Memories from the ergodic phase
the awkward dynamics of spherical mixed p-spin models

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in collaboration with
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Some motivations...

- Out of equilibrium processes are everywhere:
  - physics
  - biology
  - ecology
  - economics
  - computer science
  - ...

- Understanding off-equilibrium dynamics:
  - solving with an asymptotic ansatz
  - connecting it to thermodynamical (static) properties

Mean field spin glass models

- SG models with a **continuous** phase transition at T_c (e.g. SK model or Viana-Bray model)

$$H(\underline{\sigma}) = \sum_{(ij)\in E} J_{ij}\sigma_i\sigma_j \qquad \underline{\sigma} \in \{-1,1\}^N$$

Very difficult to study below T_c because ∞ timescales

We have surprising results! ...but not in this talk
Ask at the end if you are curious ;-)

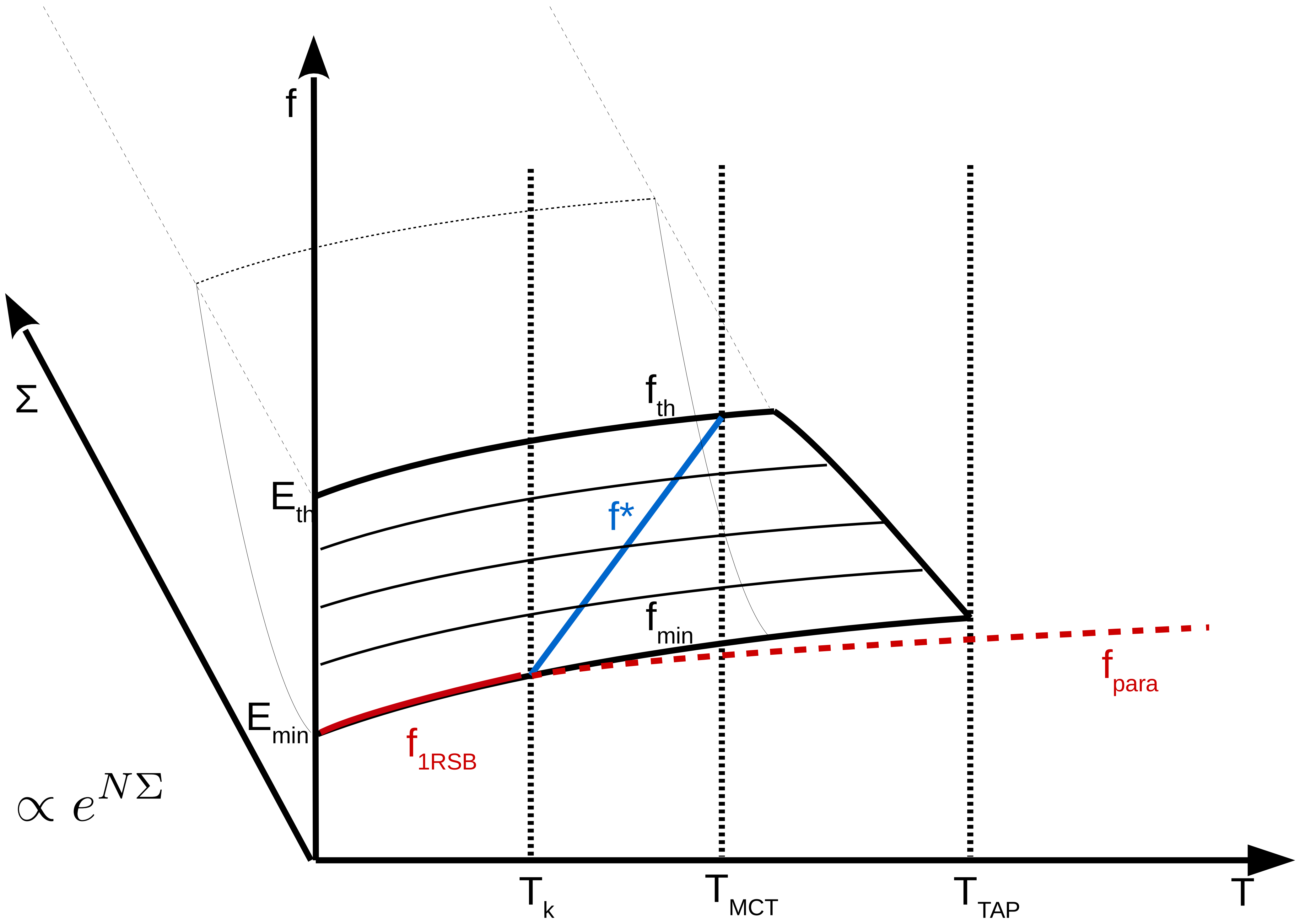
Mean field spin glass models

- SG models with a **discontinuous** phase transition (RFOT)

$$H(\underline{\sigma}) = \sum_{(i_1, i_2, \ldots, i_p) \in E} J_{i_1 \ldots i_p} \sigma_{i_1} \ldots \sigma_{i_p}$$ with p>2

	discrete variables	continuous variables
fully connected dense topology	Ising p-spin	spherical p-spin
finite connectivity sparse topology	random xorsat	???

Statics of models with RFOT



$$\#\text{states} \propto e^{N\Sigma}$$

Langevin dynamics for fully-connected spherical models

$$\dot{\sigma}_i(t) = -\frac{\partial H}{\partial \sigma_i}(\underline{\sigma}(t)) - \mu(t)\sigma_i(t) + \xi_i(t) + h_i(t)$$

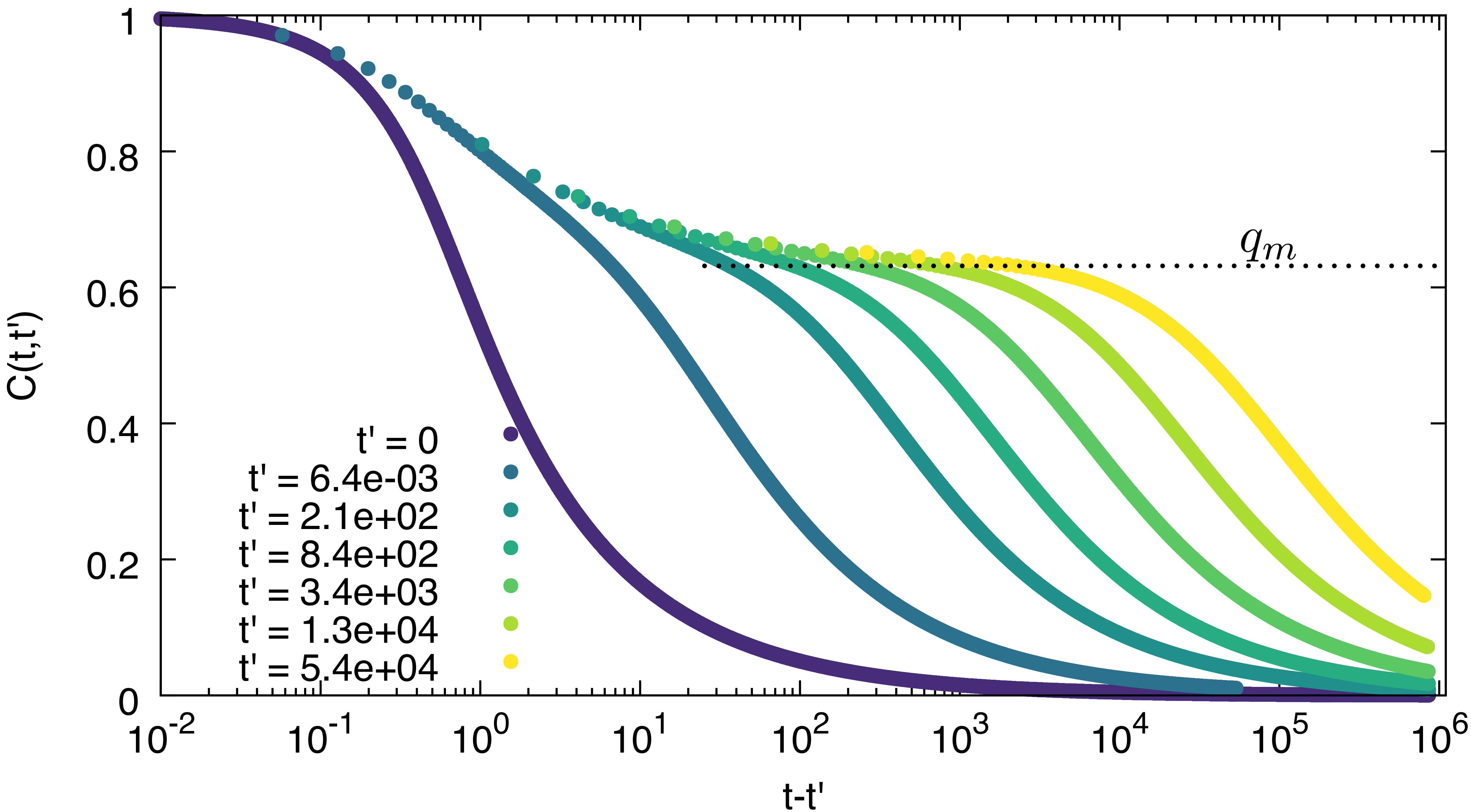
$$\langle \xi_i(t)\xi_j(t')\rangle = 2T\delta_{ij}\delta(t-t')$$

Large N limit before large times limit, closed equations in

$$C(t,t') \equiv \frac{1}{N}\overline{\langle \underline{\sigma}(t)\cdot\underline{\sigma}(t')\rangle}$$

$$R(t,t') \equiv \frac{1}{N}\sum_{i=1}^{N} \left.\frac{\delta\overline{\langle \sigma_i(t)\rangle}}{\delta h_i(t')}\right|_{h=0}$$

Spherical 3-spin model $T=0.5<T_{MCT}$ $T_0=\infty$



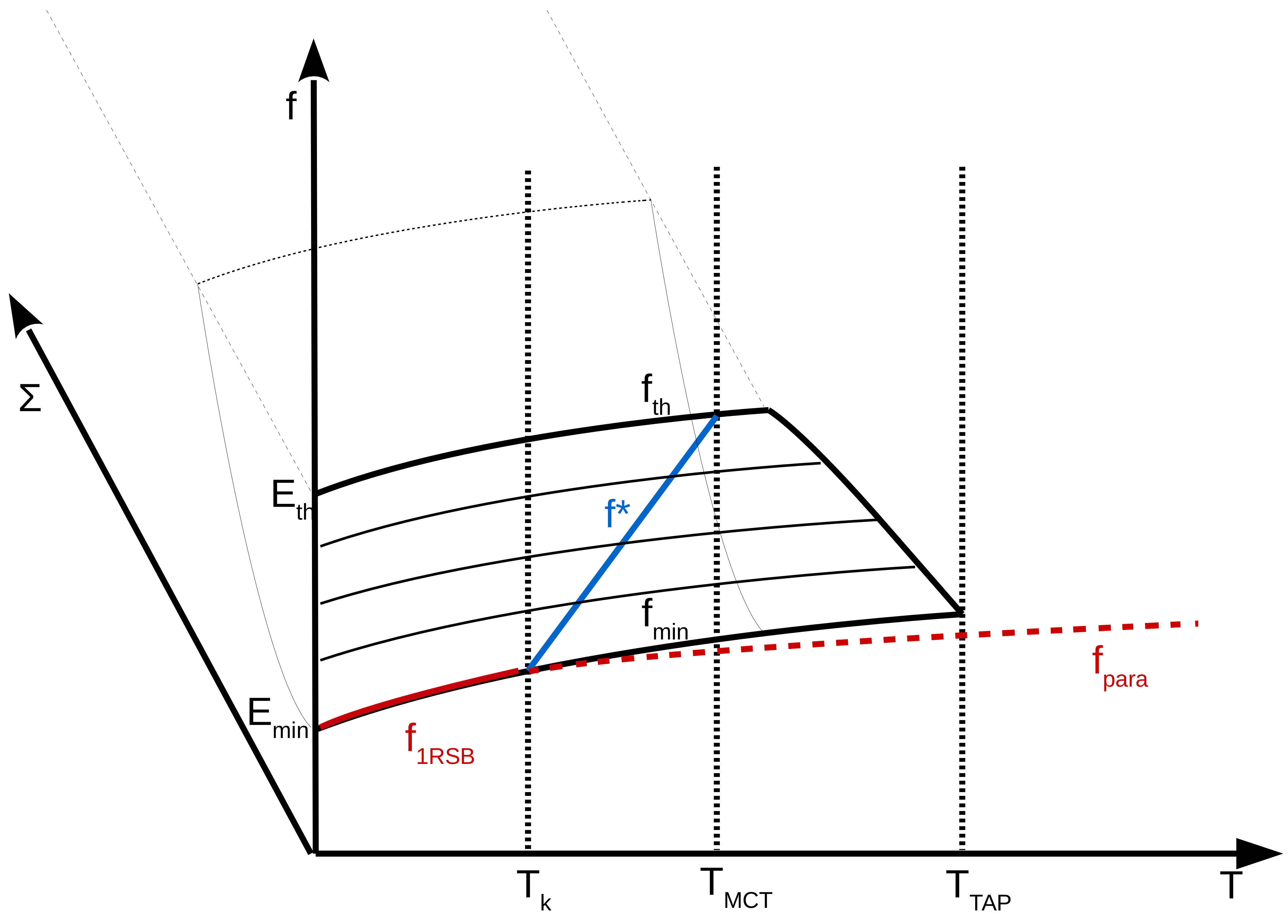
Weak ergodicity breaking : $\lim_{t\to\infty} C(t,t') = 0 \quad \forall t'$

