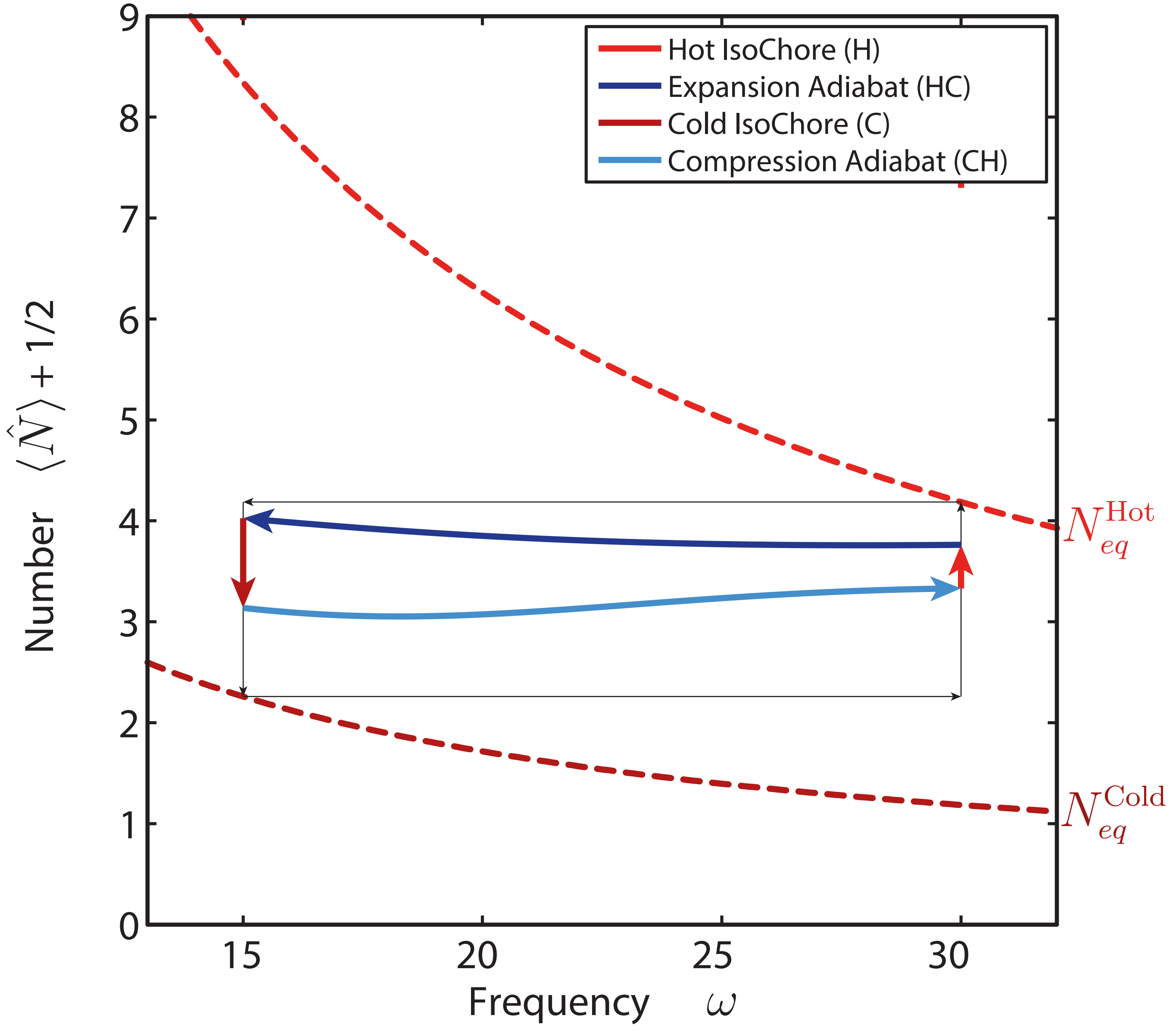

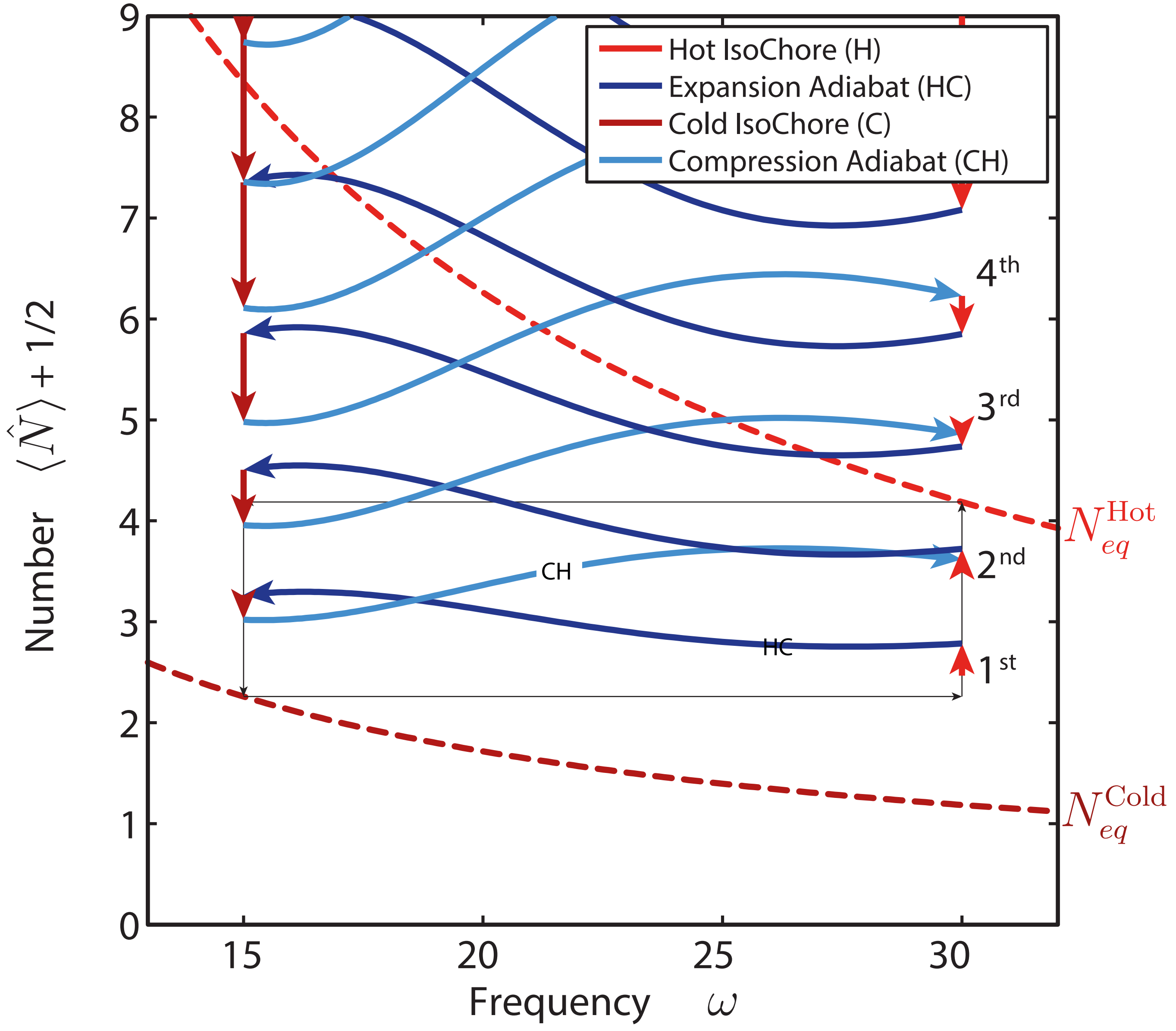

But why does it happen?

The Equations of Motion

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = +\frac{i}{\hbar}\left[\hat{H}(t), \hat{X}(t)\right] + \frac{\partial}{\partial t}\hat{X}(t)$$

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

Unitary superoperator $\mathcal{L}_H^*$

The Equations of Motion

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = +\frac{i}{\hbar}\left[\hat{H}(t), \hat{X}(t)\right] + \frac{\partial}{\partial t}\hat{X}(t)$$

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Unitary superoperator $\mathcal{L}_H^*$

$$\mathcal{L}_H^*\left(\hat{X}(t)\right) = +\frac{i}{\hbar}\left[\hat{H}(t), \hat{X}(t)\right]$$

Coupling with thermal reservoirs:

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \mathcal{L}_D^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

Dissipative Lindblad superoperator $\mathcal{L}_D^*$

- it is not unitary
- depends on $\beta = (k_B T)^{-1}$
- for the harmonic case, it includes $\hat{a}^\dagger$ and $\hat{a}$

The Lie Algebra

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \mathcal{L}_D^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

We seek for a set of operators $\{\hat{X}_1, \dots, \hat{X}_N\}$
such that:

$$\frac{d}{dt}\begin{pmatrix} \hat{X}_1 \\ \vdots \\ \hat{X}_N \end{pmatrix} = \begin{pmatrix} A_{11} & \dots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \dots & A_{NN} \end{pmatrix}\begin{pmatrix} \hat{X}_1 \\ \vdots \\ \hat{X}_N \end{pmatrix}$$

Closed with respect to the equation of motion

The Lie Algebra

Equation of motion in the Heisenberg picture:

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For $\mathcal{L}_H^*$ we have the following sufficient condition
(and a similar condition applies for $\mathcal{L}_D^*$)

$$\begin{cases} \left[i\hat{X}_h, i\hat{X}_k\right] = i\sum_k \Gamma_{hjk}\hat{X}_k, \quad \Gamma_{hjk} \in \mathbb{R} \longrightarrow \textbf{LieAlgebra} \\ \hat{H} = \sum_k c_k \hat{X}_k, \quad c_k \in \mathbb{R} \end{cases}$$

The Lie Algebra

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \mathcal{L}_D^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

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Harmonic Oscillator

$$\begin{cases} \hat{X}_1 = \hat{Q}^2 \\ \hat{X}_2 = \hat{P}^2 \\ \hat{X}_3 = \hat{D} = \hat{Q}\hat{P} + \hat{P}\hat{Q} \end{cases}$$

The Lie Algebra

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \mathcal{L}_D^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

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For $\mathcal{L}_H^*$ we have the following sufficient condition (and a similar condition applies for $\mathcal{L}_D^*$)

$$\begin{cases} \left[i\hat{X}_h, i\hat{X}_k\right] = i\sum_k \Gamma_{hjk}\hat{X}_k, & \Gamma_{hjk} \in \mathbb{R} \\ \hat{H} = \sum_k c_k \hat{X}_k, & c_k \in \mathbb{R} \end{cases} \longrightarrow$$

Harmonic Oscillator

$$\begin{cases} \hat{X}_1 = \hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2 \\ \hat{X}_2 = \hat{L} = \frac{1}{2m}\hat{P}^2 - \frac{1}{2}m\omega^2\hat{Q}^2 \\ \hat{X}_3 = \hat{C} = \frac{1}{2}\omega(t)\left(\hat{Q}\hat{P} + \hat{P}\hat{Q}\right) \end{cases}$$

The Lie Algebra

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \mathcal{L}_D^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

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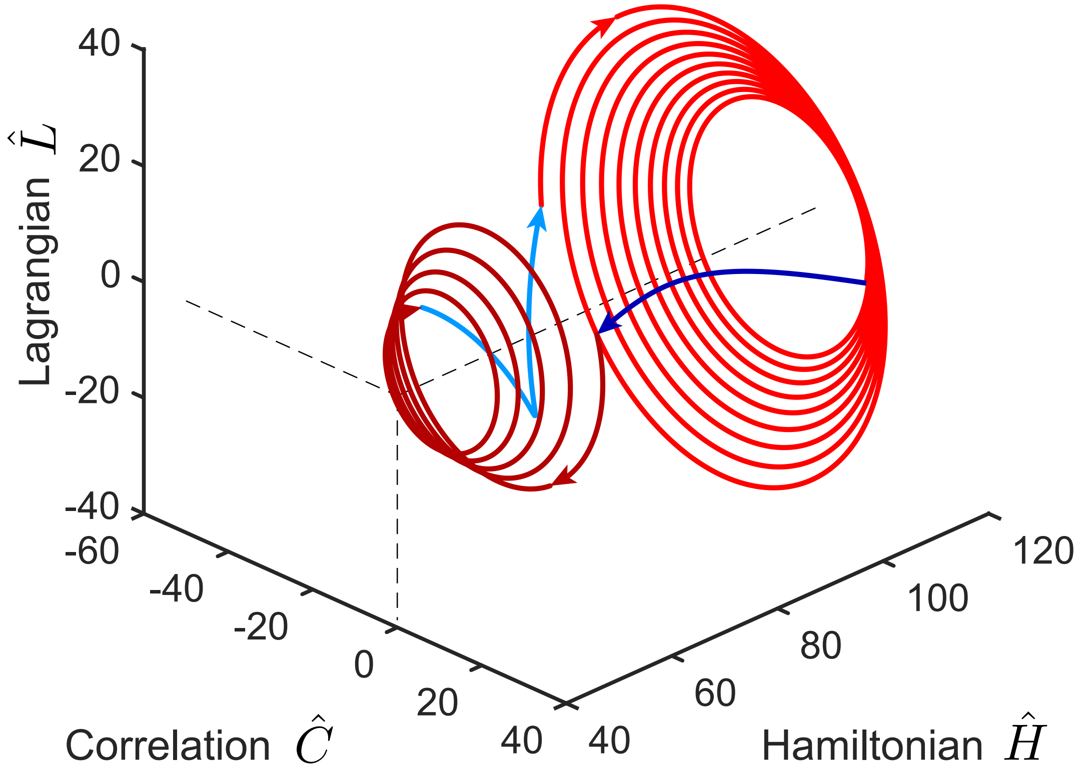


For $\mathcal{L}_H^*$ we have the following sufficient condition (and a similar condition applies for $\mathcal{L}_D^*$)

$$\begin{cases} \left[i\hat{X}_h, i\hat{X}_k\right] = i\sum_k \Gamma_{hjk}\hat{X}_k, & \Gamma_{hjk} \in \mathbb{R} \\ \hat{H} = \sum_k c_k\hat{X}_k, & c_k \in \mathbb{R} \end{cases}$$

$\longrightarrow$

Harmonic Oscillator

$$\begin{cases} \hat{X}_1 = \hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2 \\ \hat{X}_2 = \hat{L} = \frac{1}{2m}\hat{P}^2 - \frac{1}{2}m\omega^2\hat{Q}^2 \\ \hat{X}_3 = \hat{C} = \frac{1}{2}\omega(t)\left(\hat{Q}\hat{P} + \hat{P}\hat{Q}\right) \end{cases}$$

The Lie Algebra - dissipative evolution

Equation of motion in the Heisenberg picture:

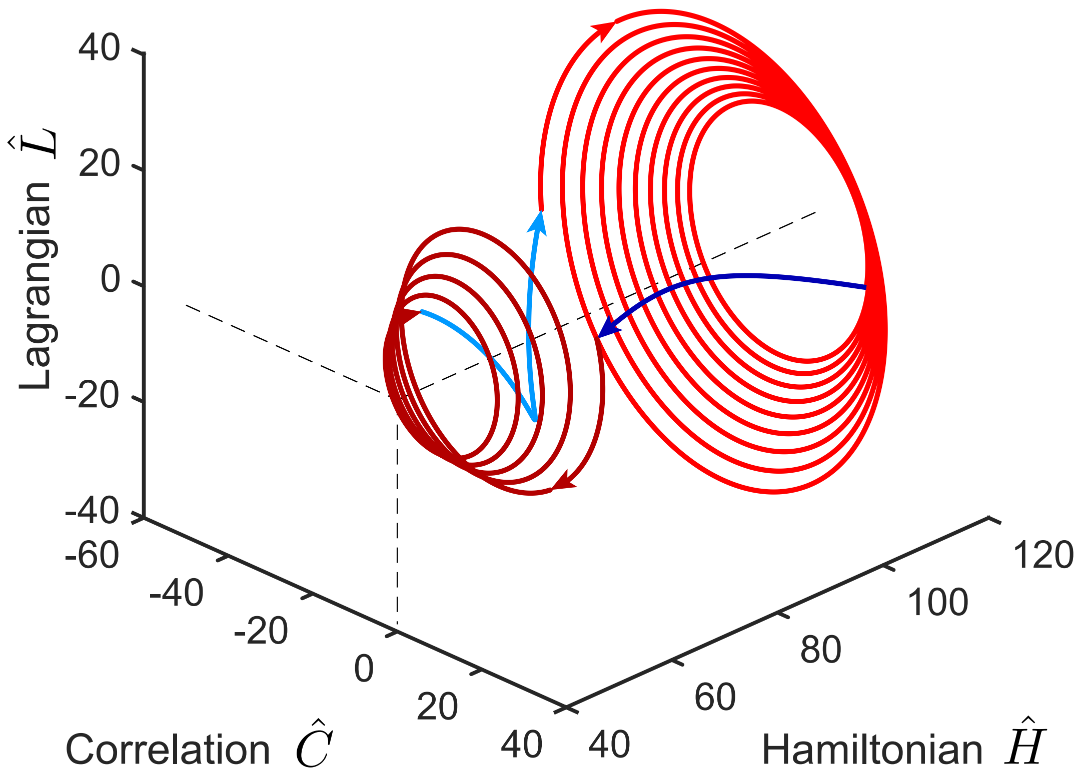
$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \mathcal{L}_D^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

We seek for a set of operators $\{\hat{X}_1, \ldots, \hat{X}_N\}$ such that:

$$\frac{d}{dt}\begin{pmatrix} \hat{X}_1 \\ \vdots \\ \hat{X}_N \end{pmatrix} = \begin{pmatrix} A_{11} & \ldots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \ldots & A_{NN} \end{pmatrix}\begin{pmatrix} \hat{X}_1 \\ \vdots \\ \hat{X}_N \end{pmatrix}$$

For $\mathcal{L}_H^*$ we have the following sufficient condition and a similar condition applies for $\mathcal{L}_D^*$ when we consider it, we need to include: $\hat{X}_4 = \hat{1}$

Expectation values



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Harmonic Oscillator

$$\begin{cases} \hat{X}_1 = \hat{H} = \frac{1}{2m}\hat{P}^2 + \frac{1}{2}m\omega^2\hat{Q}^2 \\ \hat{X}_2 = \hat{L} = \frac{1}{2m}\hat{P}^2 - \frac{1}{2}m\omega^2\hat{Q}^2 \\ \hat{X}_3 = \hat{C} = \frac{1}{2}\omega(t)\left(\hat{Q}\hat{P} + \hat{P}\hat{Q}\right) \end{cases}$$

The time-evolution equations

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\big(\hat{X}(t)\big) + \mathcal{L}_D^*\big(\hat{X}(t)\big) + \frac{\partial}{\partial t}\hat{X}(t)$$

We seek for a set of operators $\{\hat{X}_1, \ldots, \hat{X}_N\}$ such that:

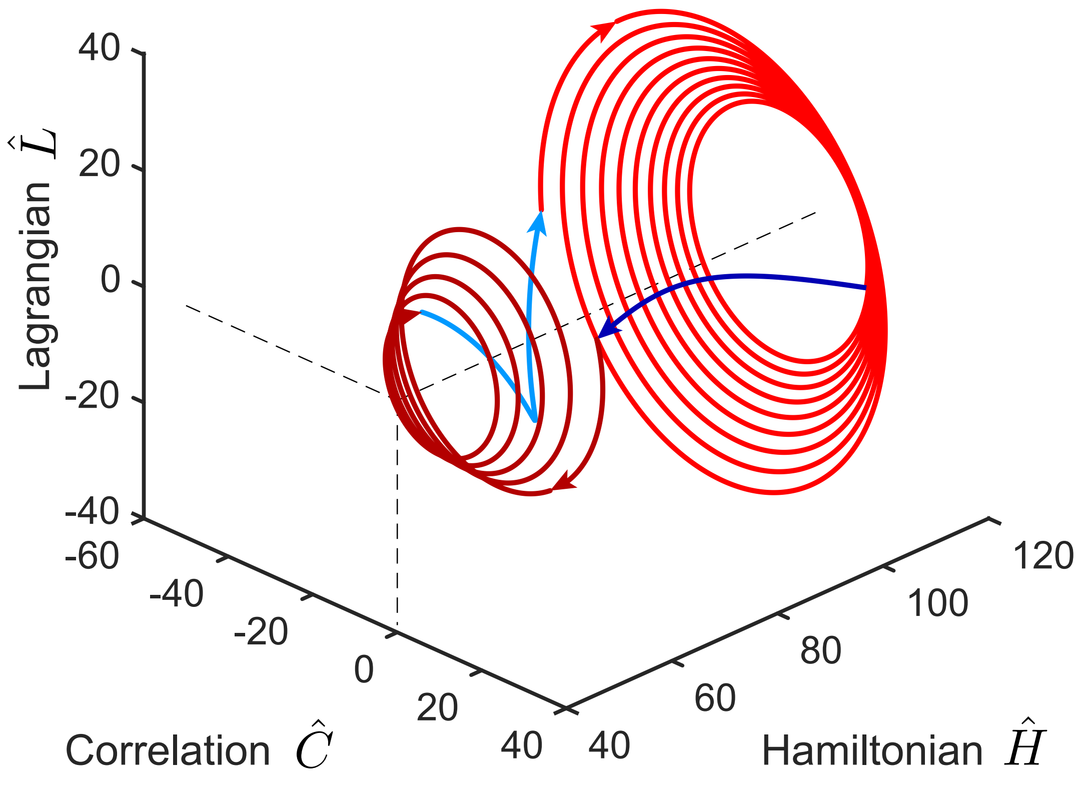
$$\frac{d}{dt}\begin{pmatrix}\hat{X}_1 \\ \vdots \\ \hat{X}_N\end{pmatrix} = \begin{pmatrix} A_{11} & \ldots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \ldots & A_{NN}\end{pmatrix}\begin{pmatrix}\hat{X}_1 \\ \vdots \\ \hat{X}_N\end{pmatrix}$$

The formal solution is:

$$\begin{pmatrix}\hat{X}_1 \\ \vdots \\ \hat{X}_N\end{pmatrix}(t) = \begin{pmatrix} U_{11} & \ldots & U_{1N} \\ \vdots & \ddots & \vdots \\ U_{N1} & \ldots & U_{NN}\end{pmatrix}\begin{pmatrix}\hat{X}_1 \\ \vdots \\ \hat{X}_N\end{pmatrix}(t=0)$$

The time-evolution matrix $\boldsymbol{U}(t)$ satisfies: $\frac{d}{dt}\boldsymbol{U}(t) = \boldsymbol{A}(t)\boldsymbol{U}(t), \quad \boldsymbol{U}(t=0) = \mathbf{1}$

Expectation values



The time-evolution equations

Equation of motion in the Heisenberg picture:

$$\frac{d}{dt}\hat{X}(t) = \mathcal{L}_H^*\left(\hat{X}(t)\right) + \mathcal{L}_D^*\left(\hat{X}(t)\right) + \frac{\partial}{\partial t}\hat{X}(t)$$

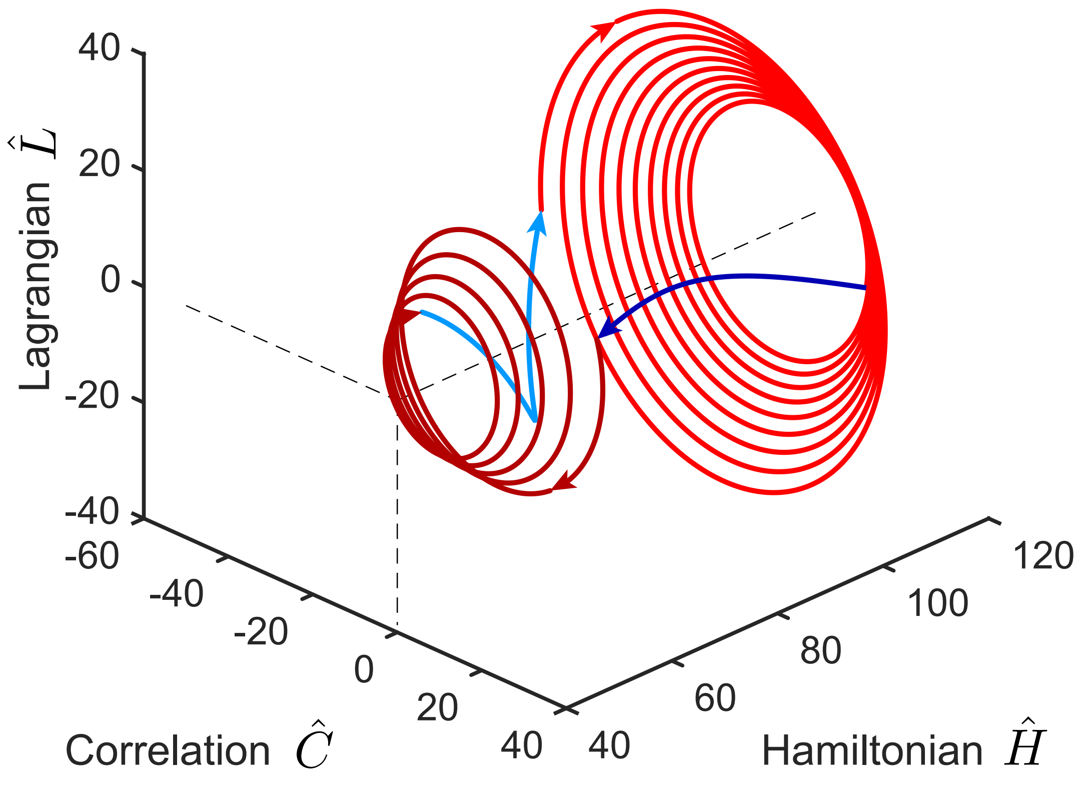
We seek for a set of operators $\{\hat{X}_1, \ldots, \hat{X}_N\}$ such that:

$$\frac{d}{dt}\begin{pmatrix} \hat{X}_1 \\ \vdots \\ \hat{X}_N \end{pmatrix} = \begin{pmatrix} A_{11} & \ldots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \ldots & A_{NN} \end{pmatrix} \begin{pmatrix} \hat{X}_1 \\ \vdots \\ \hat{X}_N \end{pmatrix}$$

In our case, we have the following structure:

$$\left(\begin{array}{c} \hat{H} \\ \hat{L} \\ \hat{C} \\ \hline \hat{1} \end{array}\right)(t) = \left(\begin{array}{ccc|c} & \tilde{\boldsymbol{U}} & & \underline{\tilde{B}} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \left(\begin{array}{c} \hat{H} \\ \hat{L} \\ \hat{C} \\ \hline \hat{1} \end{array}\right)(t=0)$$

Expectation values



Analogy with homogeneous coordinates

In the 3-dimensional space $(\hat{H}, \hat{L}, \hat{C})$:

- the vector $\underline{\tilde{B}}$ corresponds to a translation.
- the 3x3 matrix block $\tilde{\boldsymbol{U}}$ is the linear part.

$$\begin{pmatrix} \hat{H} \\ \hat{L} \\ \hat{C} \end{pmatrix}(t) = \begin{pmatrix} & \tilde{\boldsymbol{U}} & \end{pmatrix} \begin{pmatrix} \hat{H} \\ \hat{L} \\ \hat{C} \end{pmatrix}(0) + \begin{pmatrix} \underline{\tilde{C}} \end{pmatrix}$$

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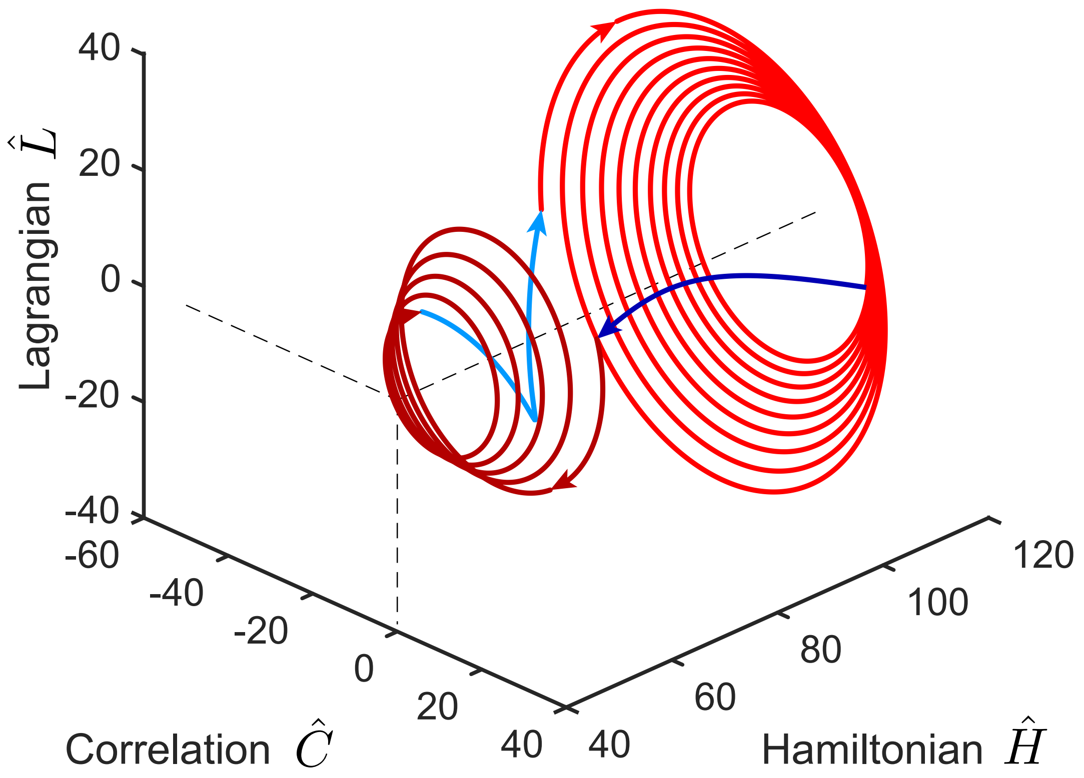