Cugliandolo-Kurchan solution

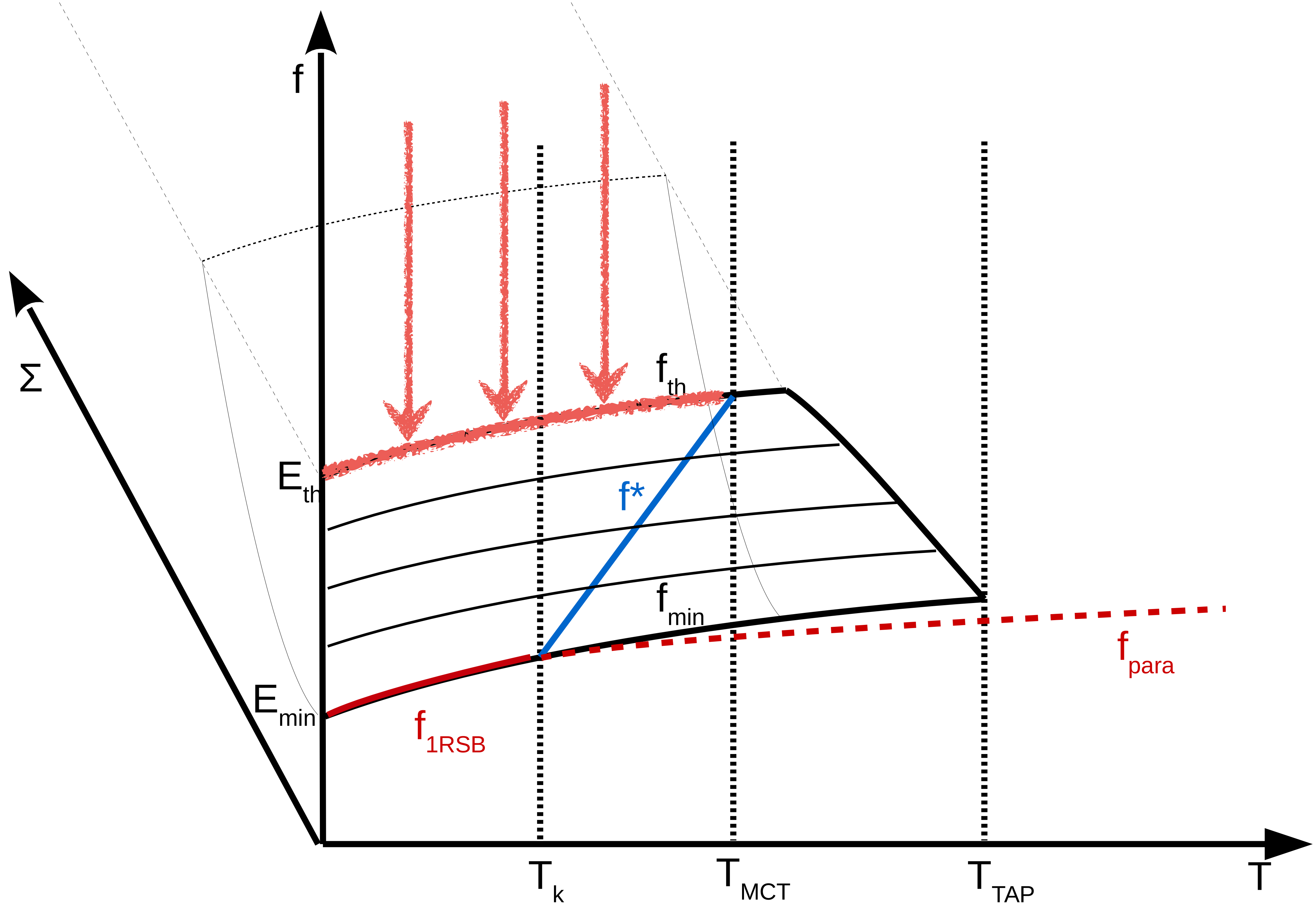
- Aging solution for $T_0=\infty$ and $T<T_d$
  - weak long term memory
  - weak ergodicity breaking: $\lim_{t\to\infty} C(t,t') = 0 \quad \forall t'$
  - $C(t,t')$ plateau value is marginal: $\frac{p(p-1)}{2} q_m^{p-2}(1-q_m)^2 = T^2$
  - energy relaxes to threshold energy
  - modified fluctuation-dissipation relation

$$TR(t,t') = X[C(t,t')]\frac{\partial C(t,t')}{\partial t'}$$

Static-dynamic connection



Static-dynamic connection



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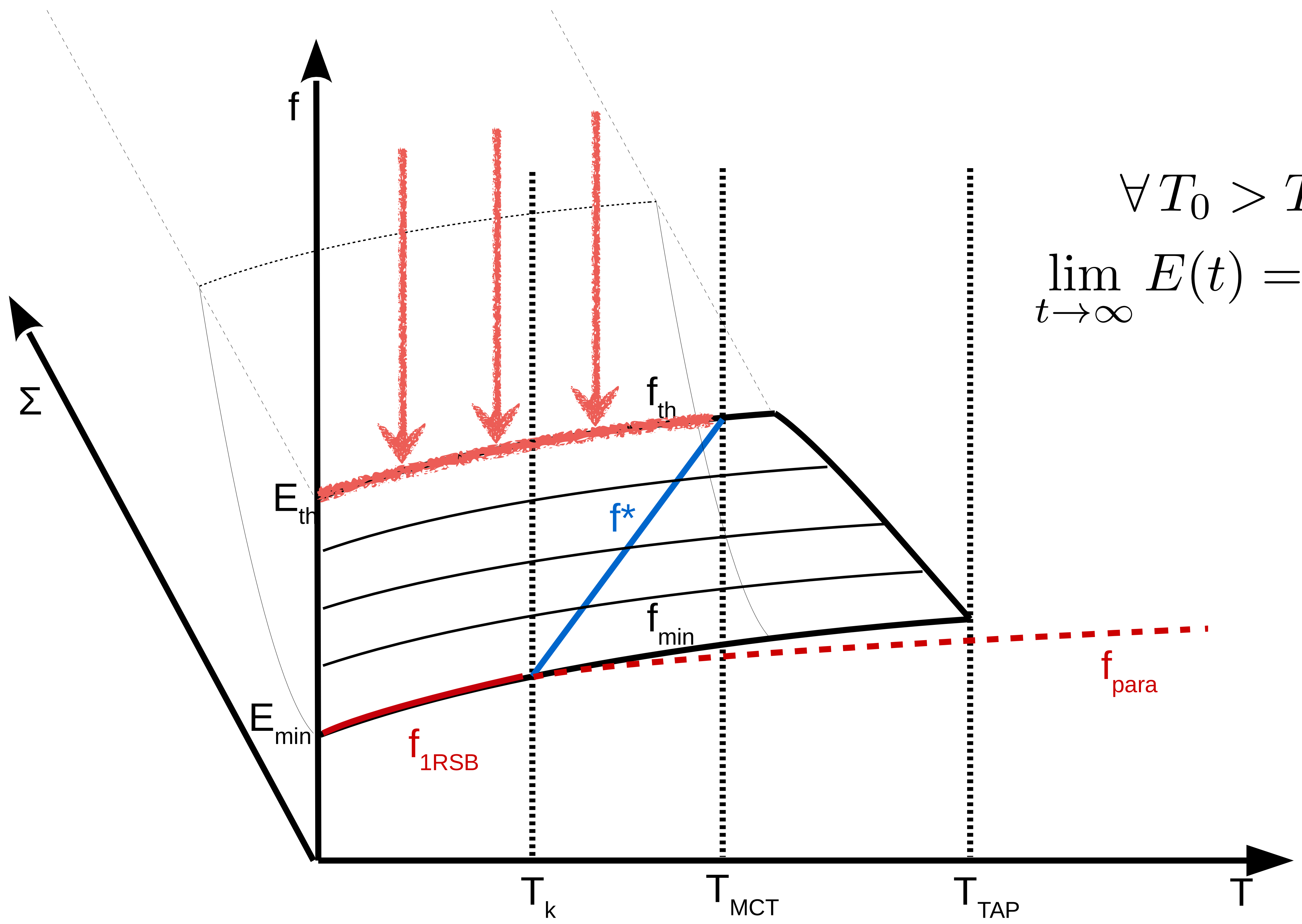
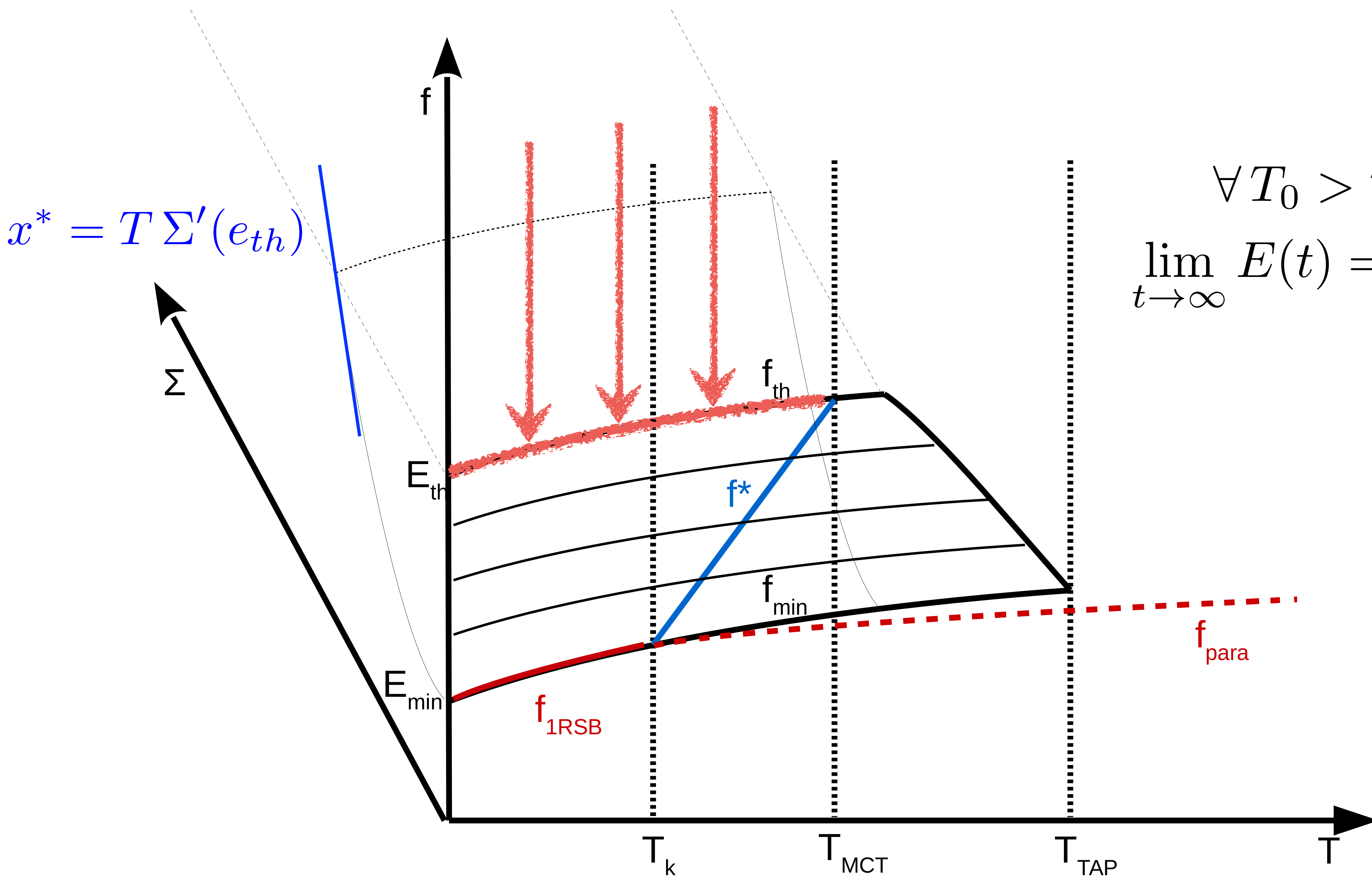


$$\forall\, T_0 > T_{\mathrm{MCT}}$$

$$\lim_{t\to\infty} E(t) = E_{th}$$

Static-dynamic connection



$$\forall\, T_0 > T_{\mathrm{MCT}}$$

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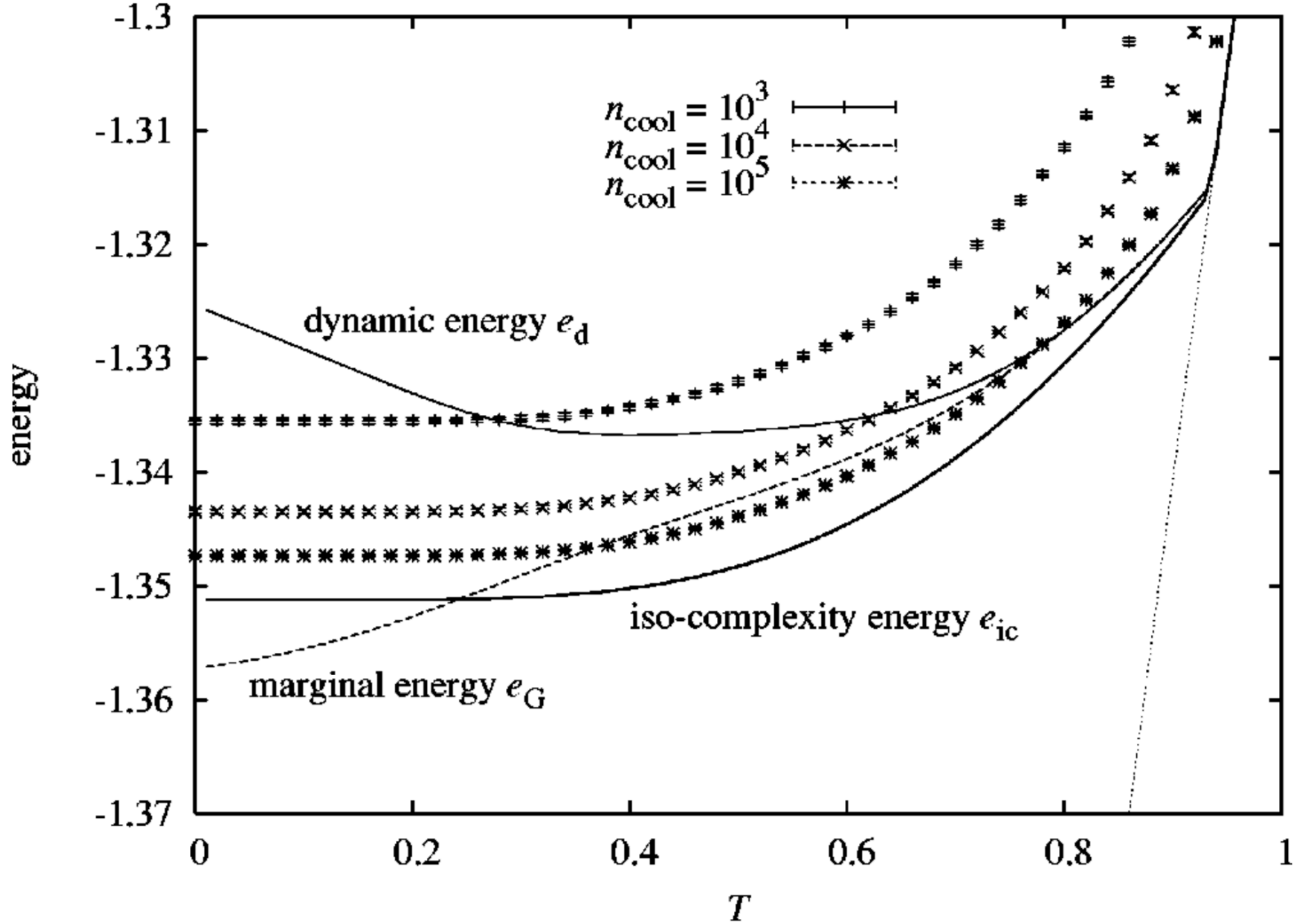
Static-dynamic connection is not always so easy!