The limit cycle

For the 3-entries vector $\underline{\tilde{X}} = (\hat{H}, \hat{L}, \hat{C})^T$

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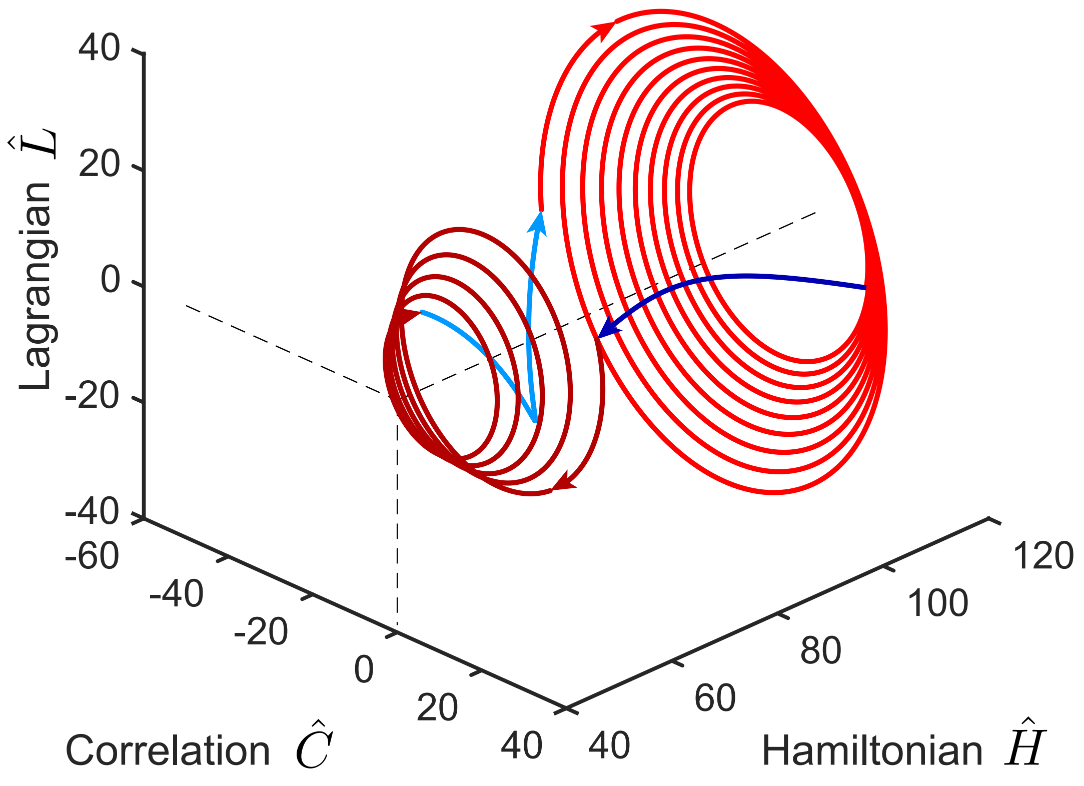
For a full cycle: $t = \tau$

For the 4-entries vector $\underline{X} = (\hat{H}, \hat{L}, \hat{C}, \hat{1})^T$ the limit cycle condition is:

$$\boldsymbol{U}(\tau)\underline{X}^0 = \underline{X}^0$$

Expectation values



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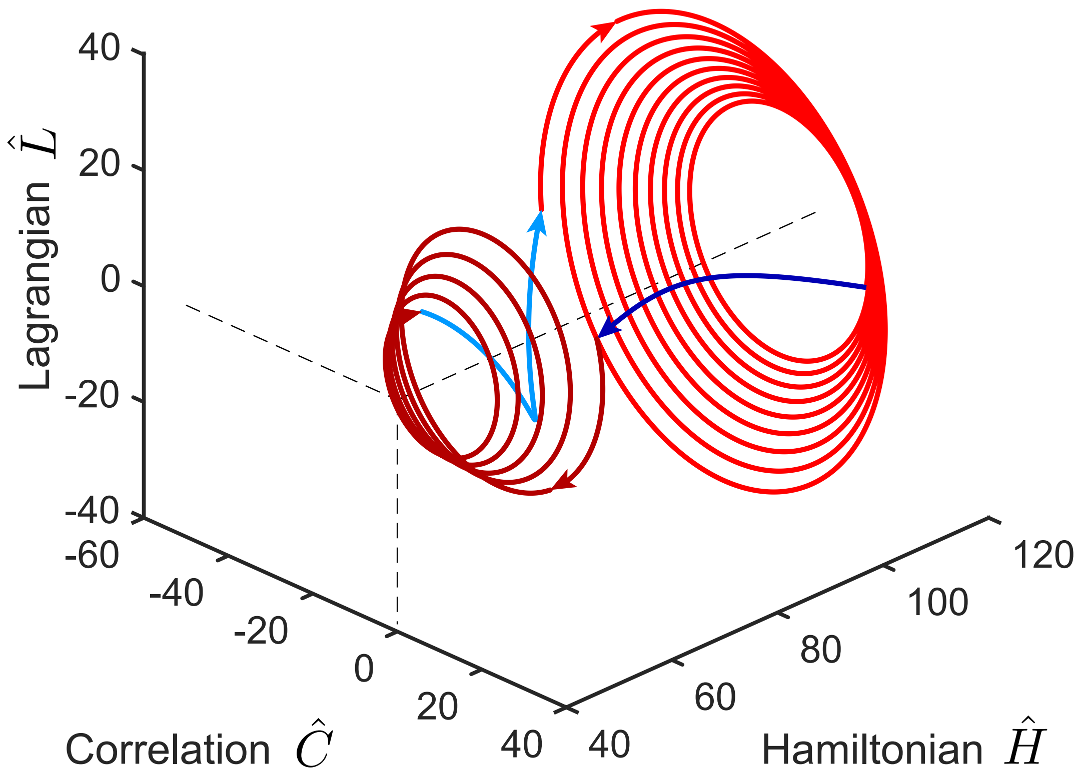
Expectation values



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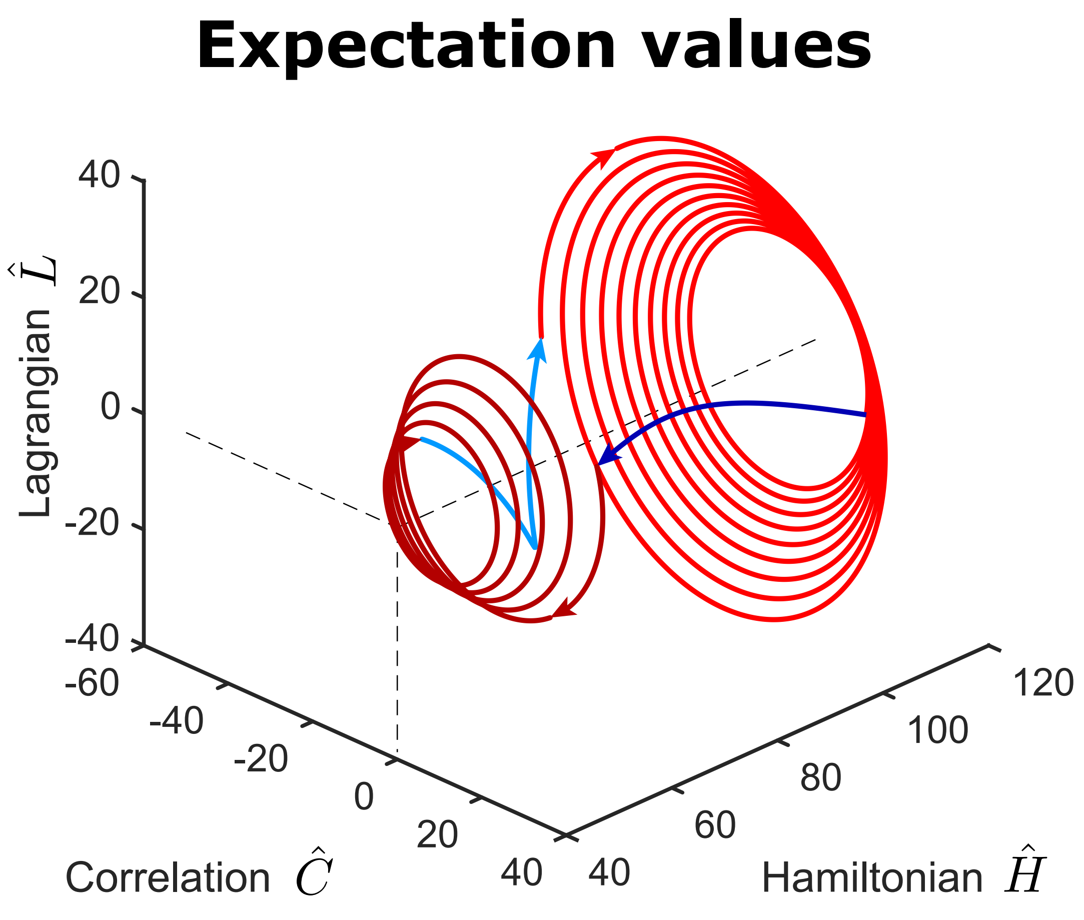

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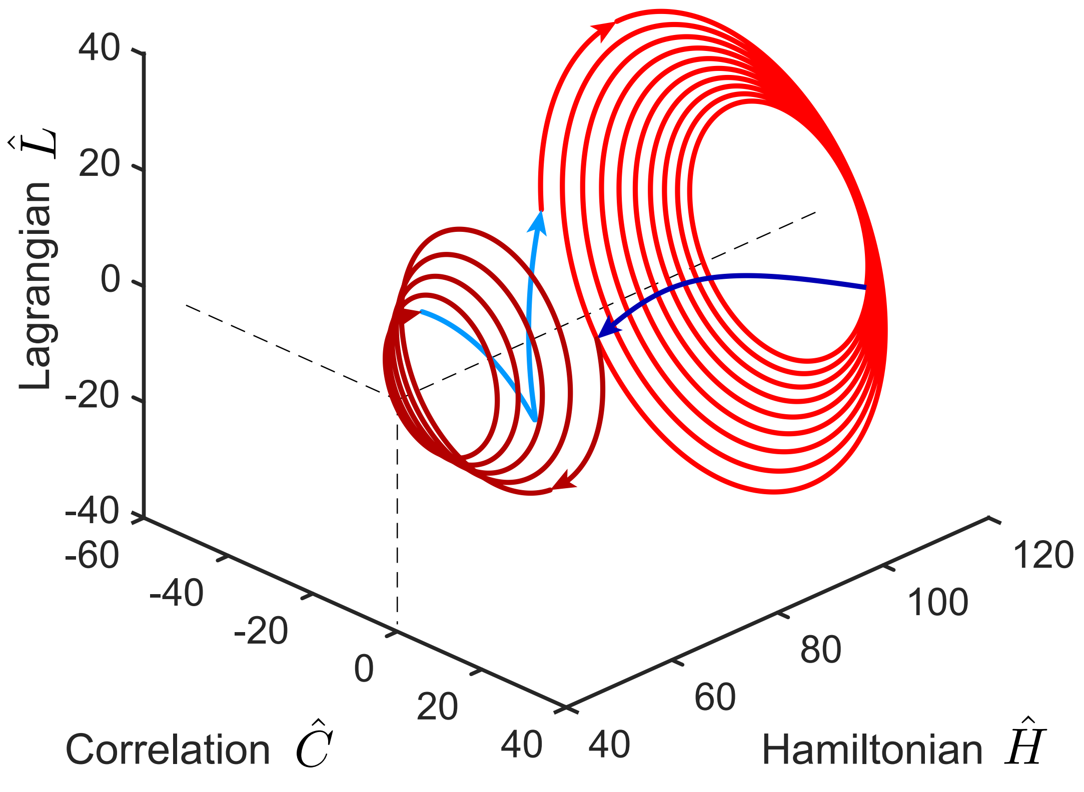
The limit cycle

Expectation values



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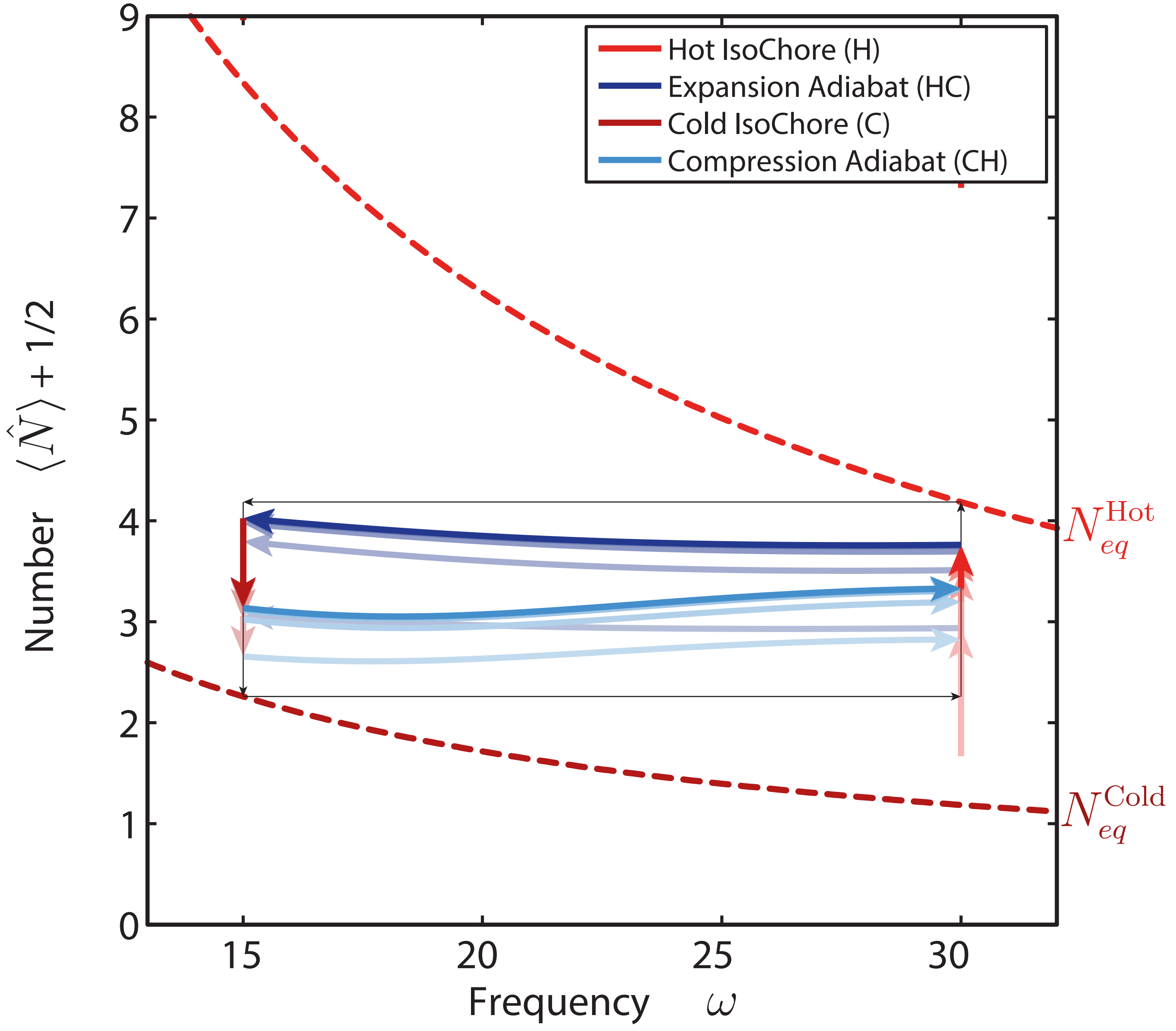
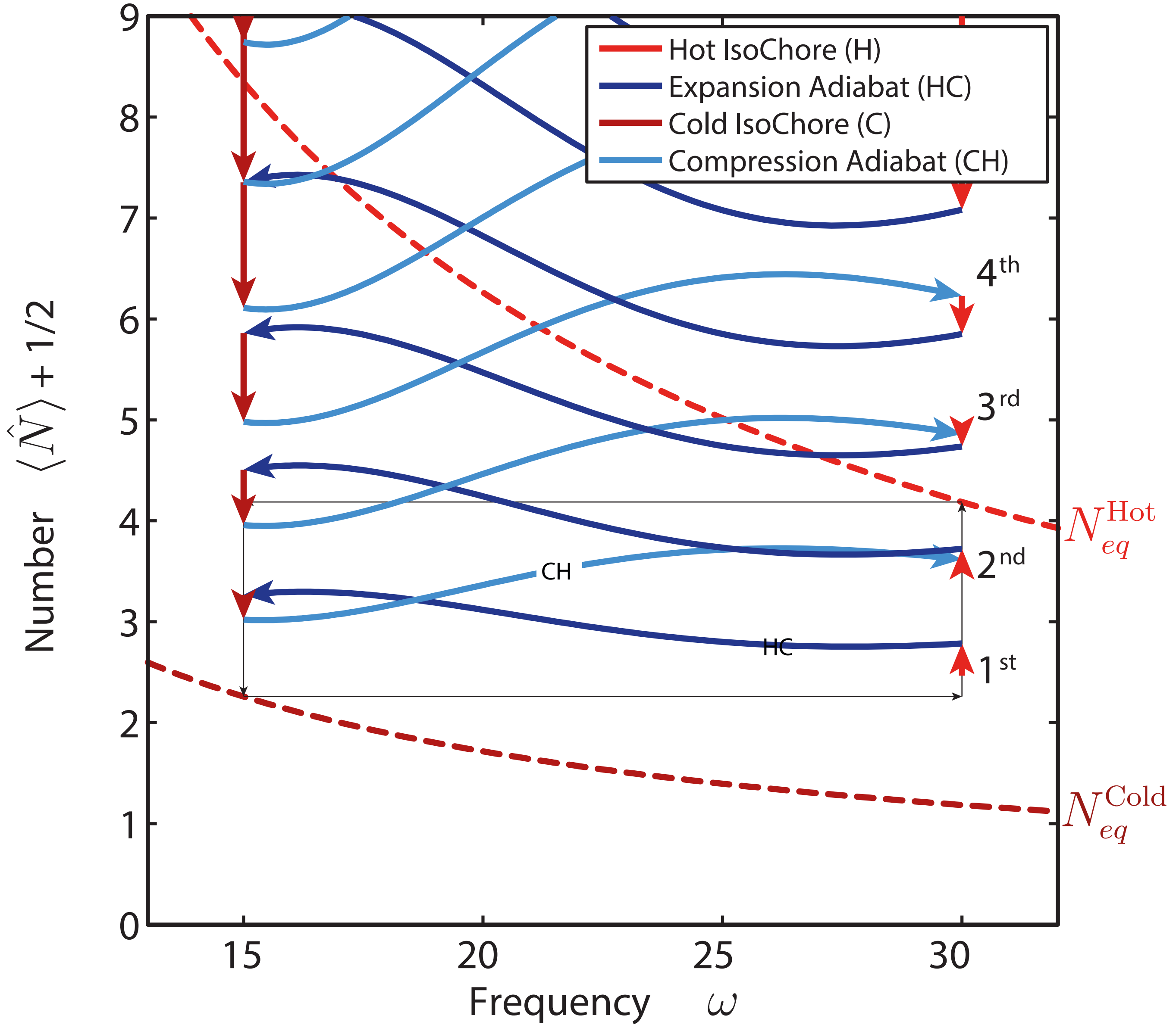
The eigenvalues of $\tilde{\boldsymbol{U}}(\tau)$ determines the stability of the limit cycle: convergent or divergent

Stability of the limit cycle





All eigenvalues of $\tilde{U}(\tau)$ have modulus strictly smaller than 1: **convergence**

At least one eigenvalue has modulus greater than /equal to 1: **divergence**

Stability of the limit cycle

An attractive (convergent) limit cycle exists if and only if all the 3 eigenvalues of $\tilde{\boldsymbol{U}}(\tau)$ have modulus strictly smaller than 1.

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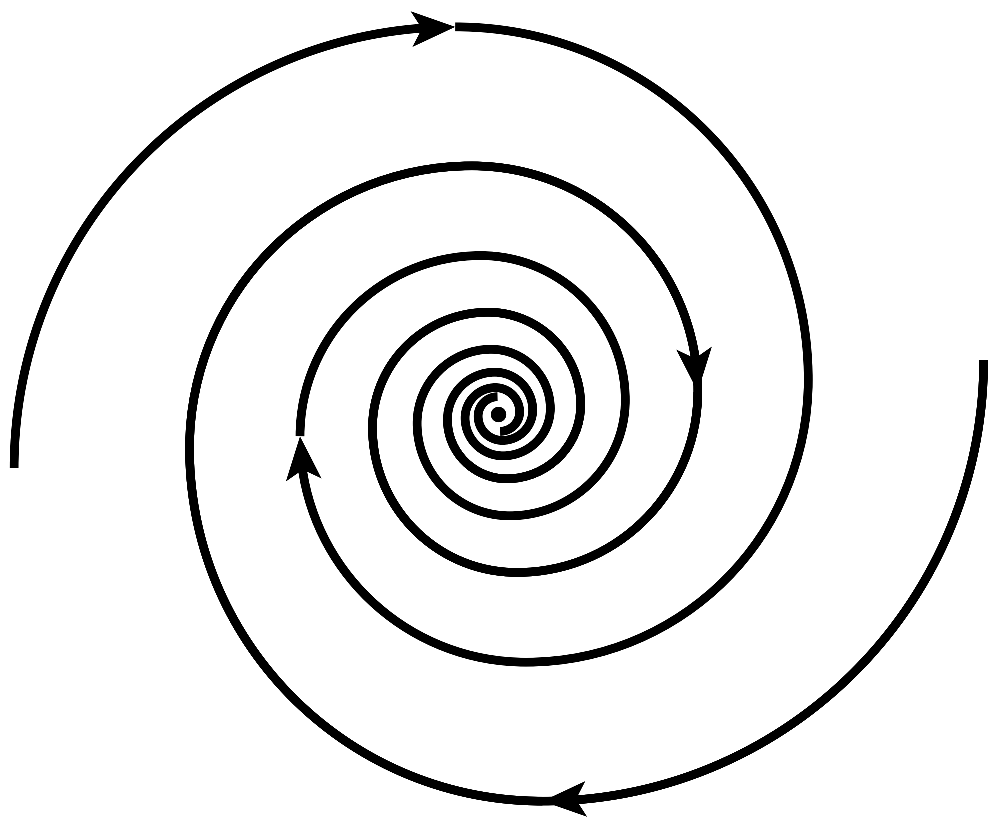
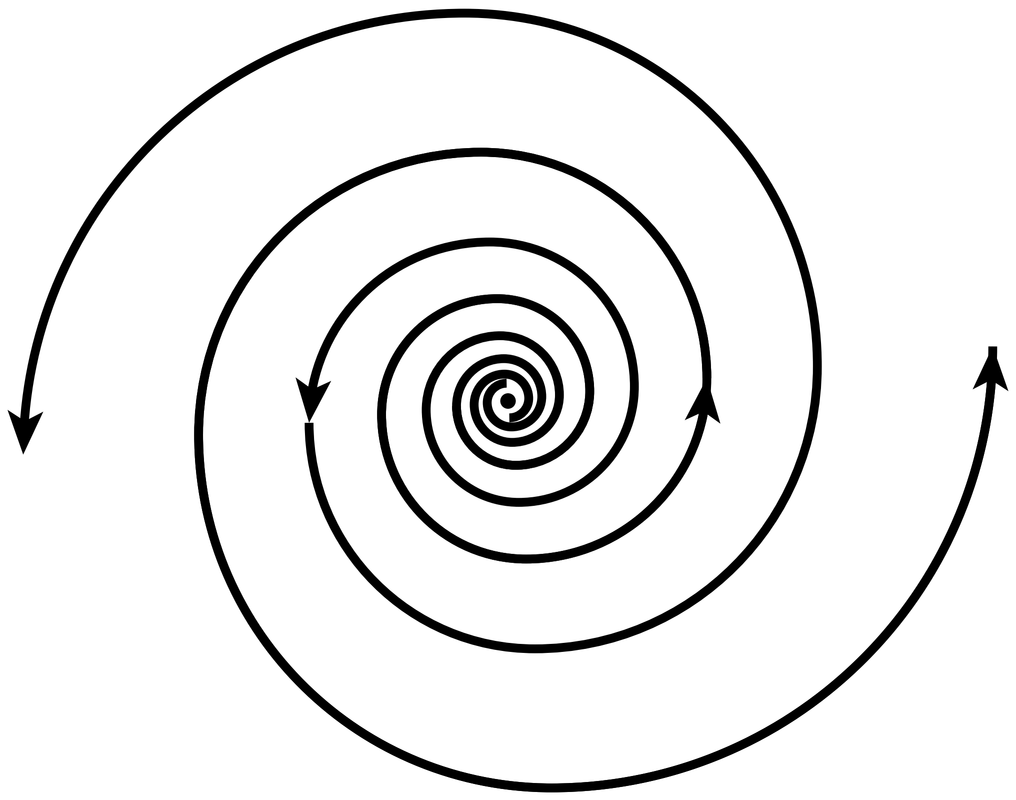
Analogous to the stability of equilibrium points for linear dynamical systems:

Stable equilibrium



Unstable equilibrium



The eigenvalues of U

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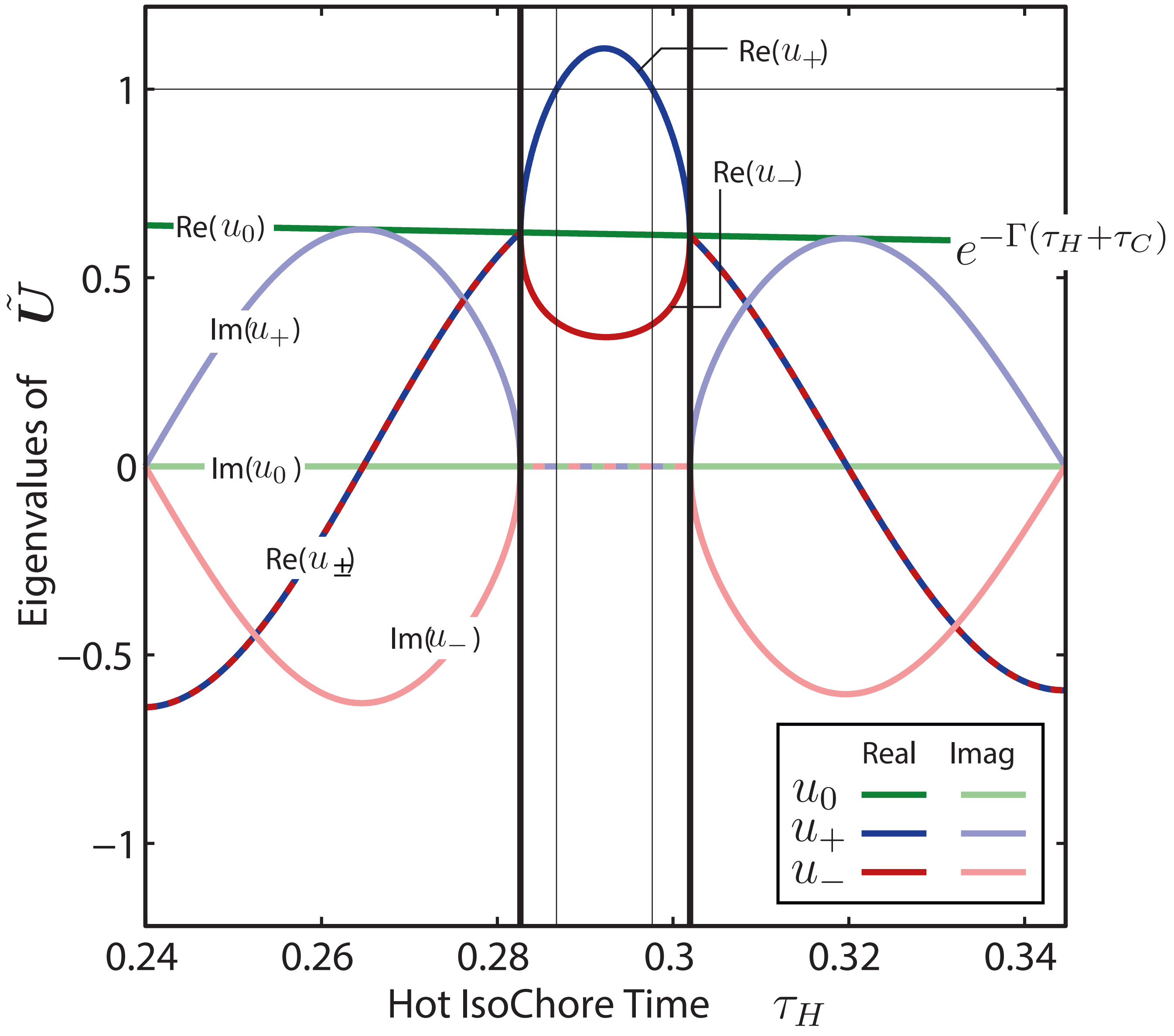