3-XORSAT
on 5-RRG
Montanari, RT
PRB (2004)

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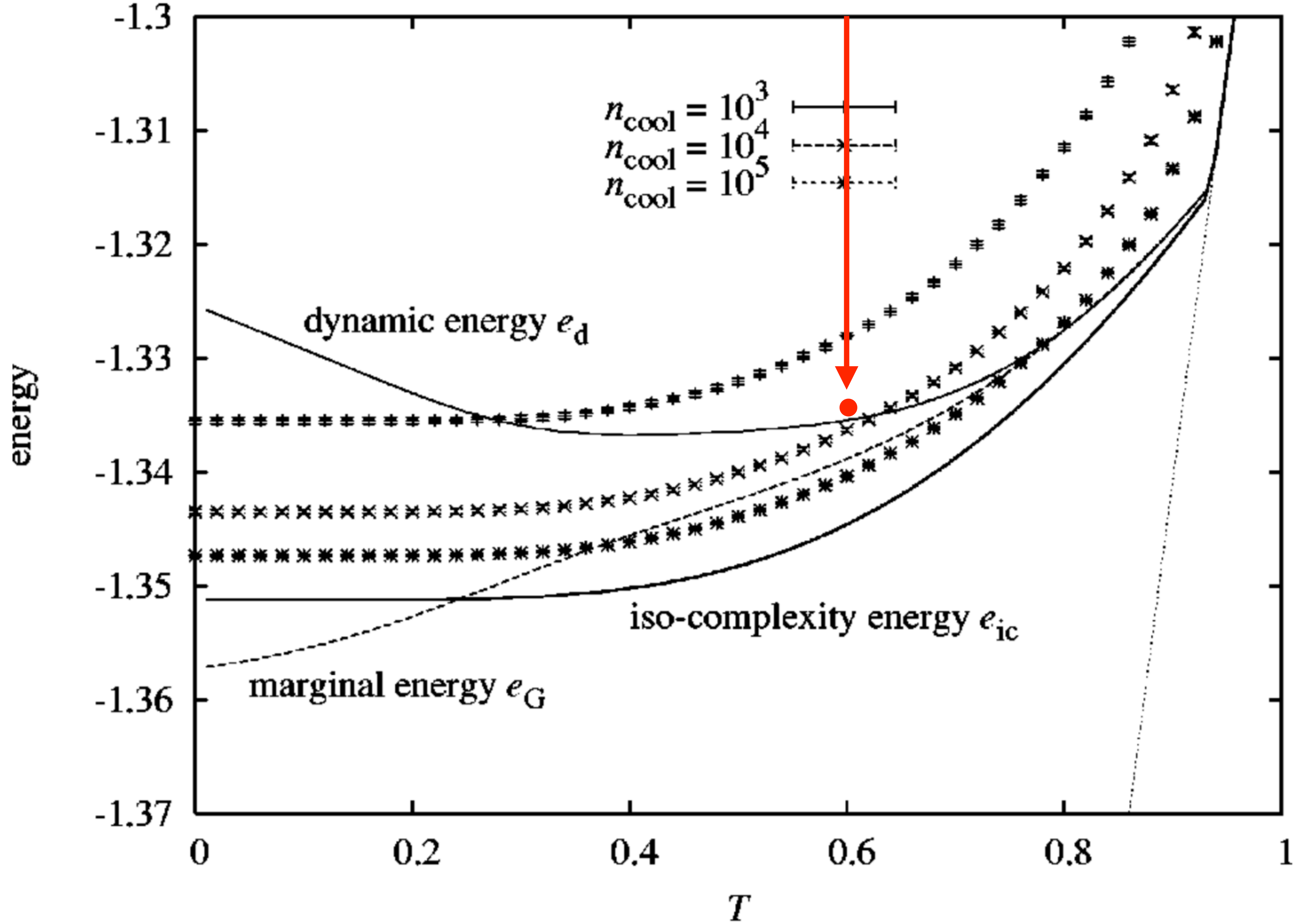
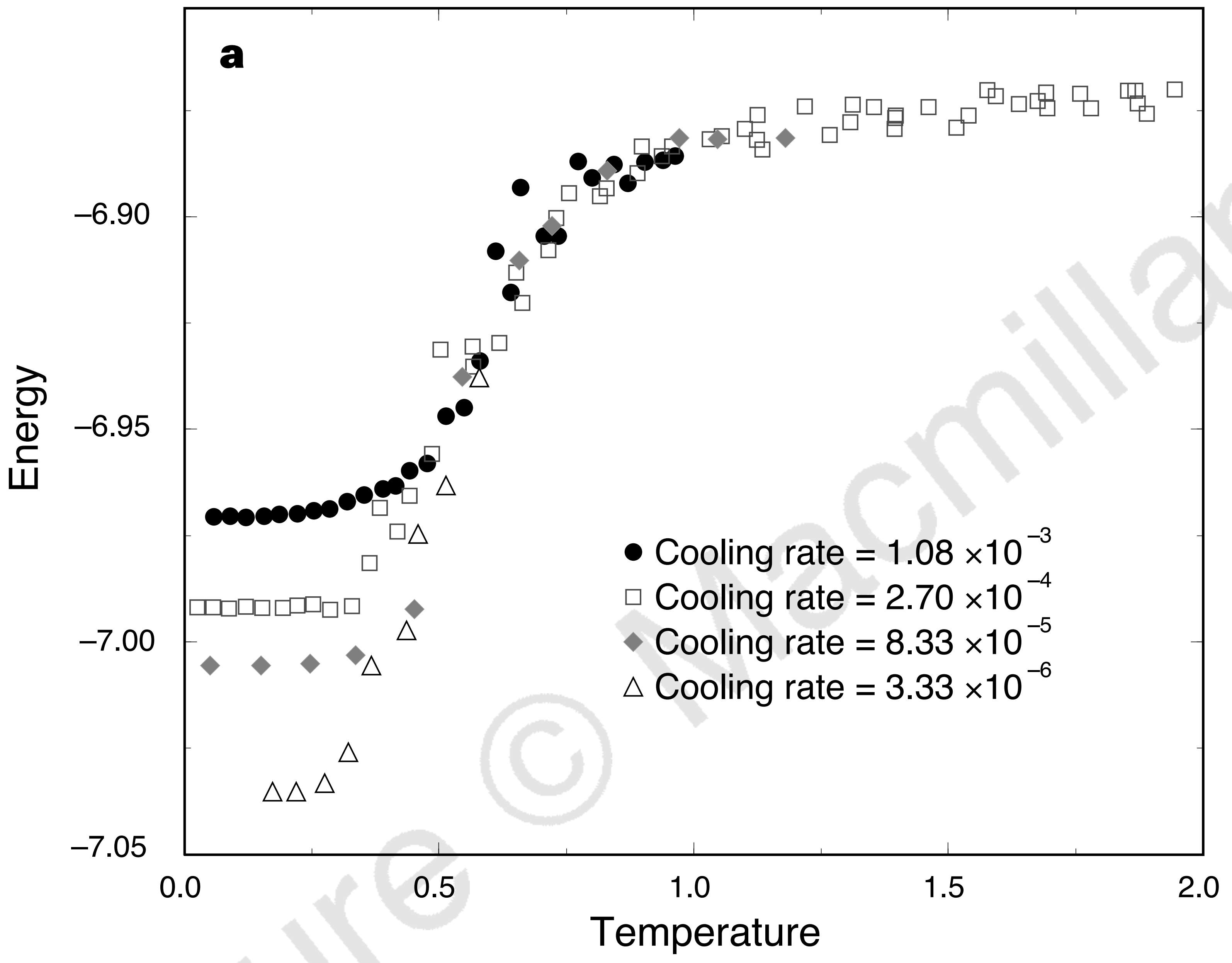


3-XORSAT
on 5-RRG
Montanari, RT
PRB (2004)

quenches
from $T_0=\infty$
to $T=0.6$

T=0 quenches in a real glass former



Sastry
Debenedetti
Stillinger
Nature (1998)

More motivations

- To find a solvable model showing the same behavior than realistic glass formers

- To solve some paradoxes in the following state process in spherical p-spin models

A general class of solvable models

- Fully connected spherical mixed p-spin model

$$H(\underline{\sigma}) = \sum_p c_p \sum_{i \leq i_1 < \ldots < i_p \leq N} J_{i_1 \ldots i_p} \sigma_{i_1} \ldots \sigma_{i_p}$$

$$\underline{\sigma} \in \mathbb{R}^N : \sum_i \sigma_i^2 = N$$

$$\overline{J_p} = 0 \quad \overline{J_p^2} = \frac{p!}{2N^{p-1}}$$

$$\frac{1}{N} \overline{H(\underline{\sigma}) H(\underline{\tau})} = \frac{1}{2} \sum_p c_p^2 \, q_{\sigma\tau}^p \equiv f(q_{\sigma\tau}) \quad q_{\sigma\tau} = \frac{1}{N} \sum_i \sigma_i \tau_i$$

$$f(q) = \frac{q^3}{2} \quad \text{(pure)} \qquad f(q) = \frac{q^3 + q^4}{2} \quad \text{(mixed)}$$

A more general class of dynamics

- Langevin dynamics at T starting thermalized at T_0

$$\dot{\sigma}_i(t) = -\frac{\partial H}{\partial \sigma_i}(\underline{\sigma}(t)) - \mu(t)\sigma_i(t) + \xi_i(t) + h_i(t)$$

$$\langle \xi_i(t)\xi_j(t')\rangle = 2T\delta_{ij}\delta(t-t') \qquad \underline{\sigma}(0) \sim \exp[-H(\underline{\sigma}(0))/T_0]$$

- These are still quenches, but can give information also on very slow annealing, under the assumption that for $T>T_0$ the annealing is at equilibrium and for $T<T_0$ the annealing is strongly out of equilibrium

Dynamical mean-field equations for spherical mixed p-spin models

- Closed set of equations in C(t,t') and R(t,t')

$$
\begin{aligned}
\partial_t C(t,t') =& -\mu(t)C(t,t') + 2TR(t',t) + \int_0^t ds f''(C(t,s))R(t,s)C(s,t') \\
&+ \int_0^{t'} ds f'(C(t,s))R(t',s) + f'(C(t,0))C(t',0)/T_0 \\
\partial_t R(t,t') =& -\mu(t)R(t,t') + \delta(t-t') + \int_{t'}^t ds f''(C(t,s))R(t,s)R(s,t') \\
\mu(t) \equiv& \, T + \int_0^t ds f''(C(t,s))R(t,s)C(t,s) \\
&+ \int_0^t ds f'(C(t,s))R(t,s) + f'(C(t,0))C(t,0)/T_0
\end{aligned}
$$

Dynamical mean-field equations for spherical mixed p-spin models

- Closed set of equations in C(t,t') and R(t,t')

$$\partial_t C(t,t') = -\mu(t)C(t,t') + 2T R(t',t) + \int_0^t ds f''(C(t,s))R(t,s)C(s,t')$$

$$+ \int_0^{t'} ds f'(C(t,s))R(t',s) + f'(C(t,0))C(t',0)/T_0$$

$$\partial_t R(t,t') = -\mu(t)R(t,t') + \delta(t-t') + \int_{t'}^t ds f''(C(t,s))R(t,s)R(s,t')$$

$$\mu(t) \equiv T + \int_0^t ds f''(C(t,s))R(t,s)C(t,s)$$

$$+ \int_0^t ds f'(C(t,s))R(t,s) + f'(C(t,0))C(t,0)/T_0$$

Smooth T dependence
Can be set to T=0

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$$\partial_t C(t,t') = -\mu(t)C(t,t') + 2TR(t',t) + \int_0^t ds f''(C(t,s))R(t,s)C(s,t')$$

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$$+ \int_0^t ds f'(C(t,s))R(t,s) + f'(C(t,0))C(t,0)/T_0$$

Smooth T dependence Can be set to T=0

Dependence on the initial condition at T_0

CK asymptotic solution is still valid

- Aging solution for $T_0=\infty$ and $T<T_d$
  - weak long term memory
  - weak ergodicity breaking: $\lim_{t\to\infty} C(t,t') = 0 \quad \forall t'$
  - $C(t,t')$ plateau value is marginal: $f''(q_m)(1-q_m)^2 = T^2$
  - energy relaxes to threshold energy
  - modified fluctuation-dissipation relation

$$TR(t,t') = X[C(t,t')]\frac{\partial C(t,t')}{\partial t'}$$

What happens for finite T_0 ?

- Simplest guess: all $T_0 > T_d$ are equivalent (ergodic phase)
- Asymptotic dynamics <-> FP potential saddle point

$$V(T|q_{12}, T_0) = \overline{\frac{-T}{Z(T')} \sum_{\underline{\sigma}} e^{-H(\underline{\sigma})/T_0} \log \left[\sum_{\underline{\tau}} e^{-H(\underline{\tau})/T} \delta(q_{12} N - \underline{\sigma} \cdot \underline{\tau}) \right]} - F(T)$$

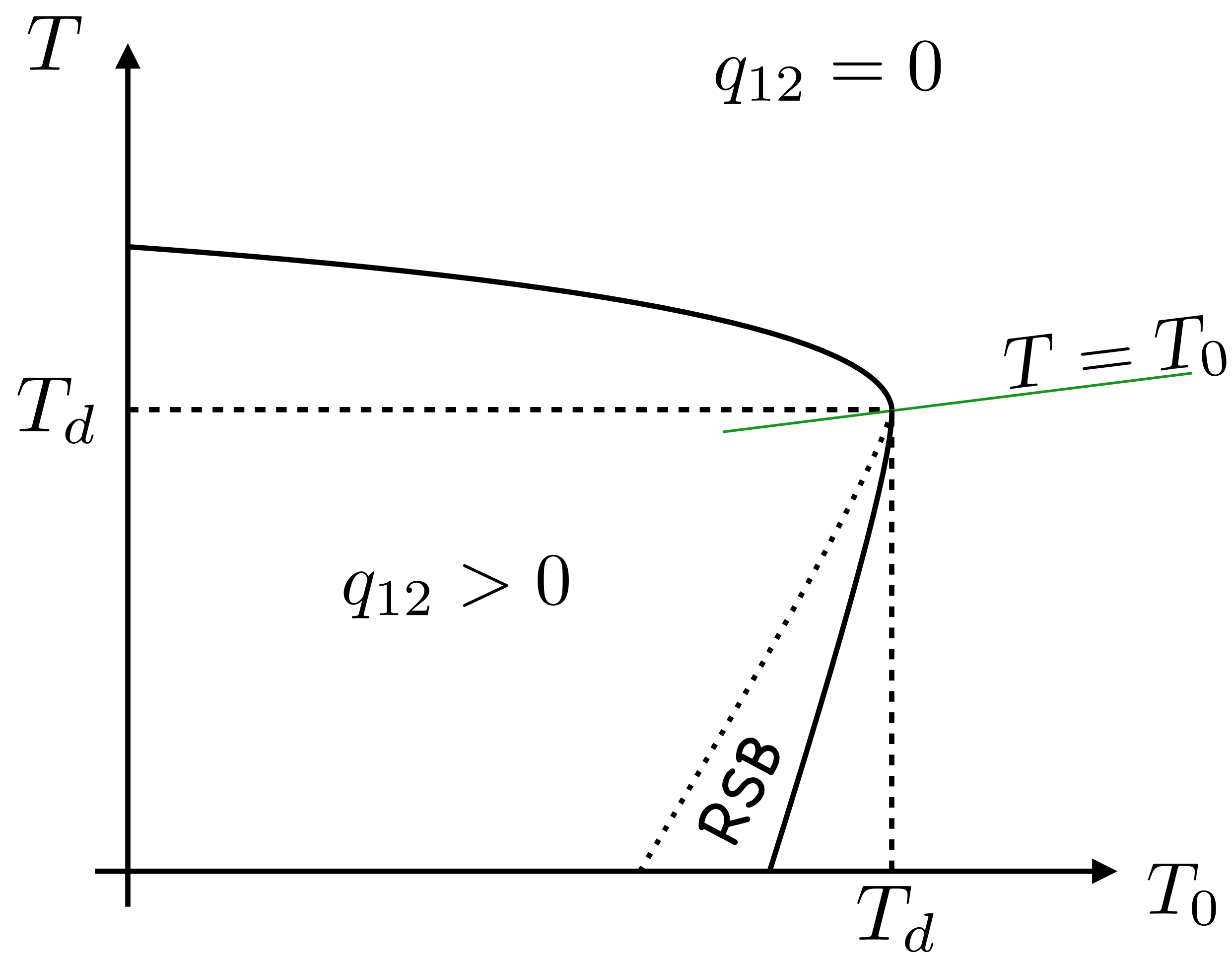
$$q_{12} = \lim_{t \to \infty} C(t, 0)$$
$$\mathcal{C}(\lambda) = \lim_{t \to \infty} C(t, \lambda t)$$
$$q_0 = \lim_{\lambda \to 0} \mathcal{C}(\lambda)$$
$$q_1 = \lim_{\lambda \to 1} \mathcal{C}(\lambda)$$
$$x = \mathcal{R}(\lambda) / \mathcal{C}'(\lambda)$$

$$q_1 = q_m$$
$$0 = \partial_{q_{12}} V$$
$$0 = \partial_{q_0} V$$
$$0 = \partial_{q_1} V$$

Barrat
Franz
Parisi
JPA (1997)

What happens for finite T_0 ?

Sun, Crisanti
Krzakala, Leuzzi
Zdeborova
JSTAT (2012)



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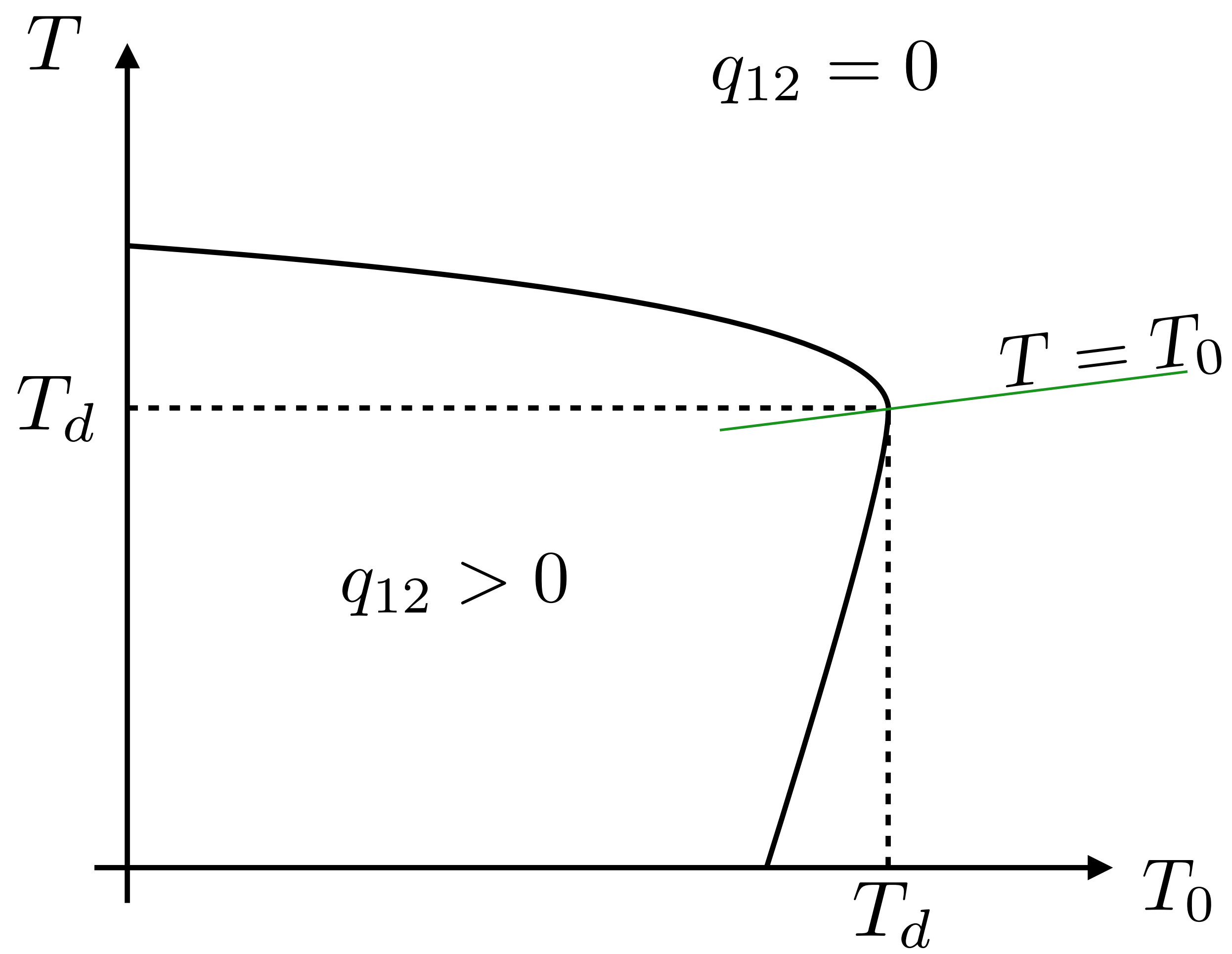

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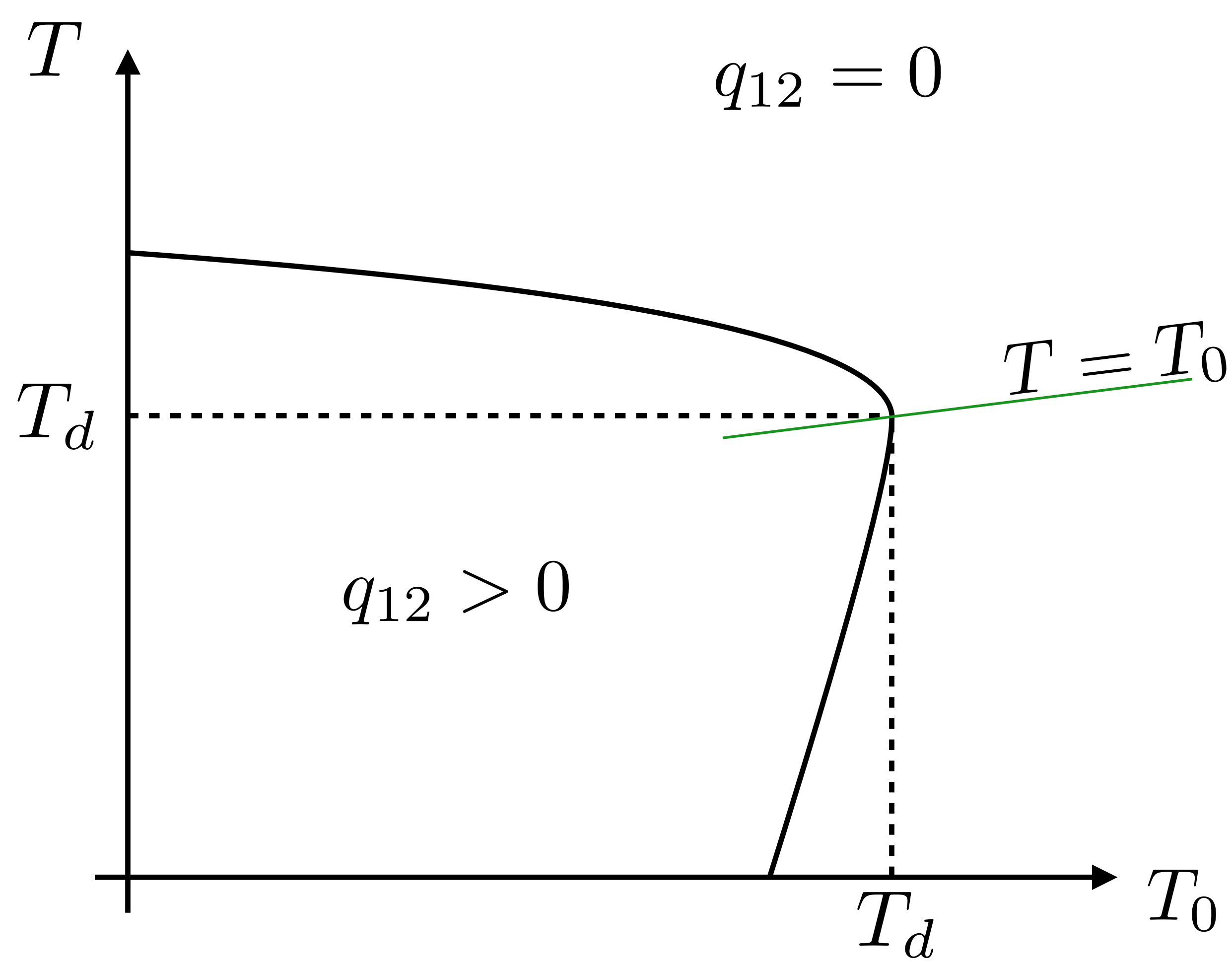

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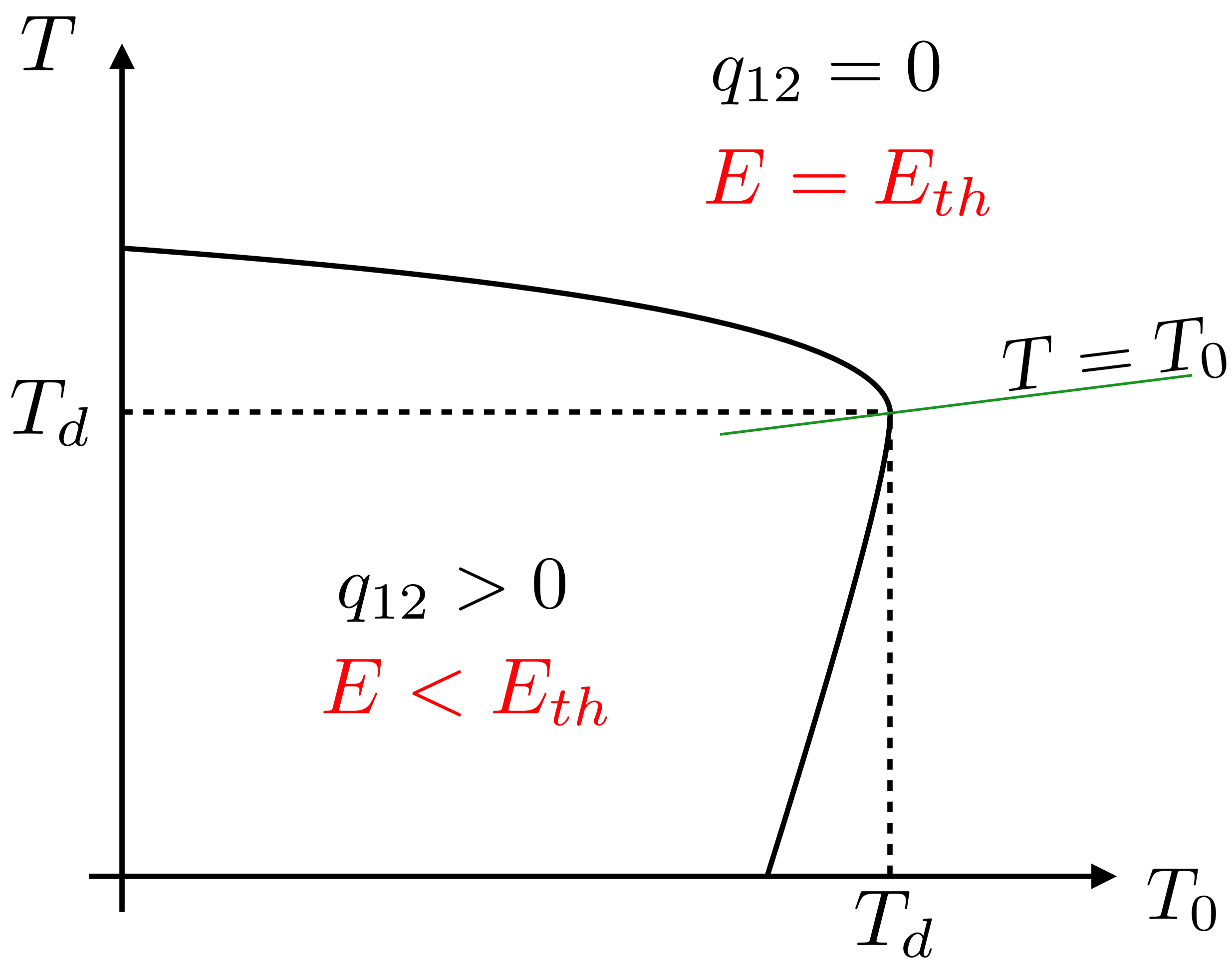
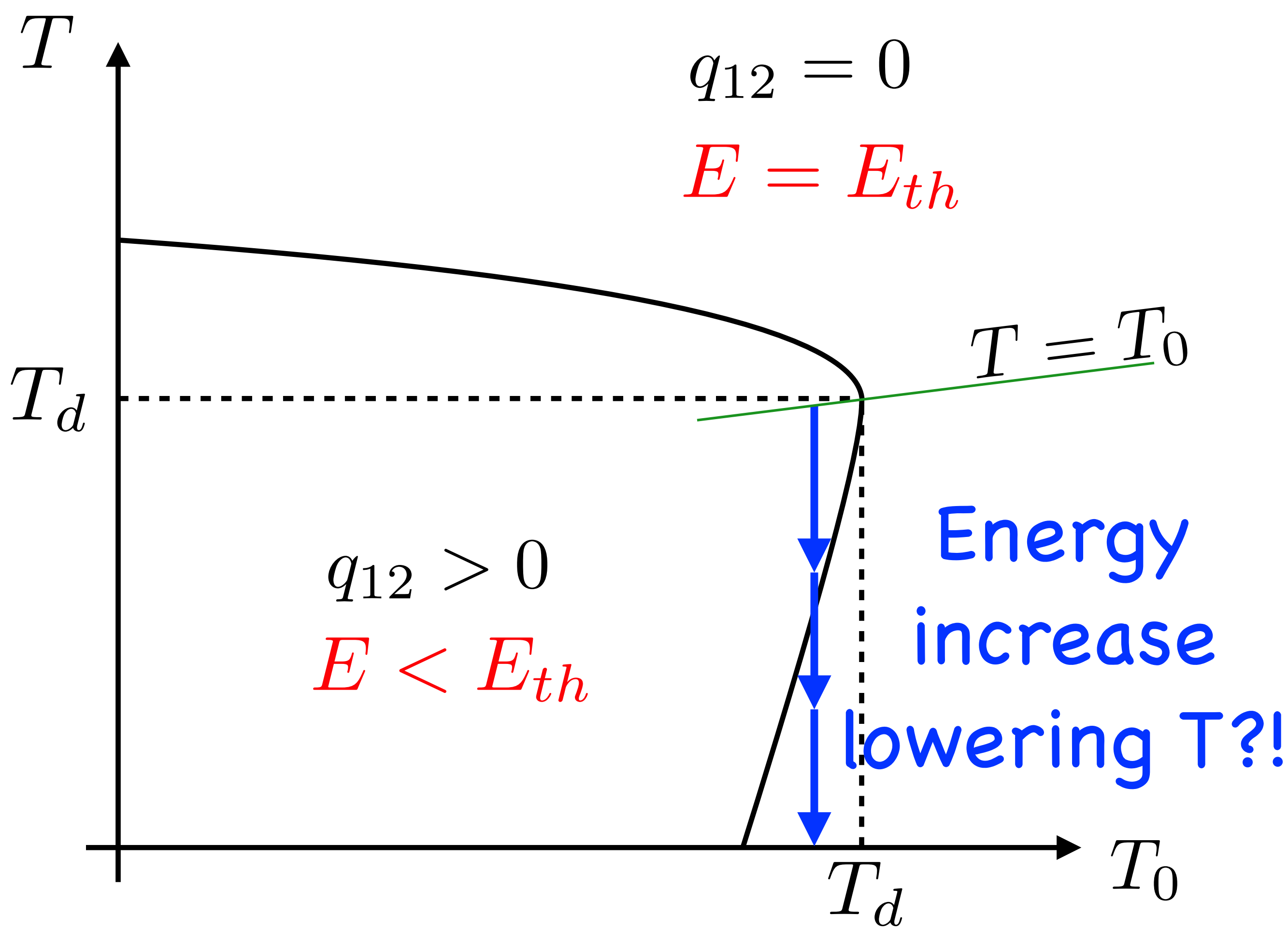