Time allocated for the steps: $\tau_H, \tau_{HC}, \tau_C, \tau_{CH}$

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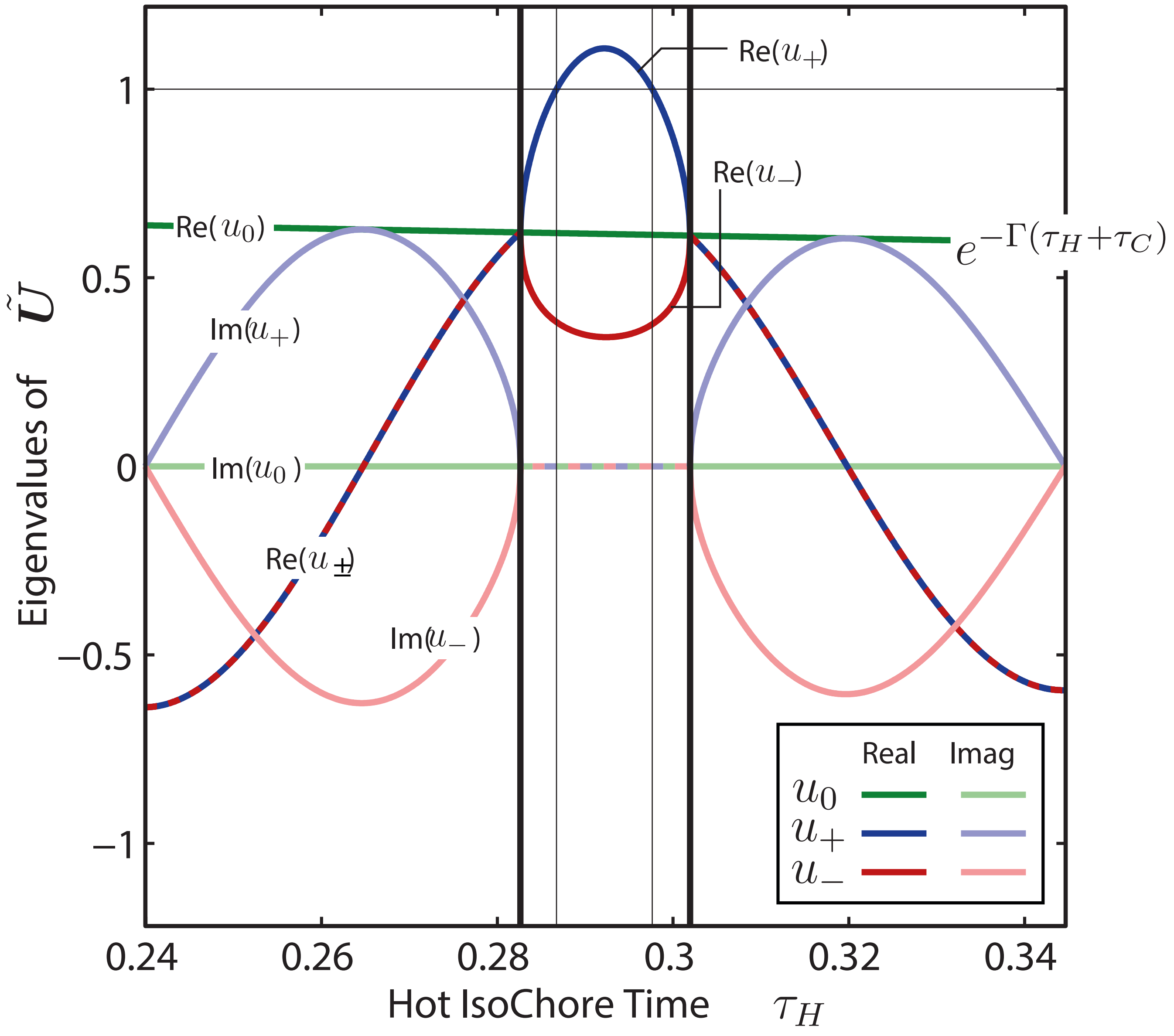

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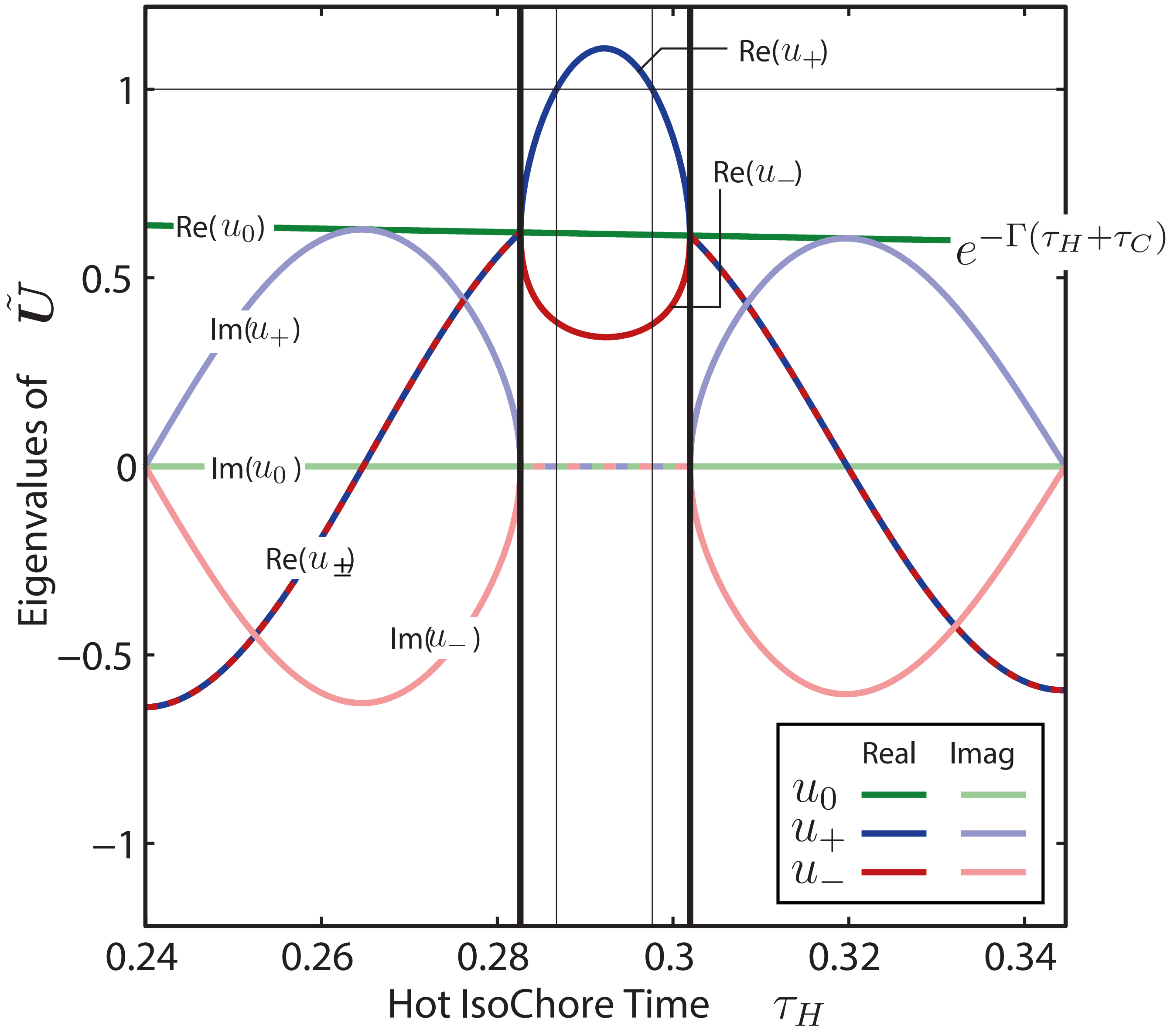

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Here Γ is the heat conductance.

We need to study $\mathcal{L}_H^*$.

If we neglect the scaling $e^{-\Gamma(\tau_H+\tau_C)}$, then the cycle converges as long as the eigen-values have modulus equal to 1.

If the matrix $\tilde{U}$ generated by $\mathcal{L}_H^*$ is orthogonal, the moduli of the eigenvalues are equal to 1.

The eigenvalues of U

An attractive (convergent) limit cycle exists if and only if all the 3 eigenvalues of $\tilde{U}(\tau)$ have modulus strictly smaller than 1.

But *why* does it happen?

The eigenvalues of U

An attractive (convergent) limit cycle exists if and only if all the 3 eigenvalues of $\tilde{\boldsymbol{U}}(\tau)$ have modulus strictly smaller than 1.

But *why* does it happen?

In the present case of a harmonic oscillator the condition that $\mathcal{L}$ is bounded cannot hold. We will assume this form for the generator with $\hat{H}$ and $\hat{F}_i$ unbounded as the simplest way to construct an appropriate model - Lindblad

(here $\hat{F}_i$ denote the Lindblad operators, i.e. $\hat{a}^\dagger$ and $\hat{a}$, in our case).

The phenomenon is linked to the properties of the underlying Lie algebra of operators.

Dynamical matrix and structure constant

The Lie algebra is defined by:

$$\left[i\hat{X}_h, i\hat{X}_k\right] = i\sum_k \Gamma_{hjk}\hat{X}_k, \quad \Gamma_{hjk} \in \mathbb{R}$$

Equation of motion:

$$\frac{d}{dt}\underline{\hat{X}} = +\frac{i}{\hbar}\left[\hat{H}, \underline{\hat{X}}\right] \quad \text{with} \quad \hat{H} = \sum_k c_k \hat{X}_k, \quad c_k \in \mathbb{R}$$

It can be written as:

$$\frac{d}{dt}\underline{\hat{X}} = \boldsymbol{A}\underline{\hat{X}} \quad \text{with} \quad a_{jk} = \frac{1}{\hbar}\sum_h c_h \Gamma_{hjk}$$

The structure constant Γ_{hjk} is always antisymmetric w.r.t. an exchange of the first 2 indexes.

If it is invariant under cyclic permutation, then it is also antisymmetric w.r.t. exchange of the last 2 indexes.

When this happens, the dynamical matrix $\boldsymbol{A}$ is skew symmetric.

Dynamical matrix and limit cycle

The time-evolution operator obeys:

$$\frac{d}{dt}\boldsymbol{U}(t) = \boldsymbol{A}(t)\boldsymbol{U}(t), \quad \boldsymbol{U}(t=0) = \mathbf{1}$$

The formal solution is:

$\boldsymbol{U}(t) = \exp\left(\boldsymbol{\Omega}(t)\right)$ with $\boldsymbol{\Omega}(t)$ from Magnus expansion (nested $\boldsymbol{A}(t)$ commutators)

If $\boldsymbol{A}(t)$ is skew-symmetric, so is $\boldsymbol{\Omega}$.

If $\boldsymbol{\Omega}$ is skew-symmetric, $\boldsymbol{U}$ is orthogonal.

If $\boldsymbol{U}$ is orthogonal, the moduli of its eigenvalues are equal to 1.

When we consider the scaling $e^{-\Gamma(\tau_H+\tau_C)}$, convergence is guaranteed.

When the dynamical matrix $\boldsymbol{A}(t)$ generated by $\mathcal{L}_H^*$ is skew-symmetric, the existence of a limit cycle is guaranteed.

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The structure constant

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- For a compact semisimple Lie algebra there is always a basis for which the structure constant is invariant under cyclic permutation of the indices.

The adjoint representation consists of the set $\{\mathrm{ad}_{i\hat{X}_h}\}$ of the transformations that performs the commutations:

$$\mathrm{ad}_{i\hat{X}_h}(i\hat{X}) := [i\hat{X}_h, i\hat{X}]$$

For any two elements $X, Y \in \mathrm{span}\left(\{\mathrm{ad}_{i\hat{X}_h}\}\right)$

$$K(X, Y) := \mathrm{Trace}(X \circ Y)$$

- Semisimple Lie Algebra: K is non-degenerate
- Compact Lie Algebra: K is negative semi-definite

- Compact and semisimple: K is negative definite → it can be used as scalar product.

$$\langle X|Y\rangle = -K(X, Y)$$

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We equipped the Lie Algebra with a scalar product

$$\langle X|Y\rangle = -K(X,Y)$$

Now we can construct an ortho-normal basis $\{A_h\}$ for the Lie Algebra:

$$\langle A_i|A_j\rangle = \delta_{ij}$$

In this basis, the structure constant is invariant under cyclic permutation of the indices.

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The spin system

For a compact semisimple Lie algebra the existence of a limit cycle is guaranteed.

The Lie algebra associated to the harmonic oscillator is not:
the killing form is degenerate.

For the "spin system" the Lie algebra generates 3D rotations:

$$\left[\hat{B}_1, \hat{B}_2\right] = +\sqrt{2}i\hat{B}_3$$

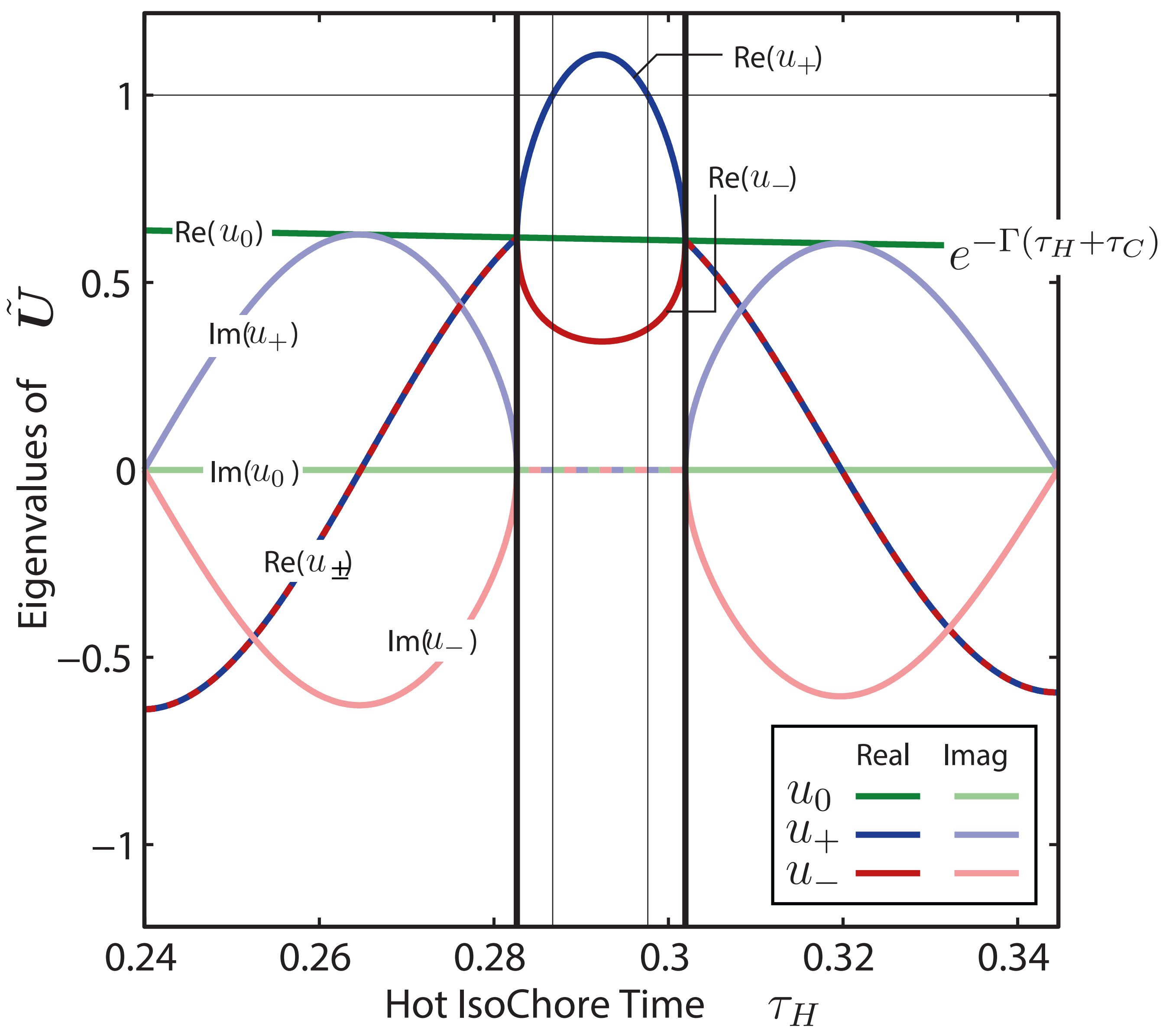
$$\left[\hat{B}_2, \hat{B}_3\right] = +\sqrt{2}i\hat{B}_1$$