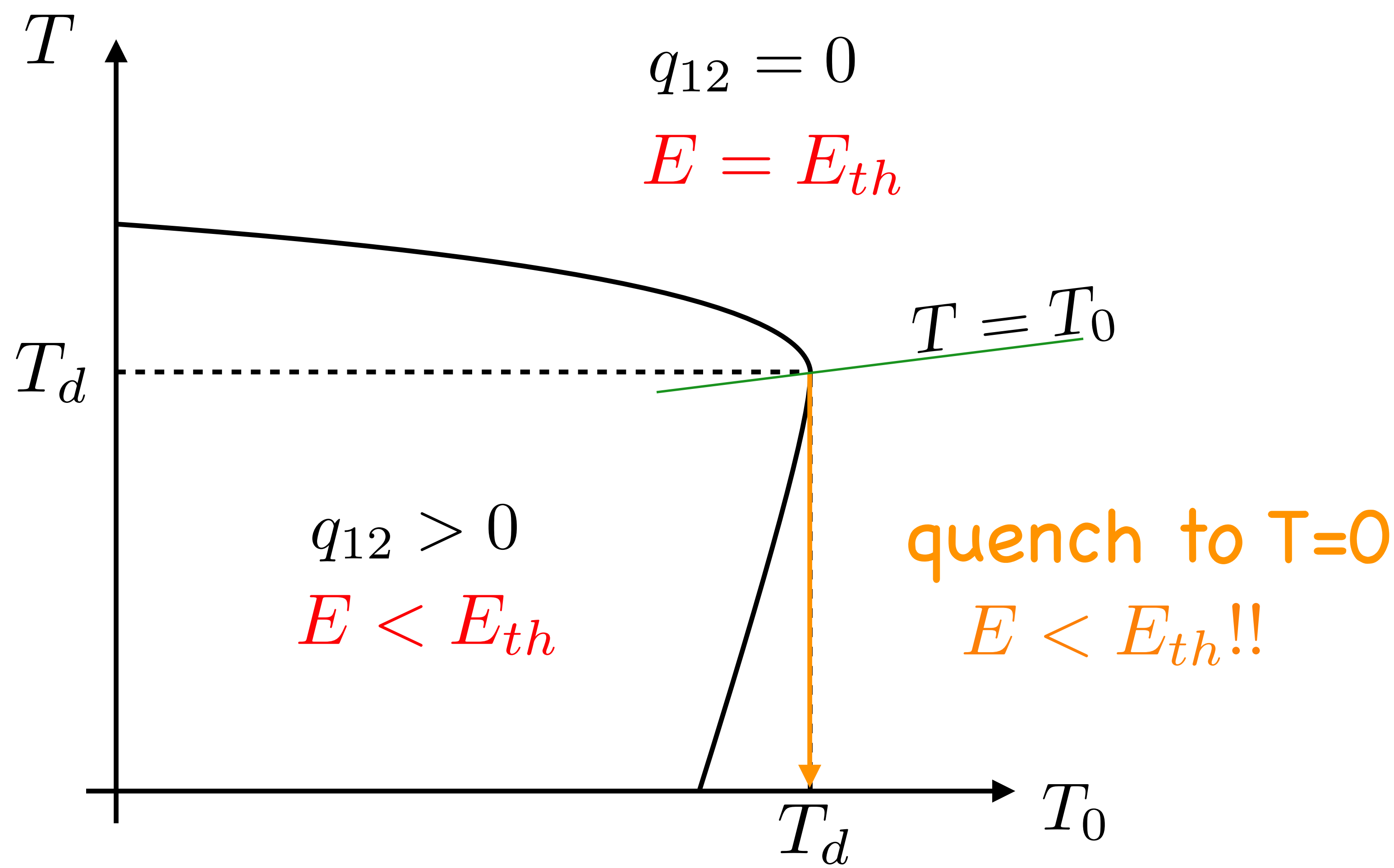
$$E = E_{th} - \beta_0 f(q_{12}) + \beta x f(q_0)$$

What happens for finite T₀ ?



$$E = E_{th} - \beta_0 f(q_{12}) + \beta x f(q_0)$$

What happens for finite T_0 ?



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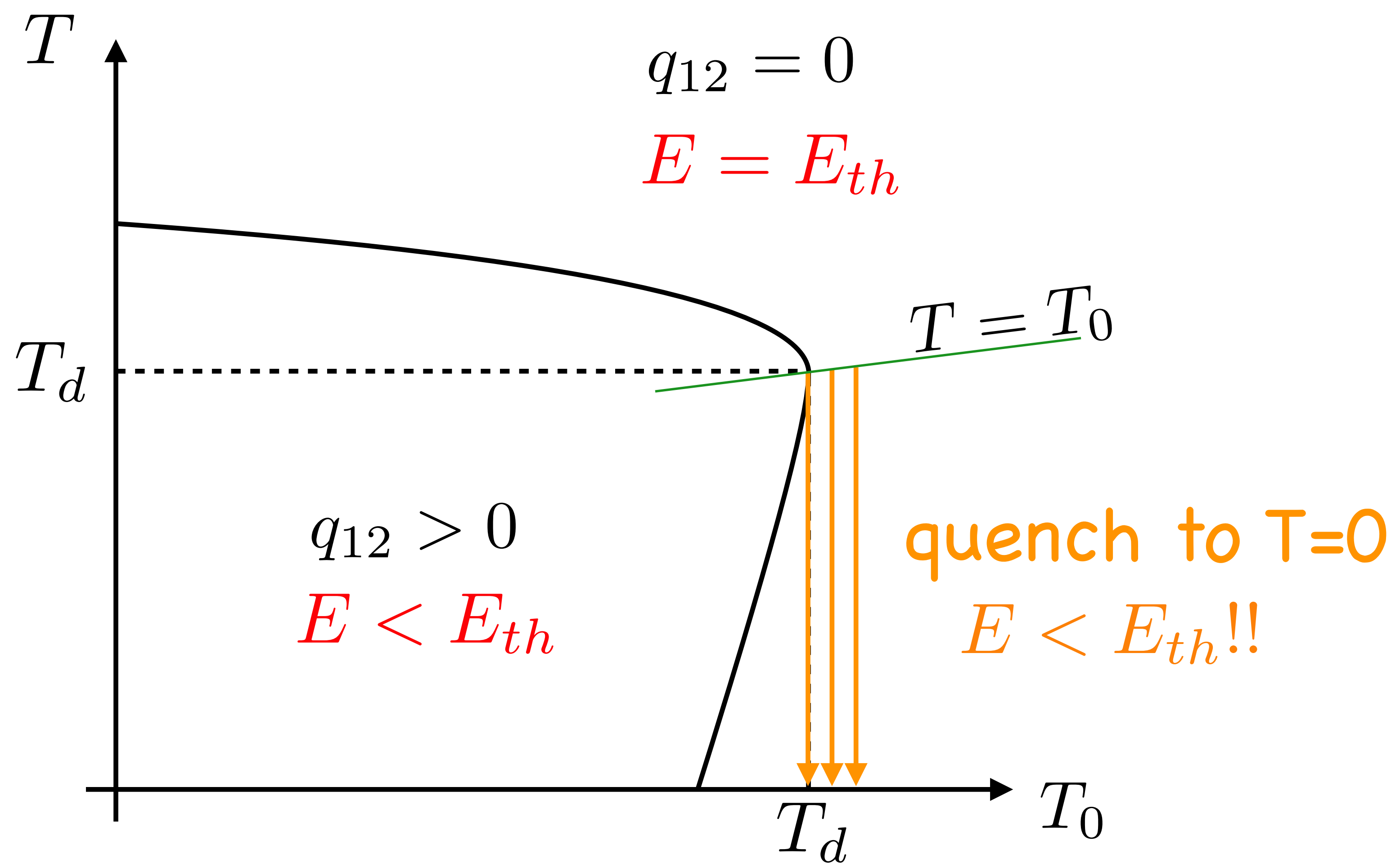
What happens for finite T_0 ?



$$E = E_{th} - \beta_0 f(q_{12}) + \beta x f(q_0)$$

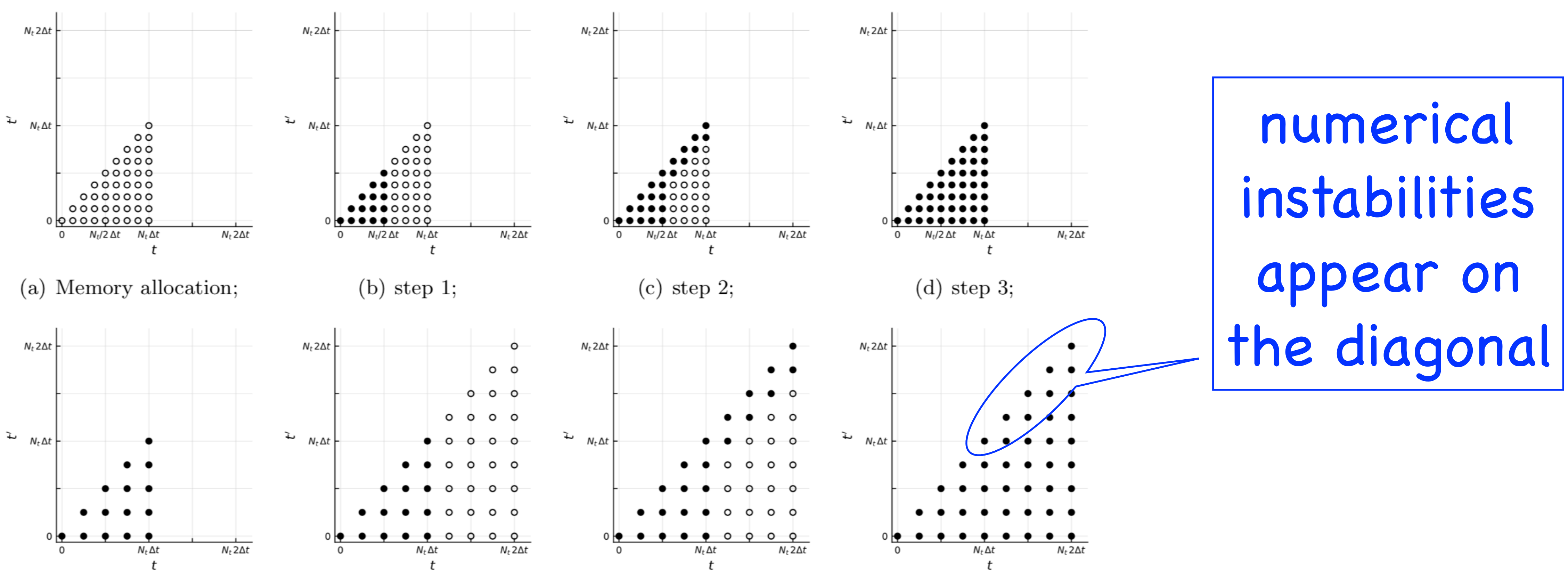
What we have done

- Fix T=0 (quenches by gradient descent)
- For many different values of T_0
  (hereafter we call it T, it is the only temperature...)
  - Integrate dynamical mean-field equations in the $N=\infty$ limit and guess the large time asymptotic behavior
  - Compute constrained complexity of minima to try a statics-dynamics connection
  - Minimize numerically the energy in finite size systems

How to integrate the equations

- We use a <u>fixed</u> time step Δt
  Then we extrapolate in the limit $\Delta t \to 0$
  This is a safe procedure!