$$\left[\hat{B}_3, \hat{B}_1\right] = +\sqrt{2}i\hat{B}_2$$

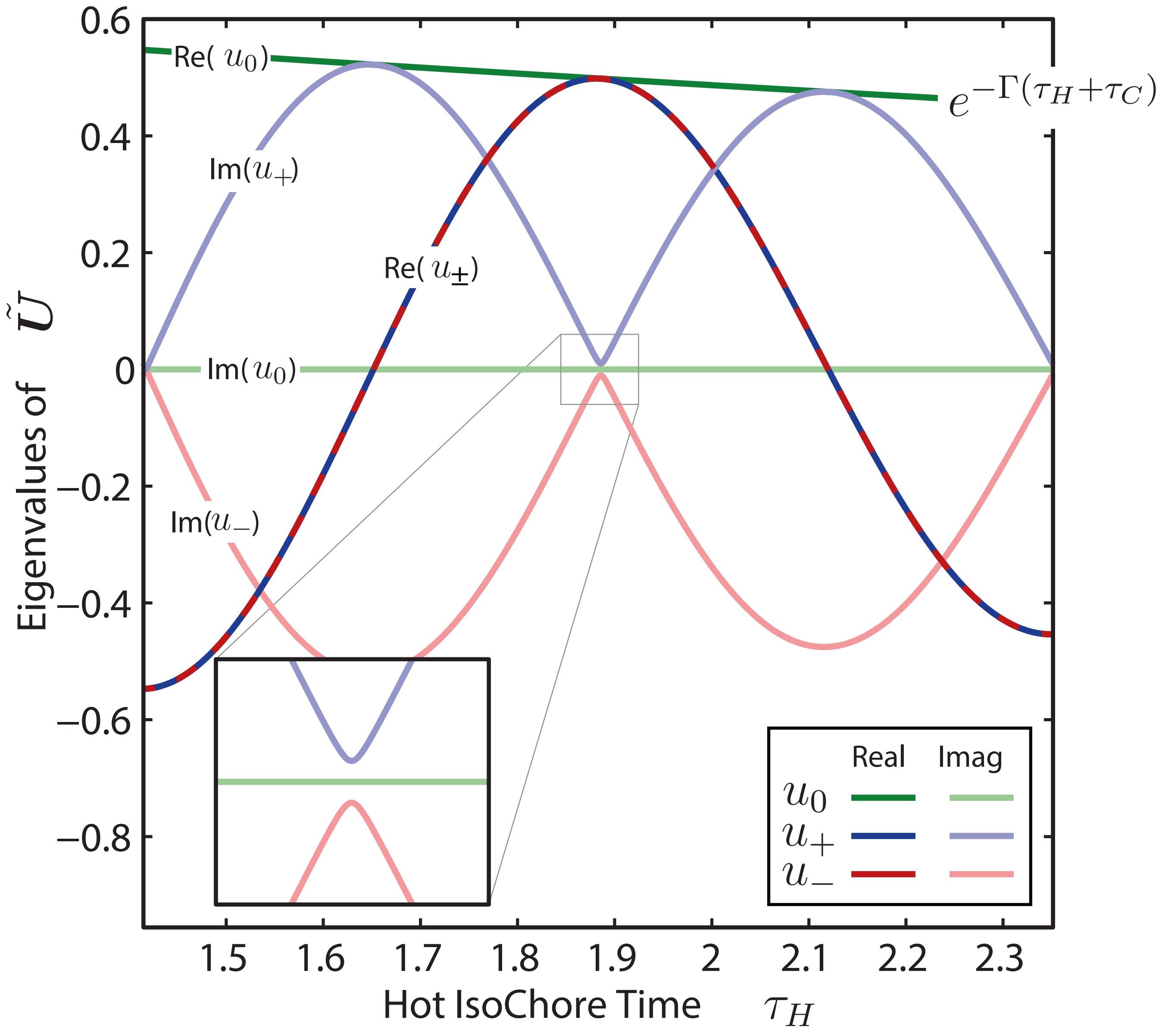
The limit cycle is always stable.

The spin system

Harmonic oscillator



Spin system



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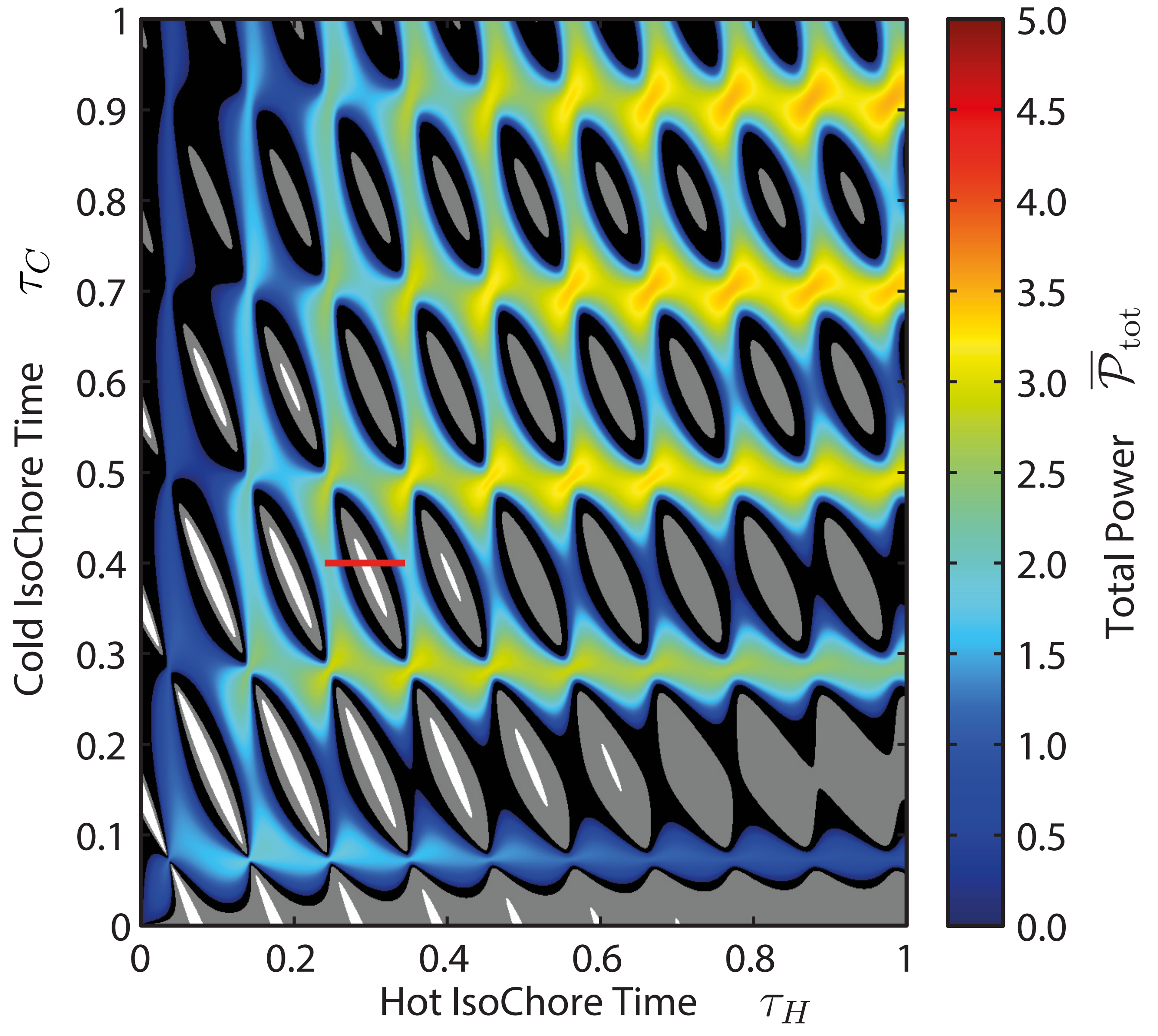

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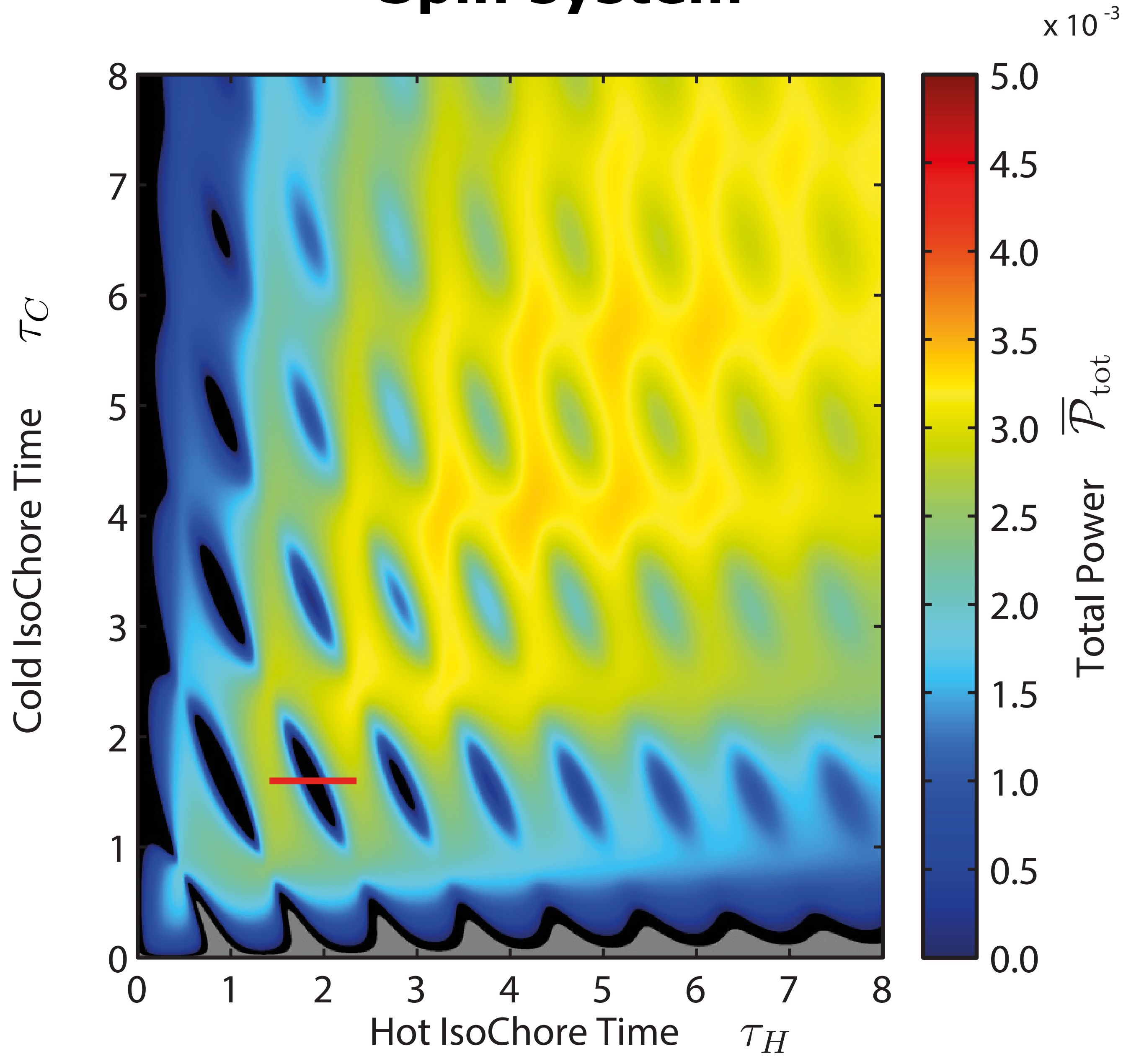
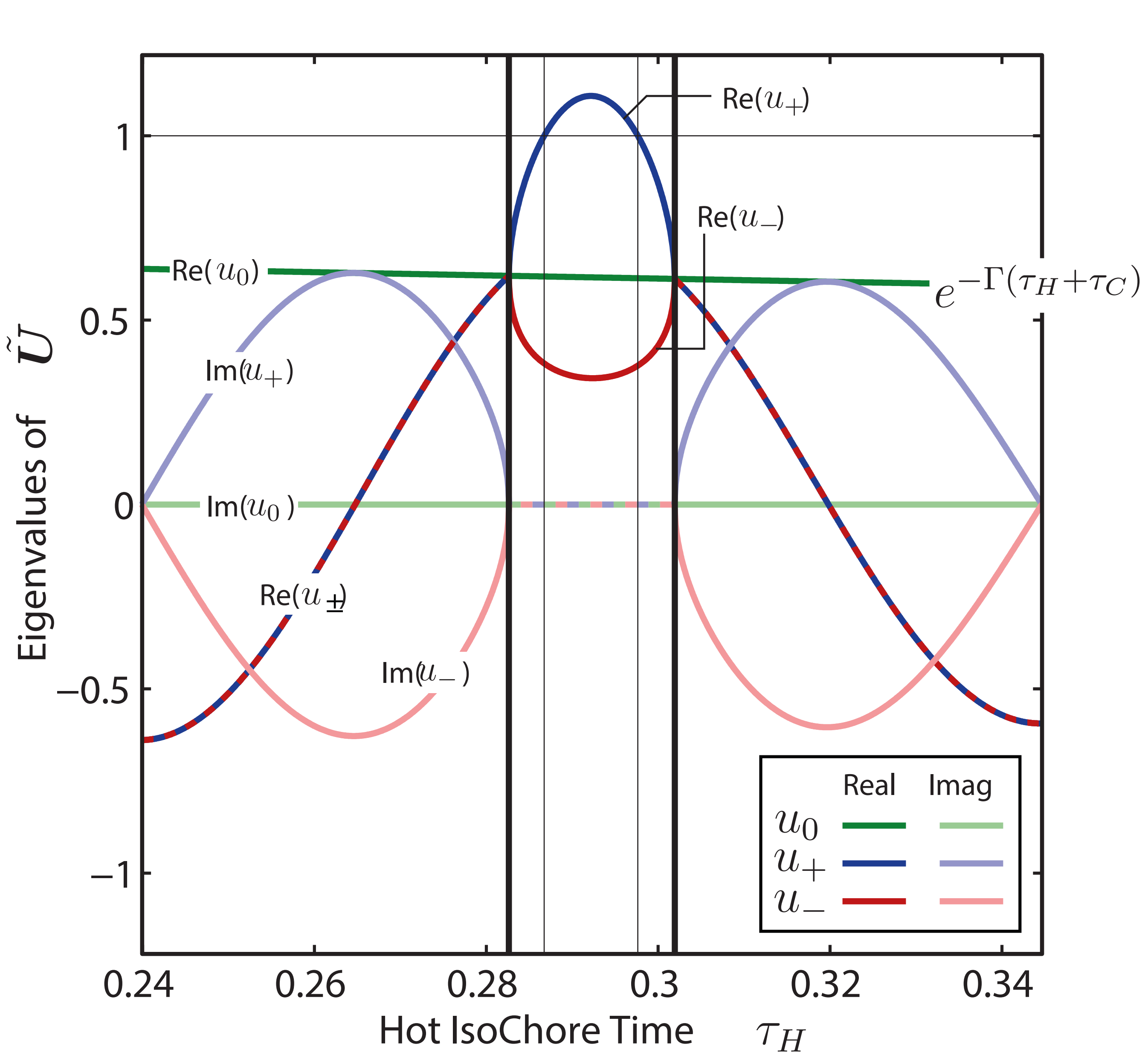
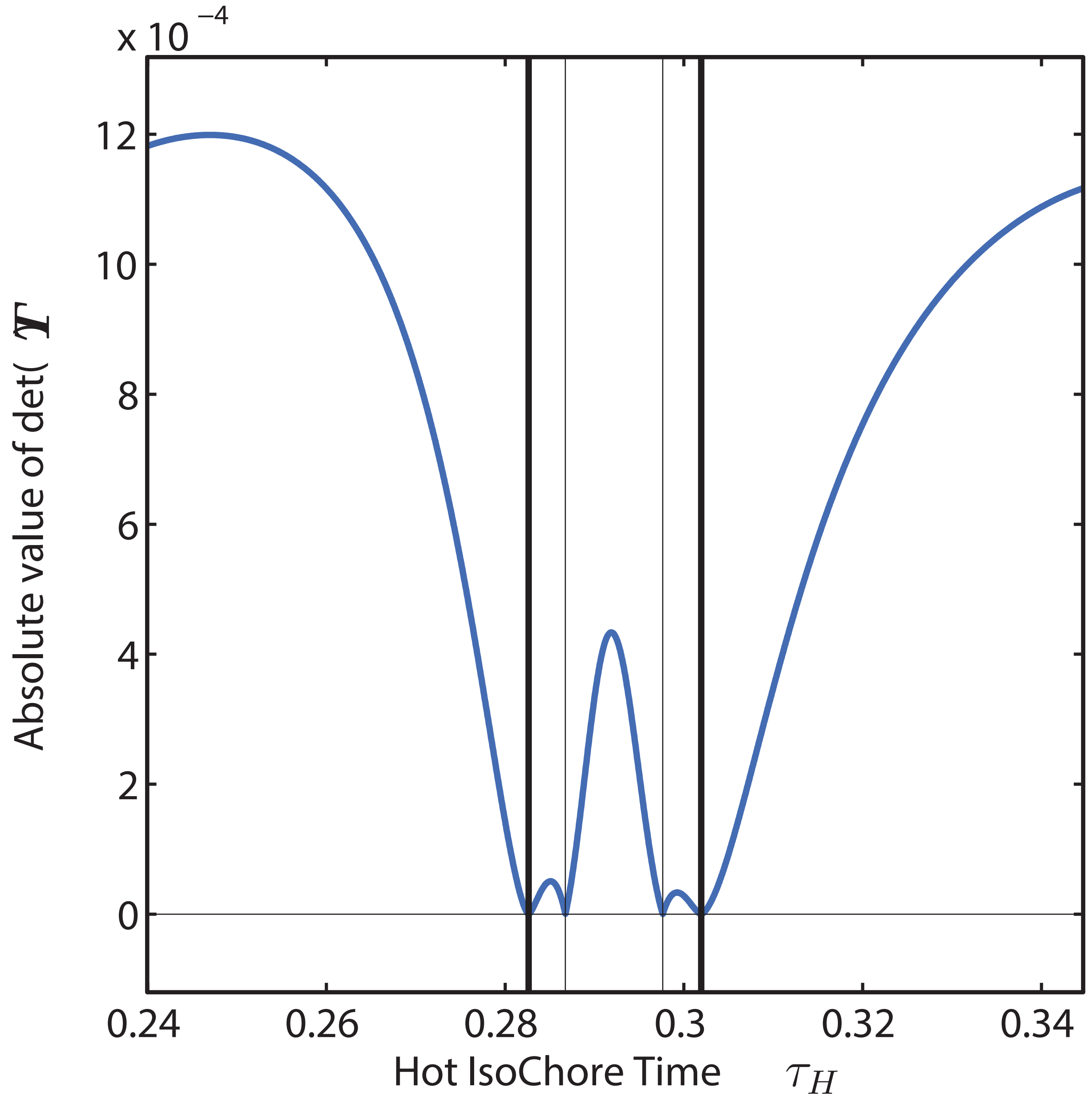