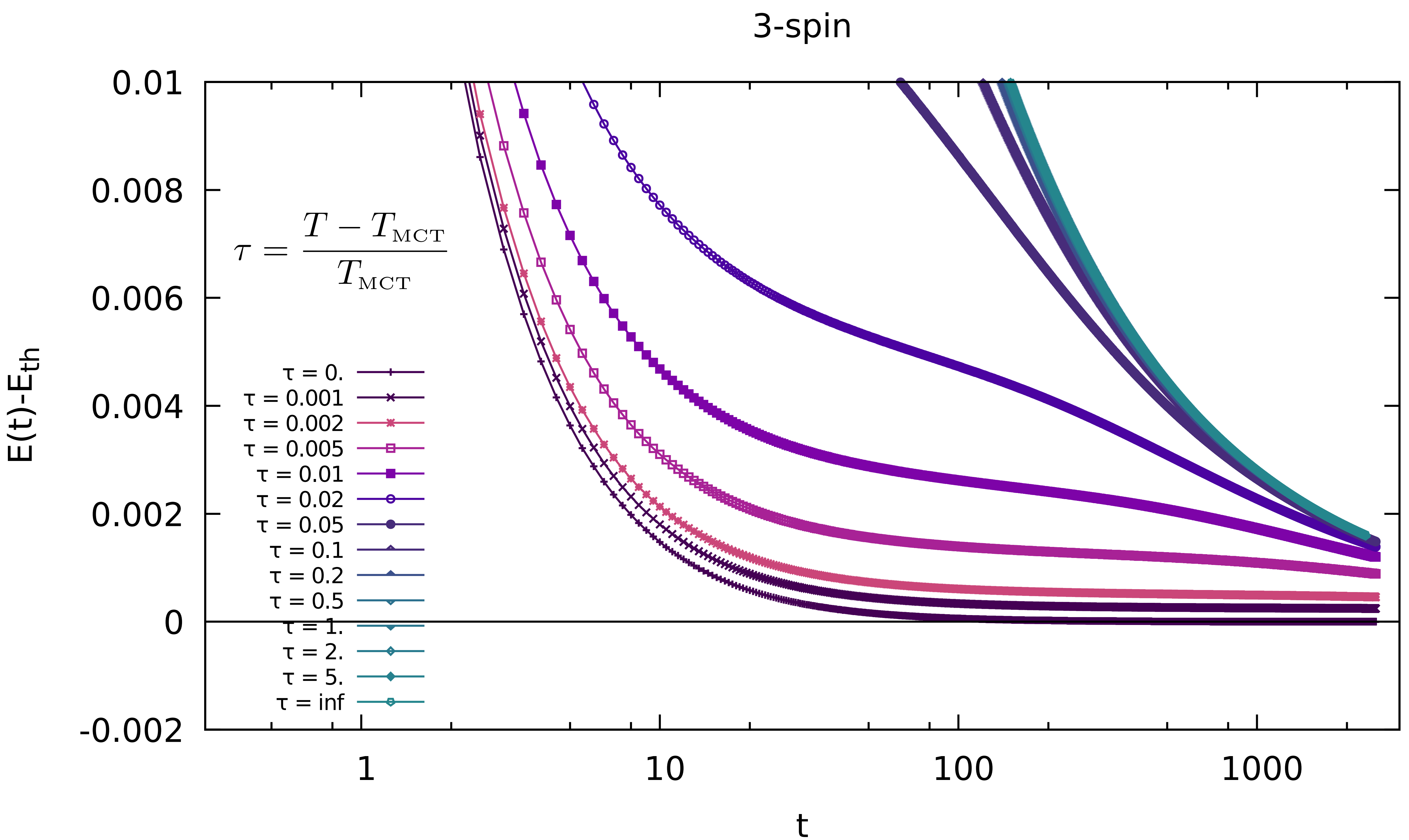
- A <u>variable</u> time step does not work for mixed models with discontinuous phase transition...



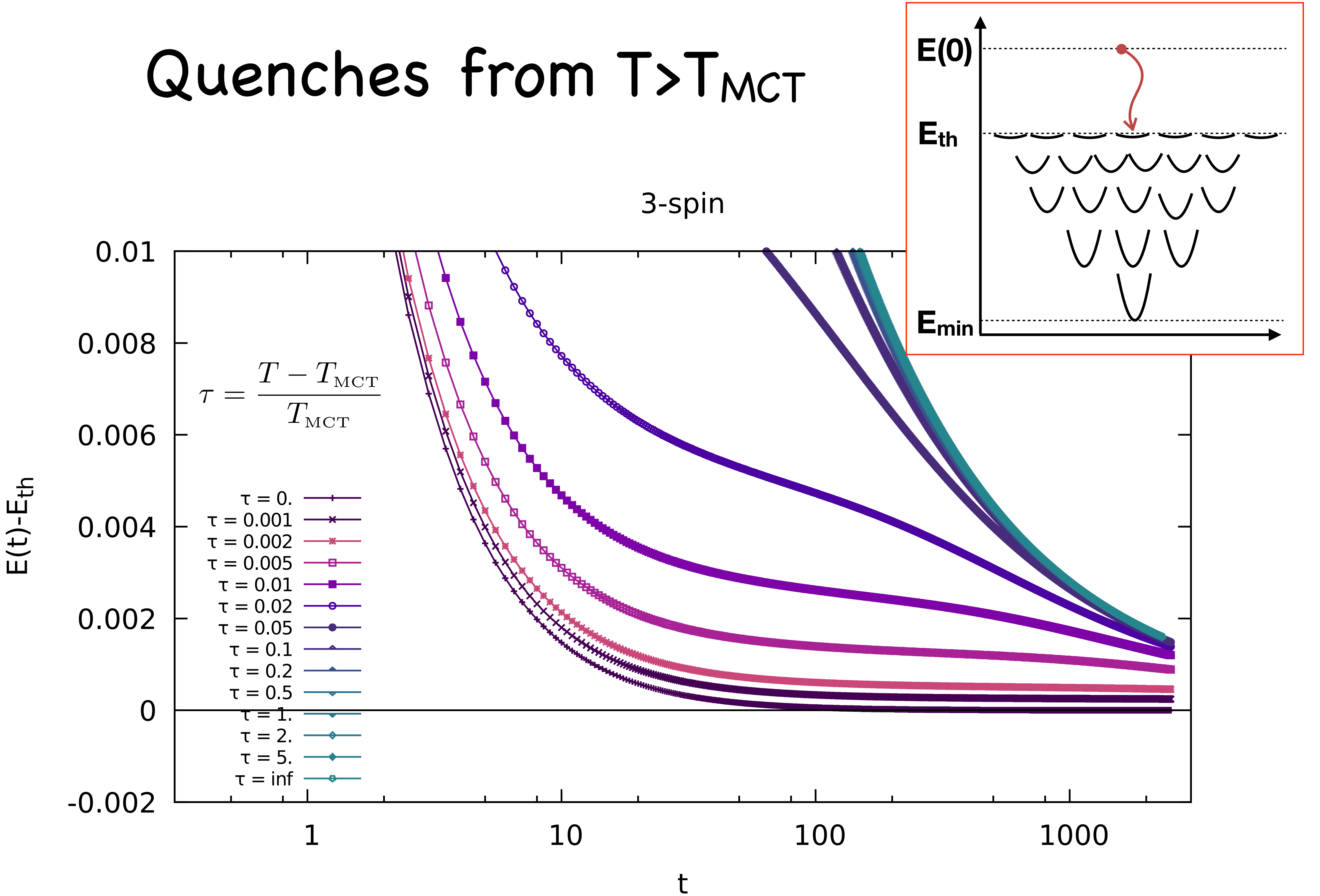
(a) Memory allocation; (b) step 1; (c) step 2; (d) step 3;

(e) step 4.1; (f) step 4.2; (g) step 2; (h) step 3.

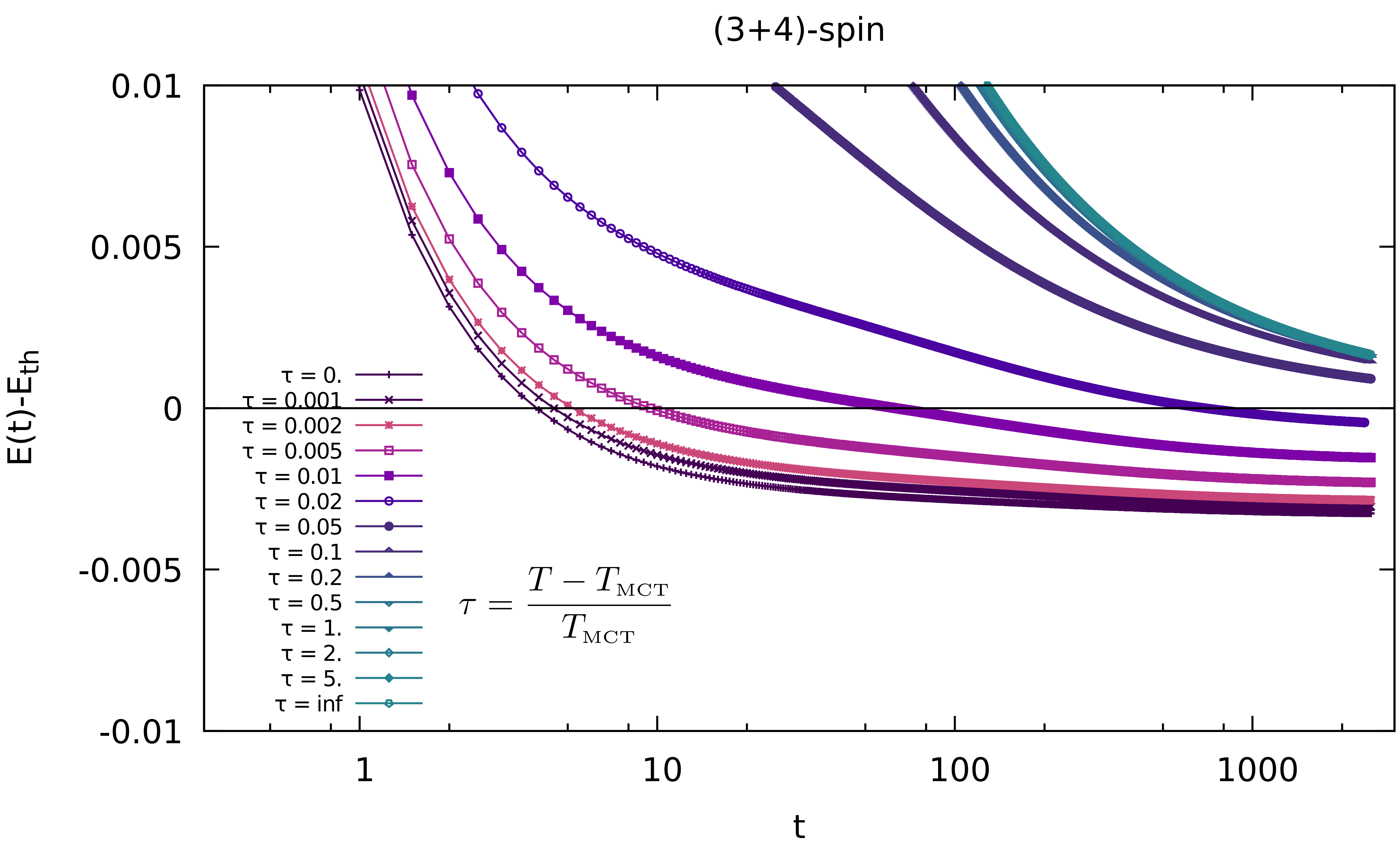
Quenches from T>T_{MCT}



Quenches from T>T$_{MCT}$



Quenches from $T>T_{MCT}$



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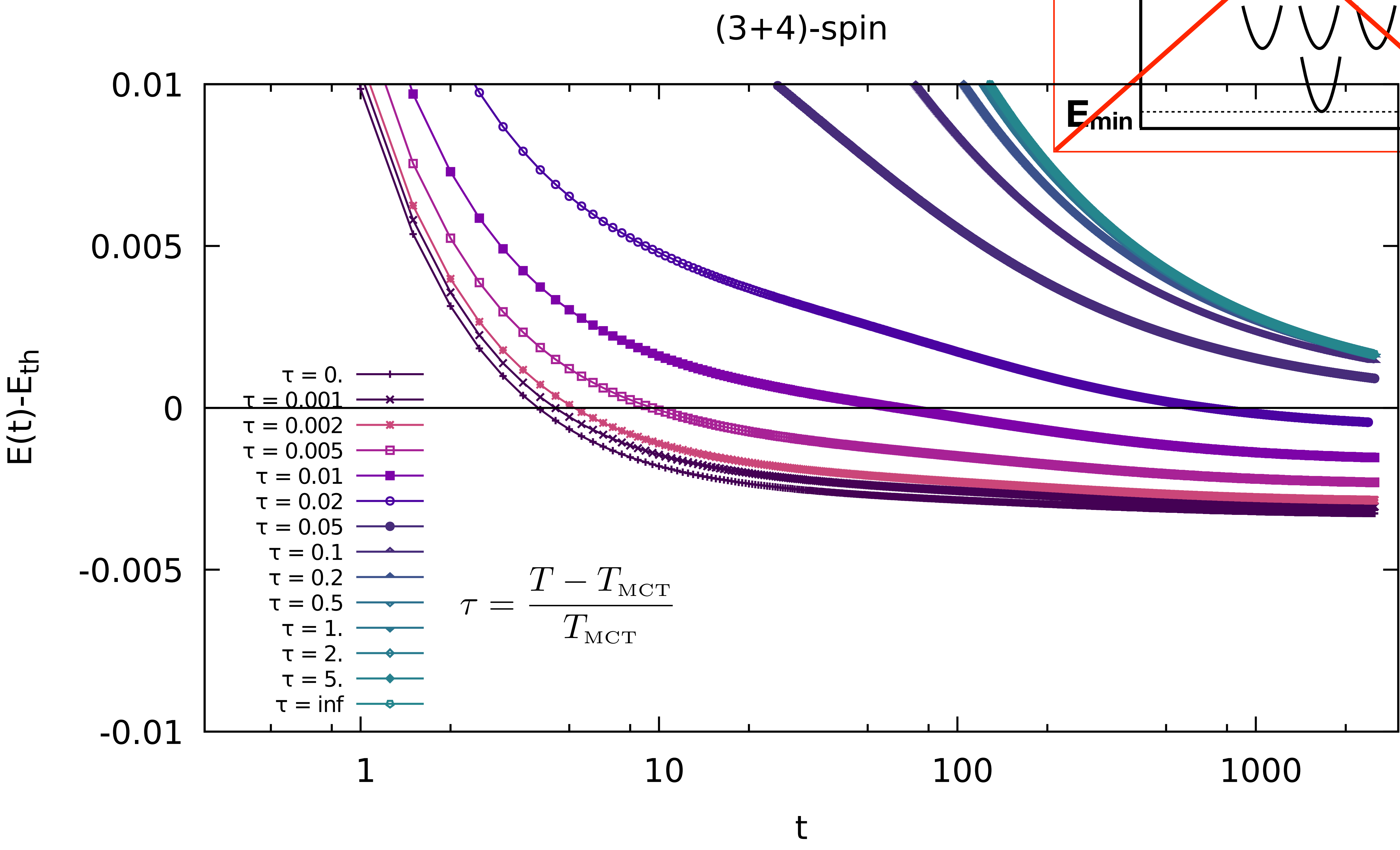
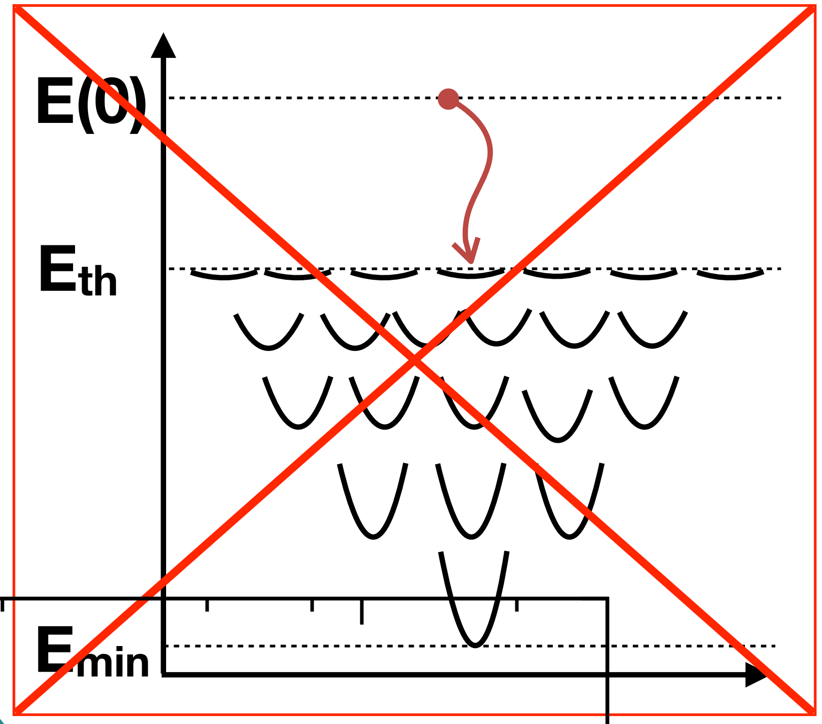
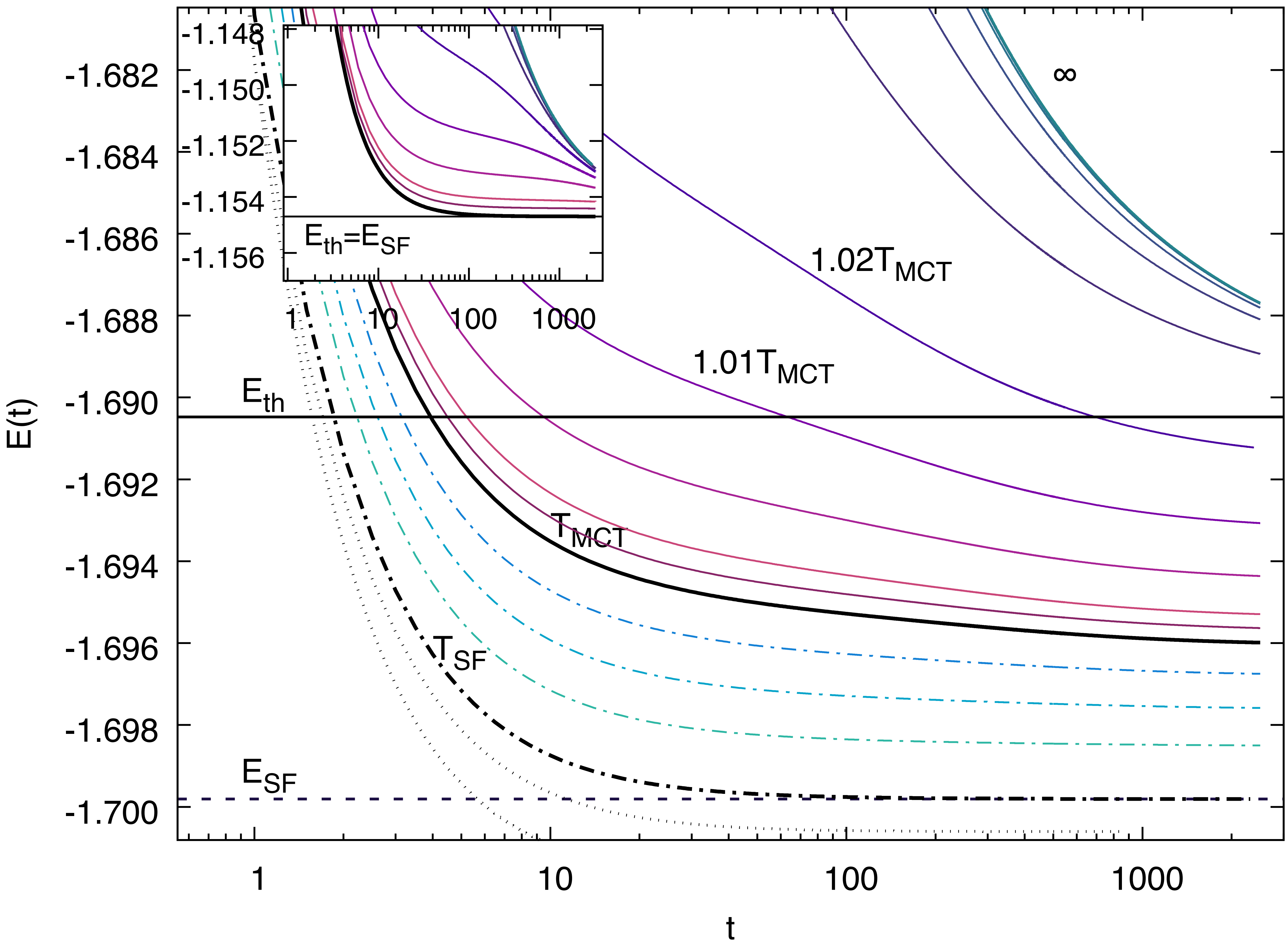