Exceptional points - non-hermitian degeneracy

The eigenvectors coalesce: the dimension of the corresponding eigenspace is defective





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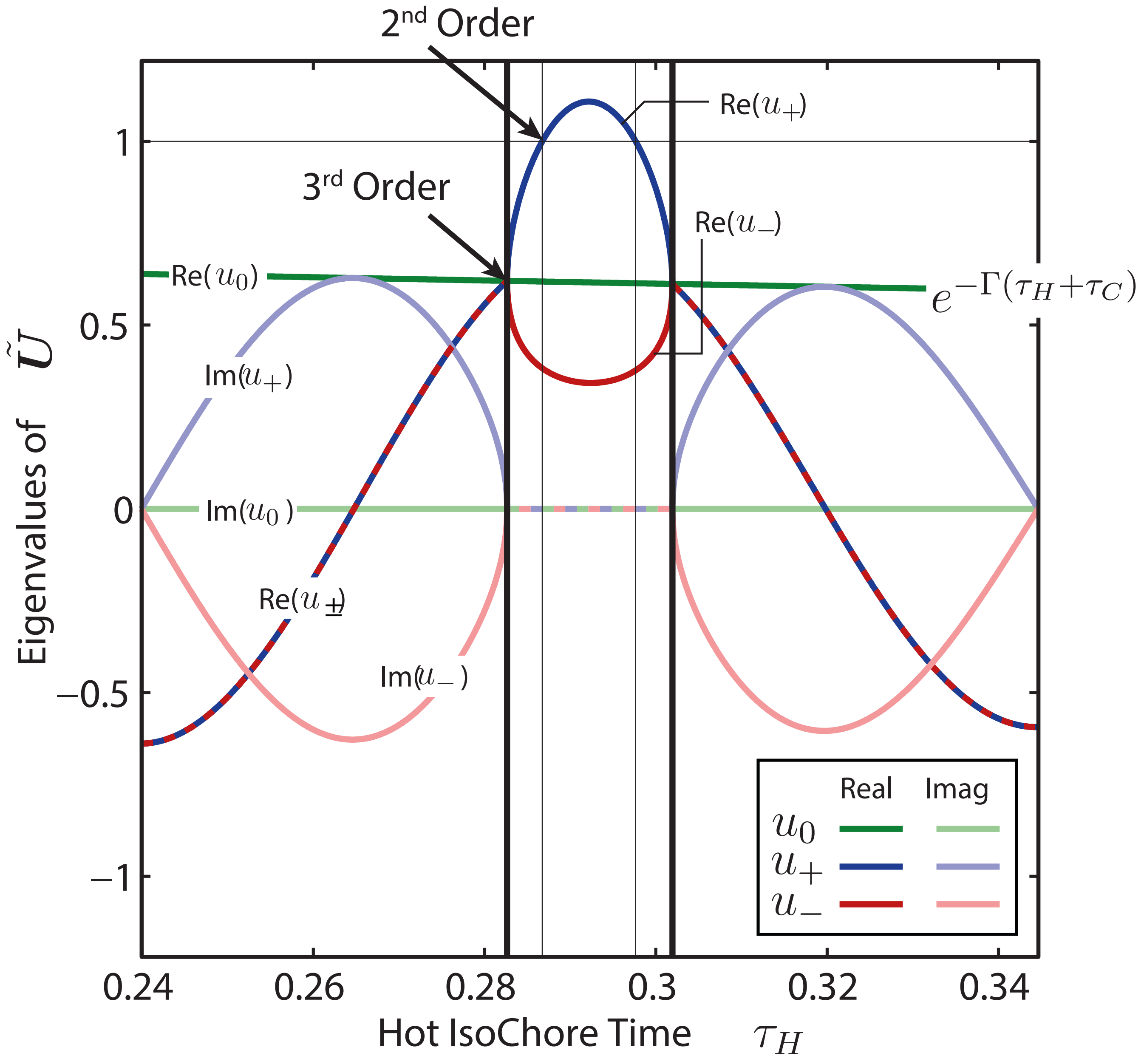
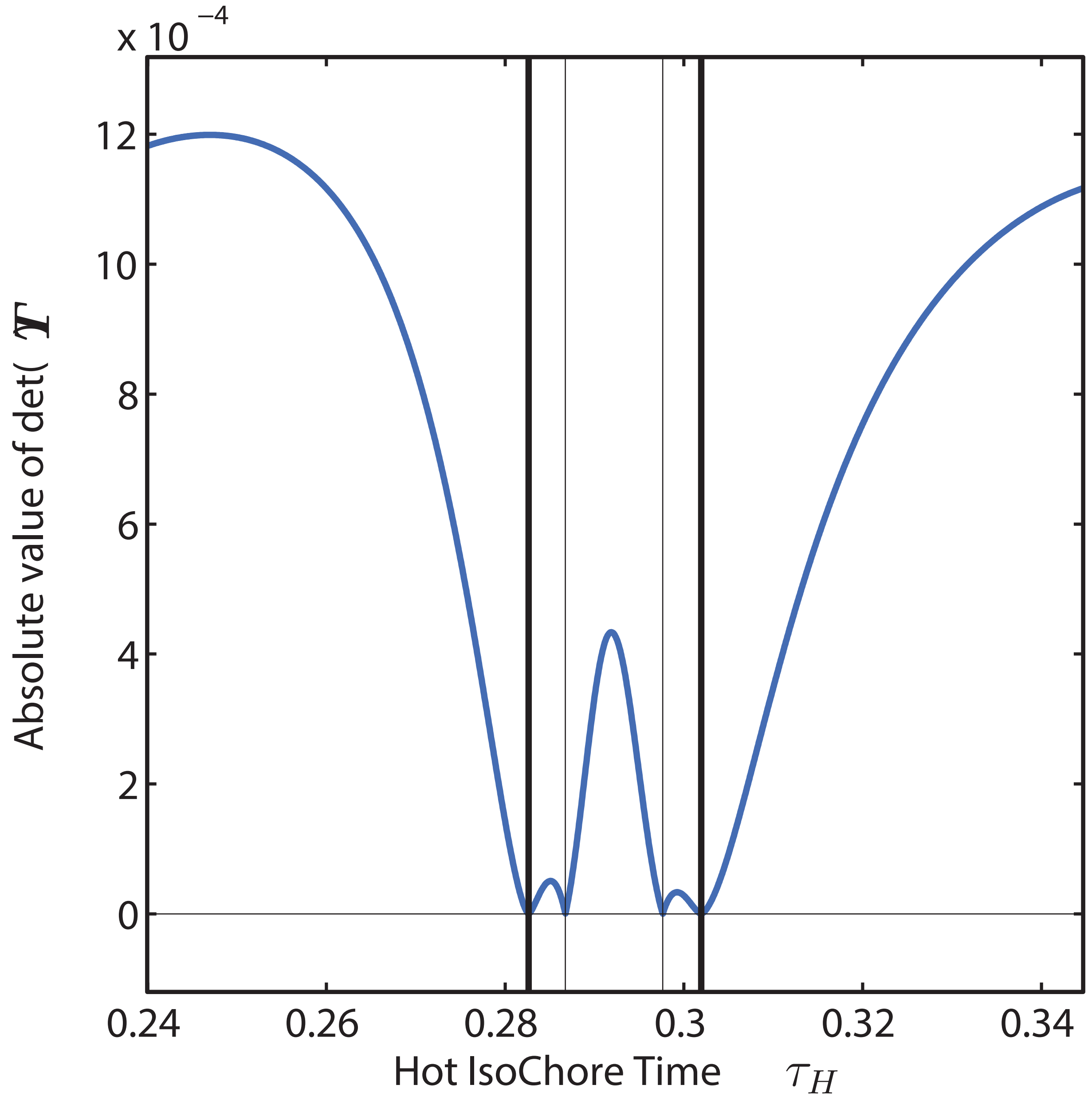
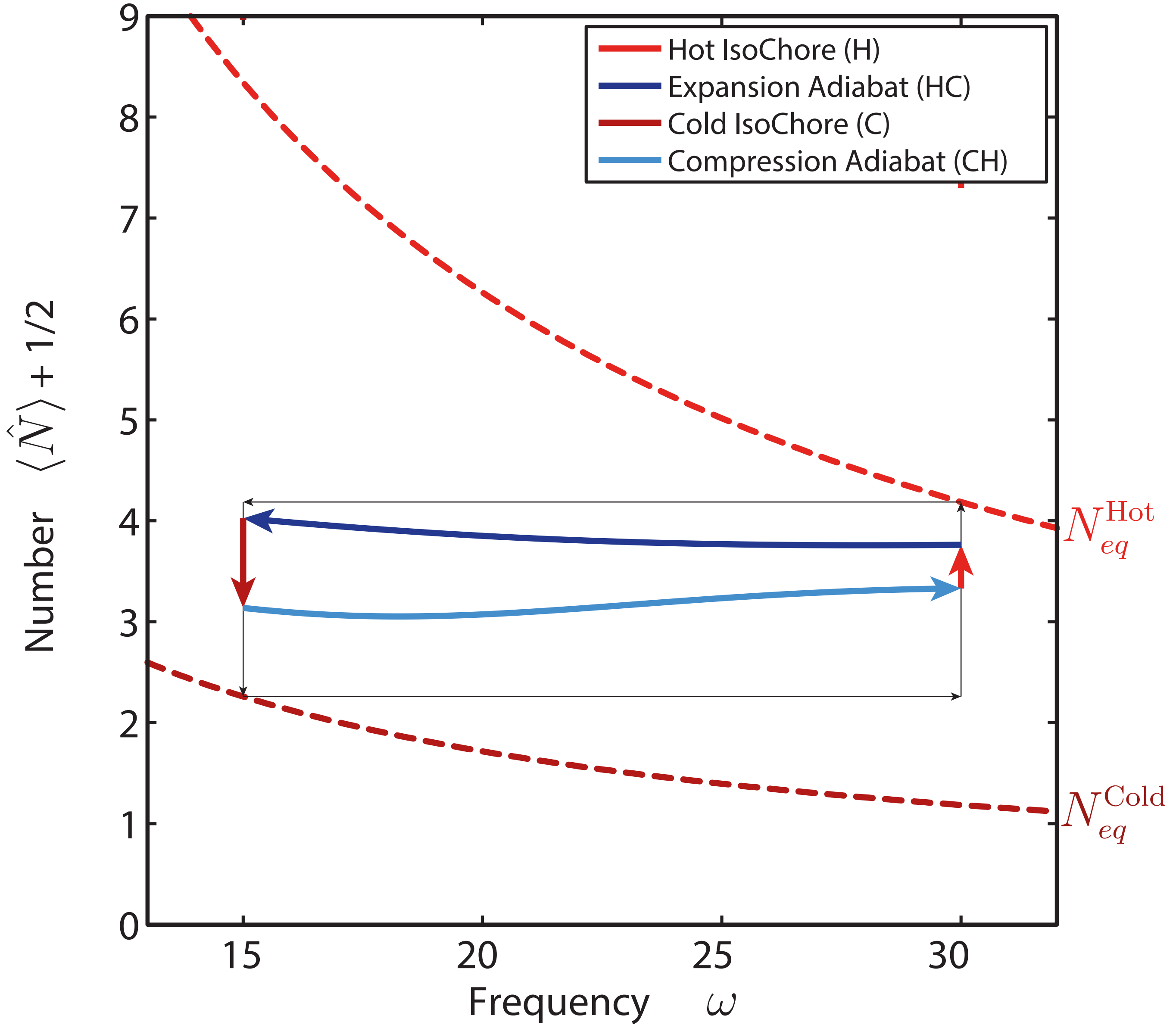




Quantum friction



The power is given by:

$$\mathcal{P}(t) = \frac{d}{dt}\langle \hat{H} \rangle = \frac{d}{dt}\left(\sum_n P_n(t)\varepsilon_n(t)\right)$$

Decomposed into two contributions:

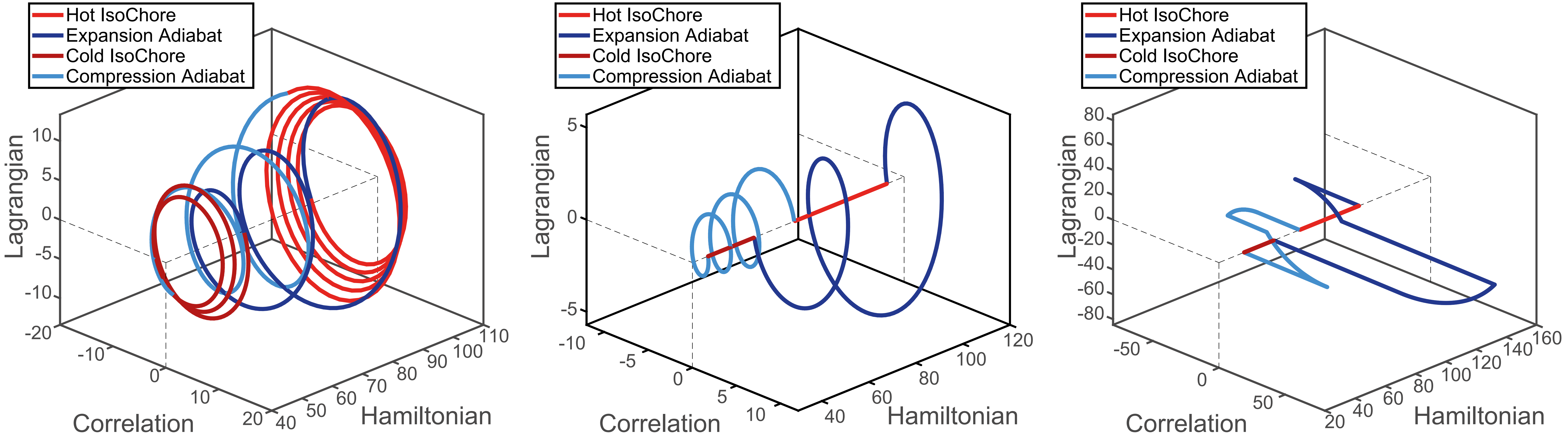
$$\mathcal{P}(t) = \underbrace{\sum_n \dot{P}_n \varepsilon_n}_{\textbf{Frictional}} + \underbrace{\sum_n P_n \dot{\varepsilon}_n}_{\textbf{External}}$$

Quantum friction limits the amount of work.

It is zero in the quasi-static regime.

Can we get rid of it in finite-time?

Quantum friction - frictionless cycles



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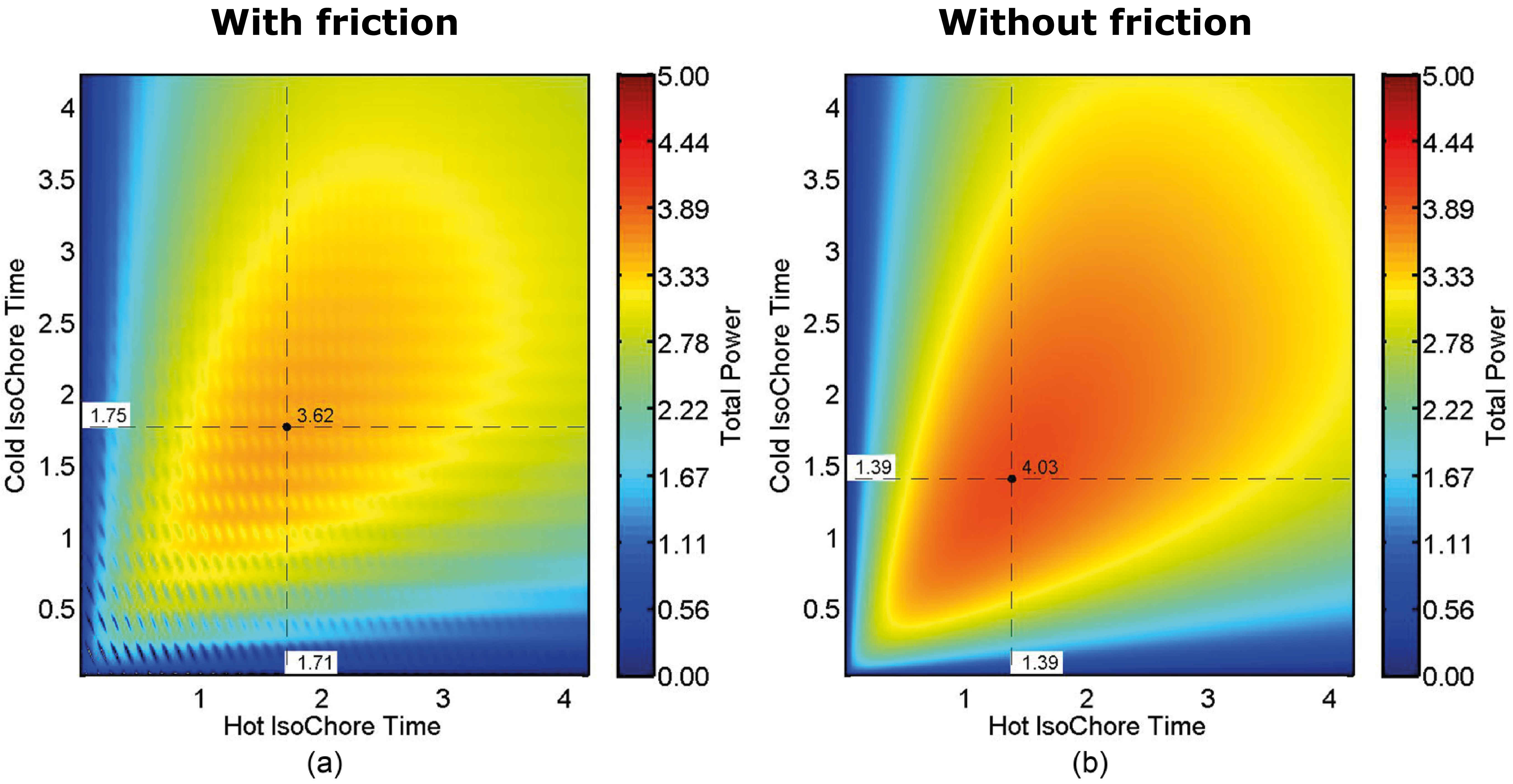

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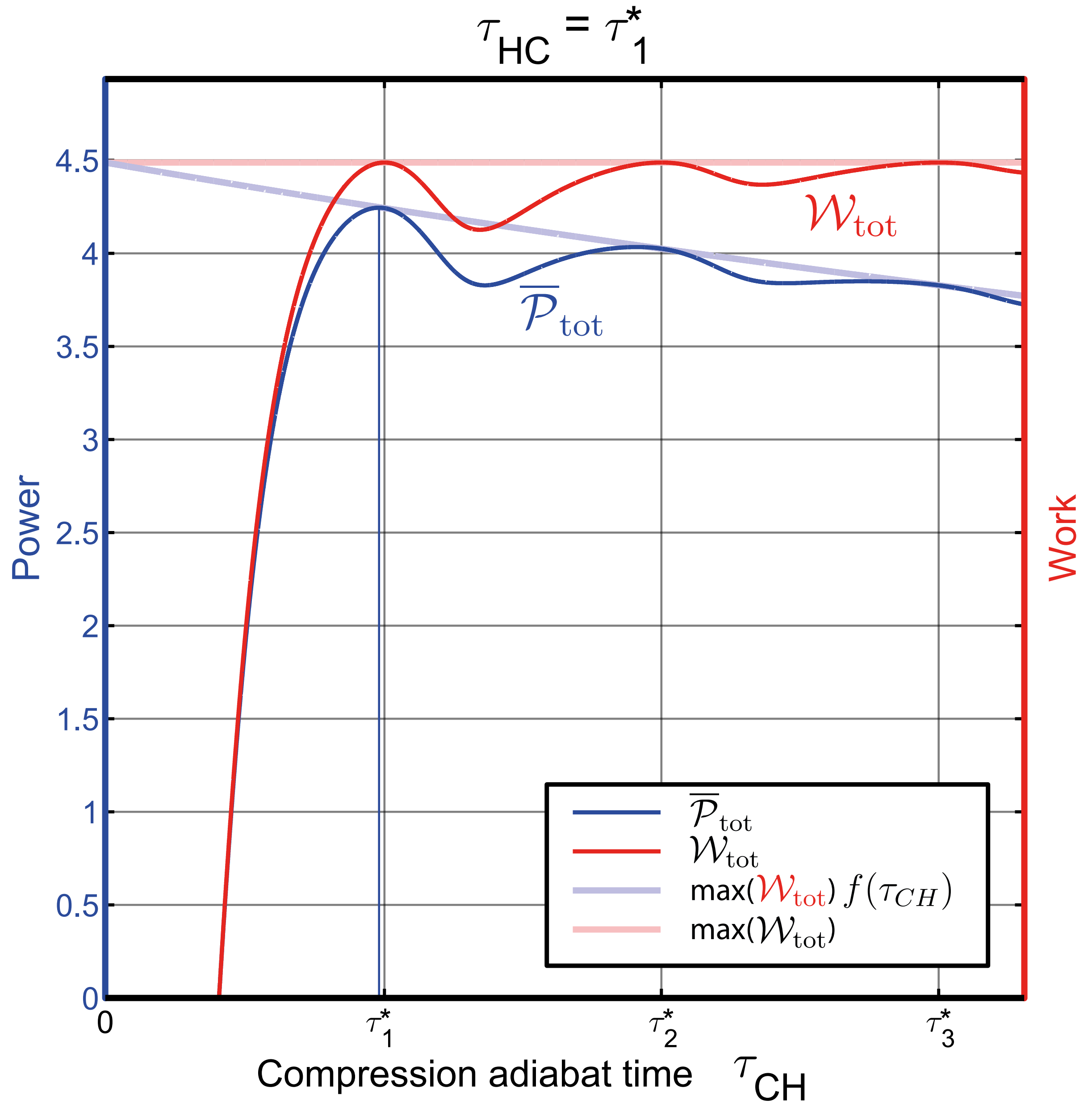
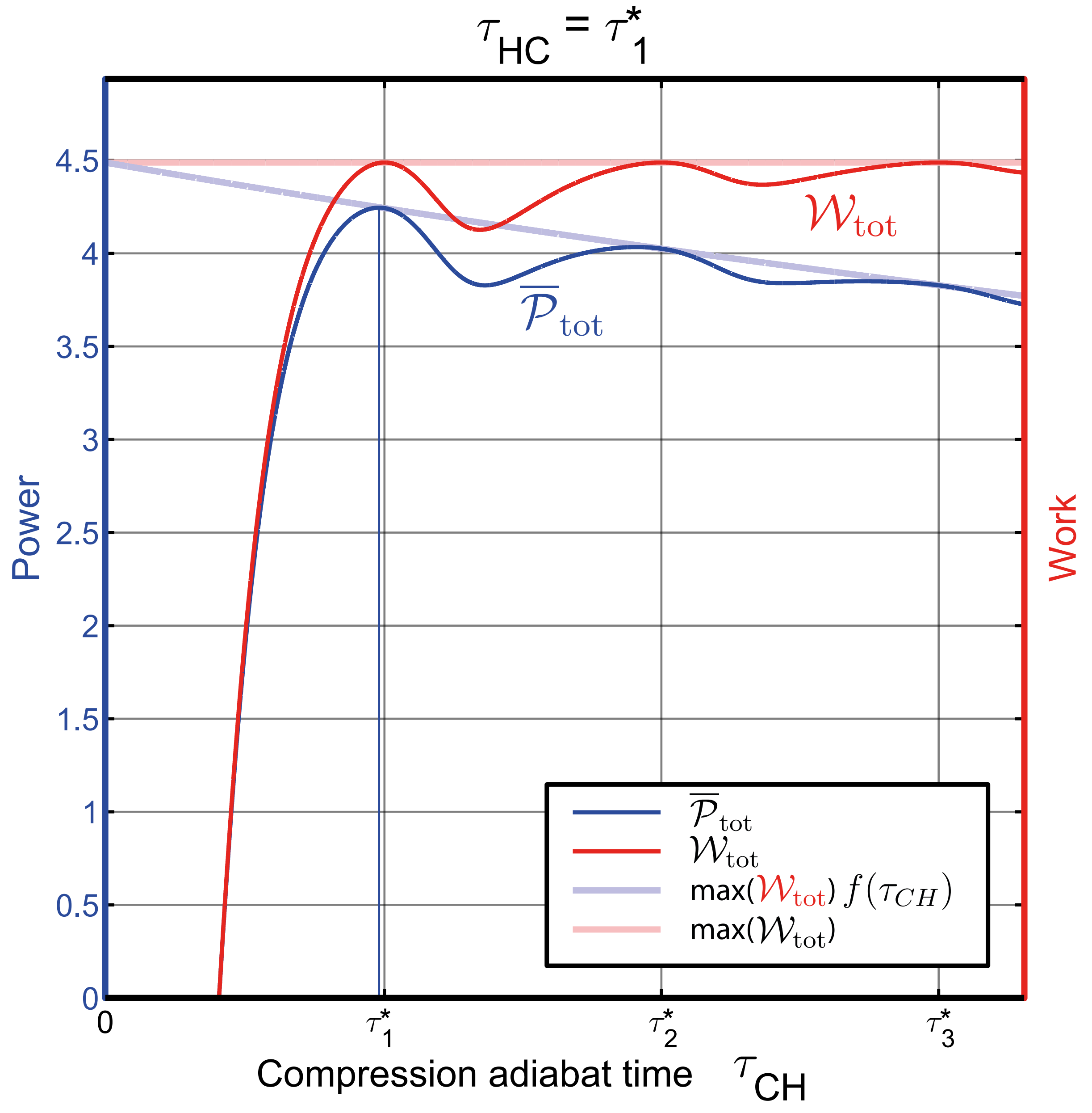


Quantum friction limits the amount of work.

Frictionless cycles give maximum work.

If the goal is maximum power it is still convenient to allow for some friction so that the duration of the cycle is reduced.

Quantum friction - frictionless cycles



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At some point we will get around to publishing the quartic result :)