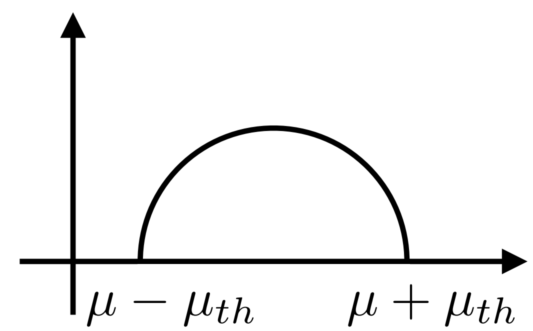


A broader range of temperatures



Radial reaction μ determines the local stability

- Hessian spectrum is a shifted semicircle law



$$\mu_{th} = 2\sqrt{f''(1)}$$

minima have $\mu > \mu_{th}$ and saddles have $\mu < \mu_{th}$

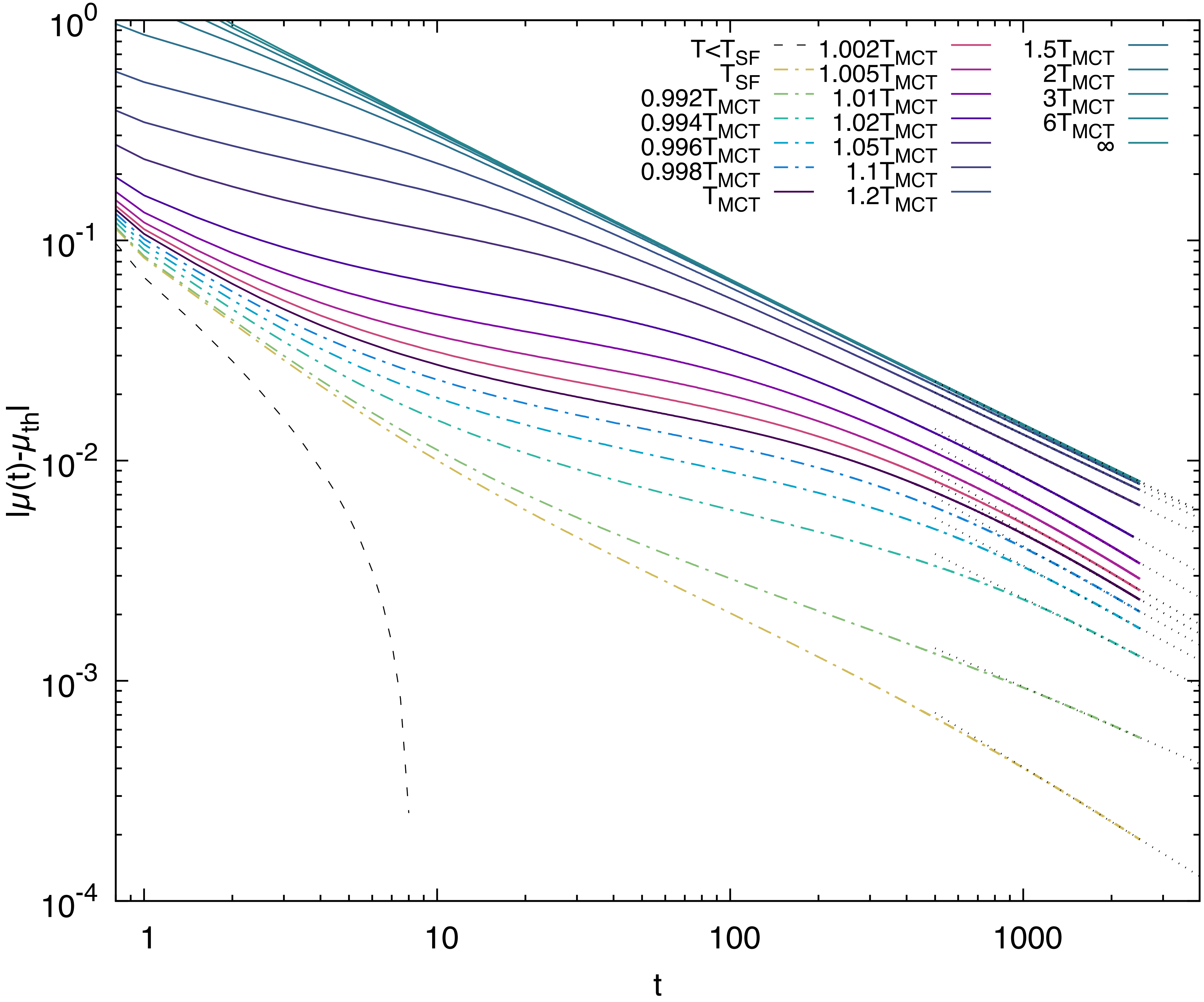
- Main difference between pure and mixed models

$$e = \sum_p c_p^2 \, e_p \qquad \mu = -\sum_p c_p^2 \, p \, e_p$$

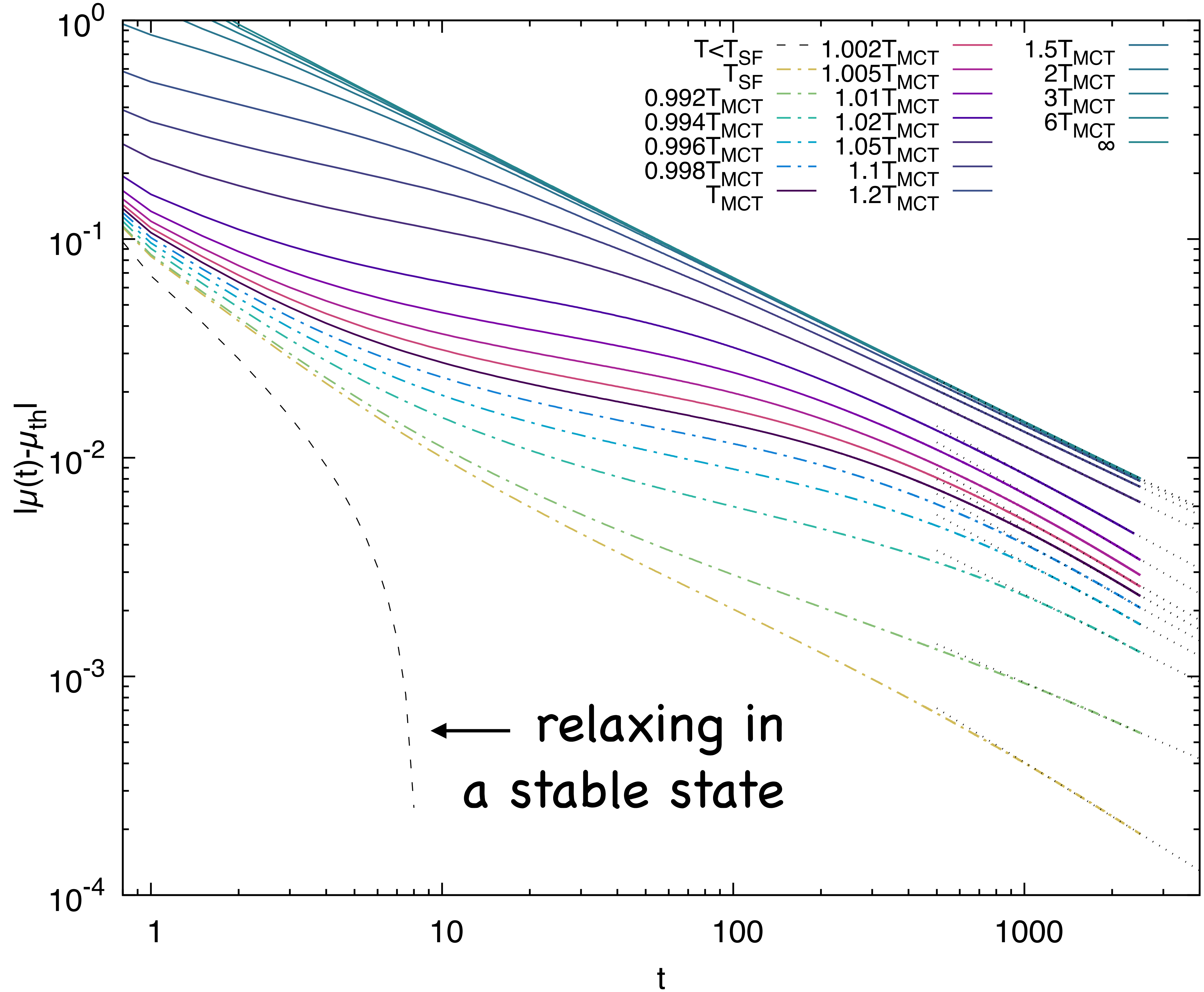
pure model marginal states concentrate at $e_{th} = -\dfrac{\mu_{th}}{p}$

mixed model has marginal states at different energies!

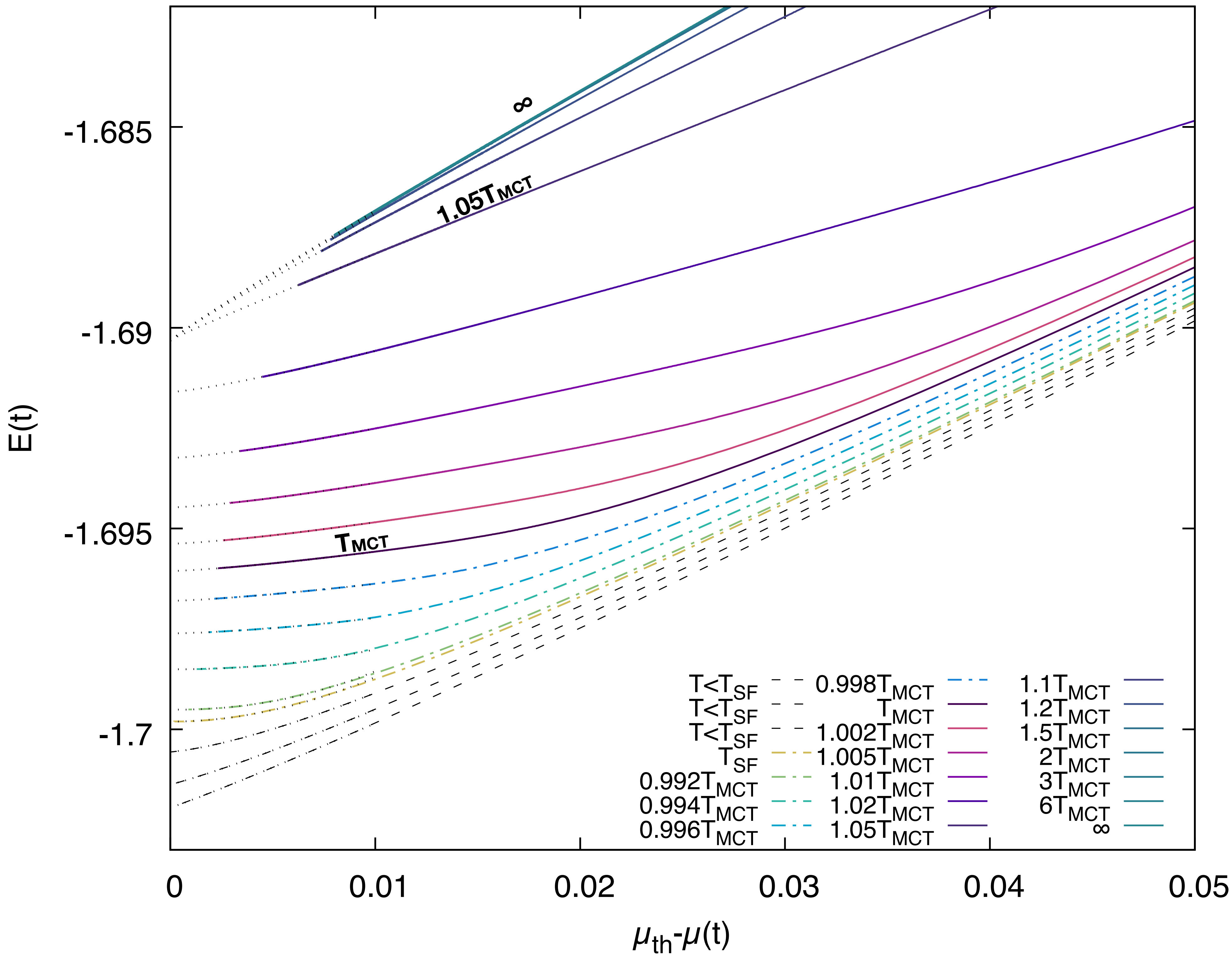
Radial reaction in the (3+4)-spin



Radial reaction in the (3+4)-spin



Energy vs radial reaction



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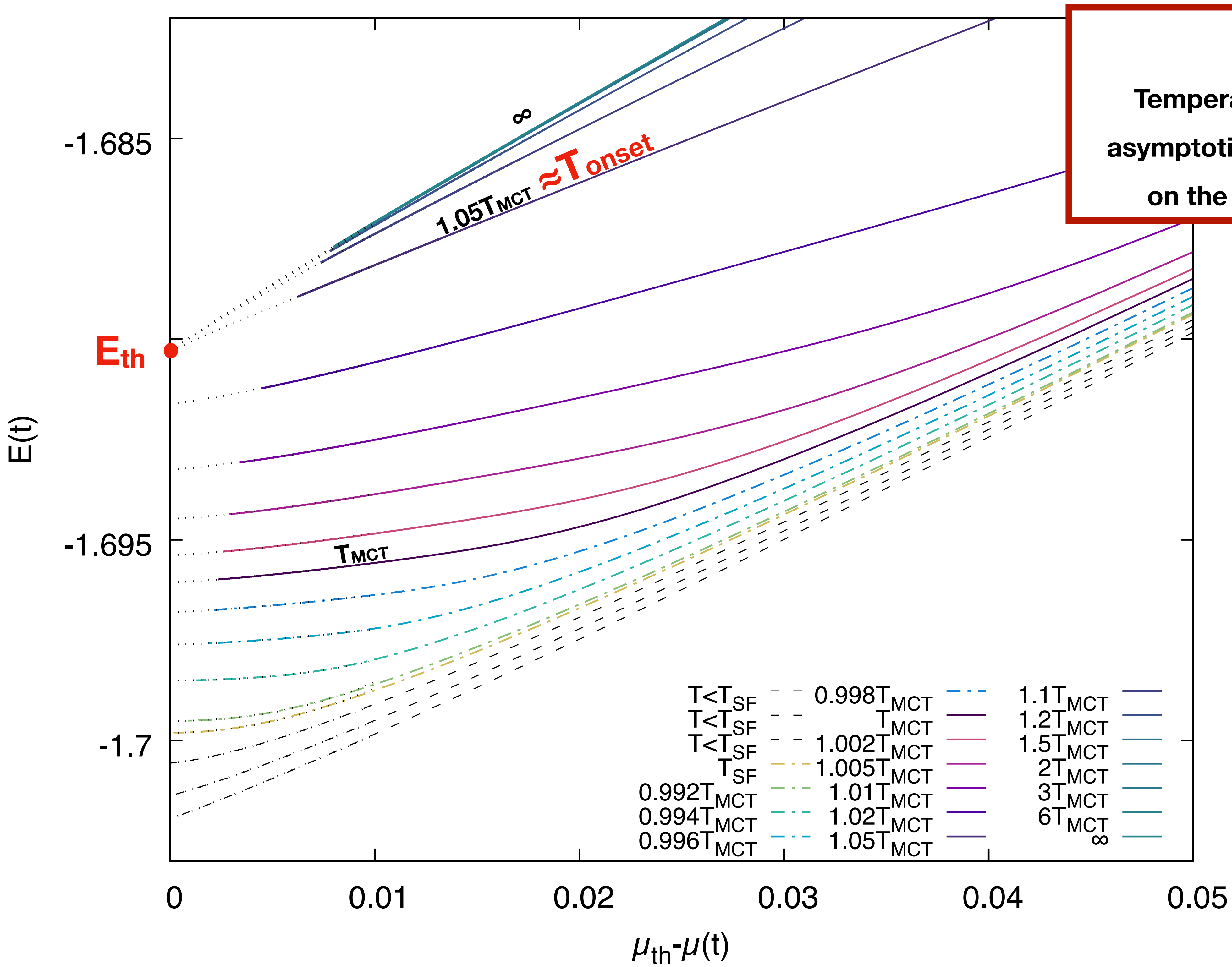
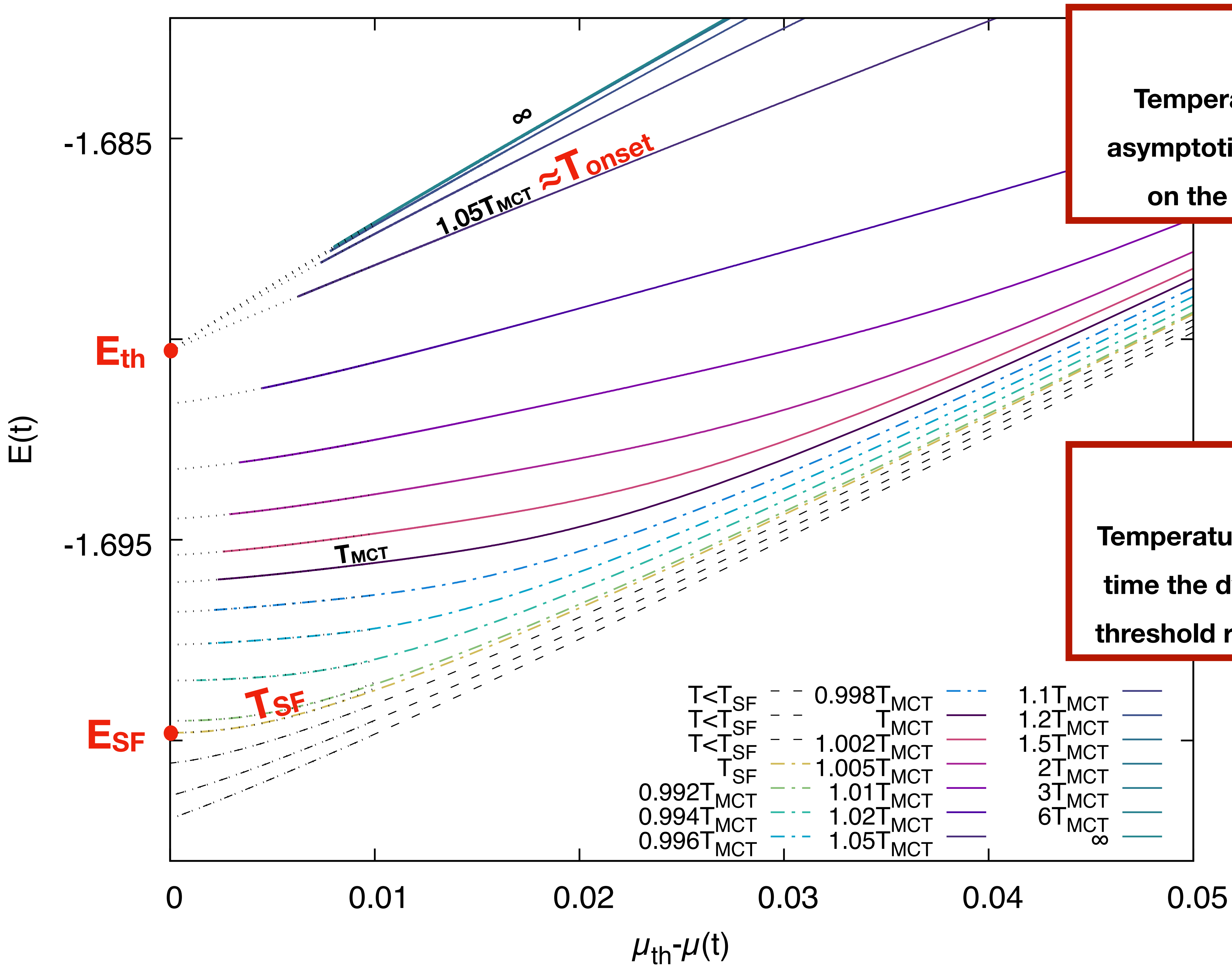


T_{onset}

Temperature above which the asymptotic energy is independent on the starting temperature

Energy vs radial reaction



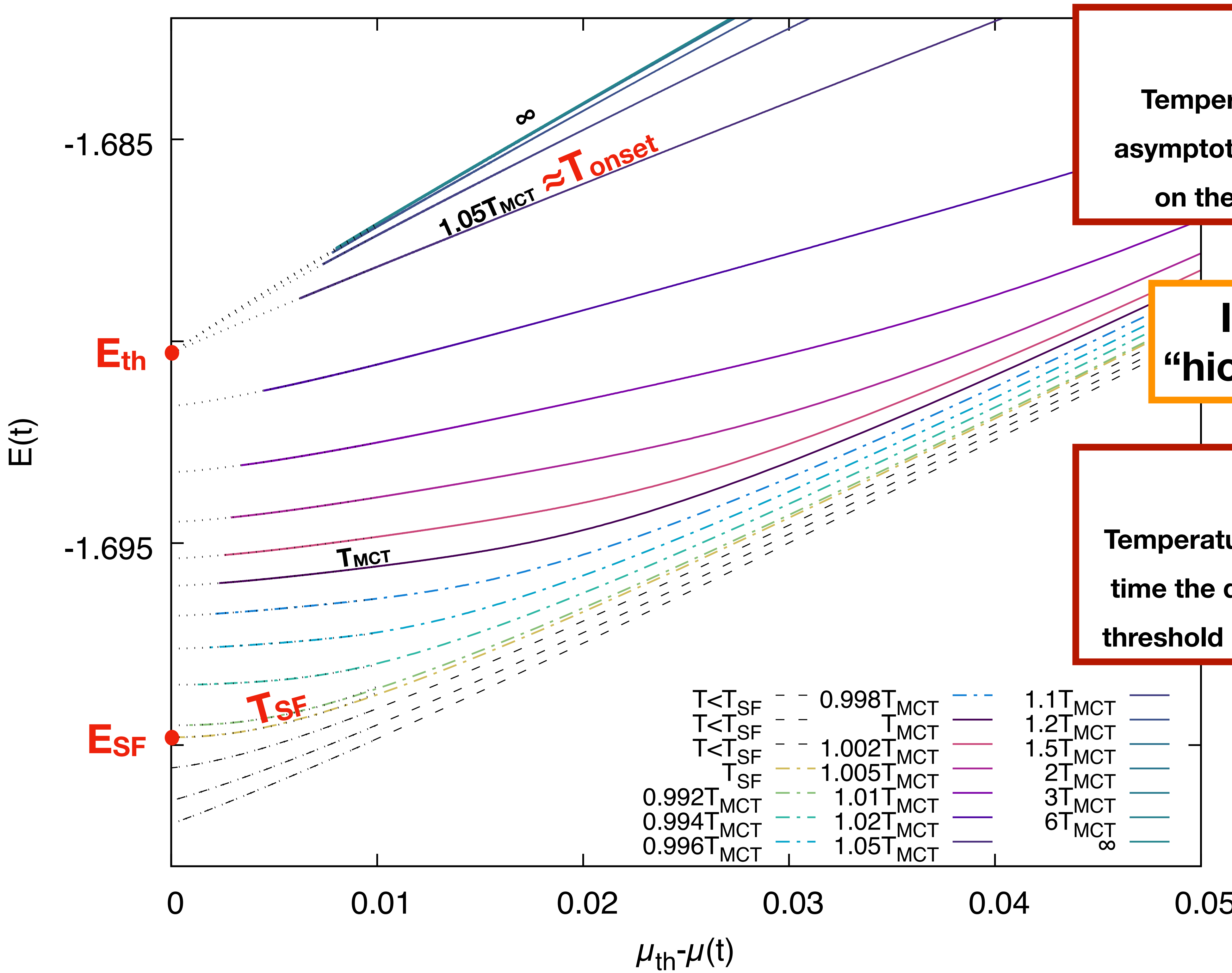
T_{onset}

Temperature above which the asymptotic energy is independent on the starting temperature

T_{SF}

Temperature below which in a finite time the dynamics goes above the threshold radial reaction ($\mu > \mu_{th}$)

Energy vs radial reaction



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In between "hic sunt leones"

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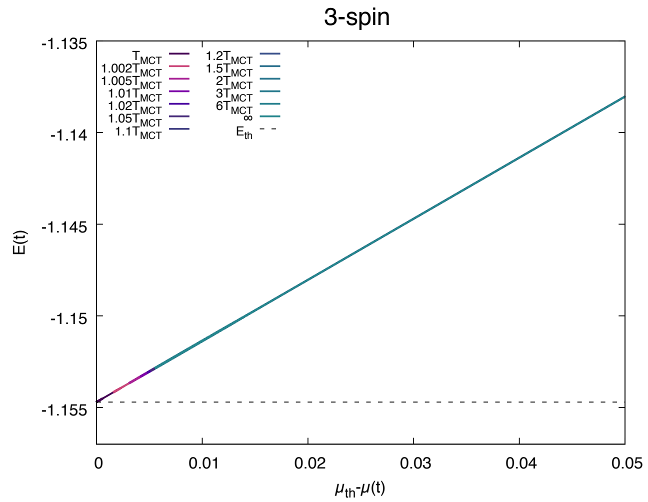
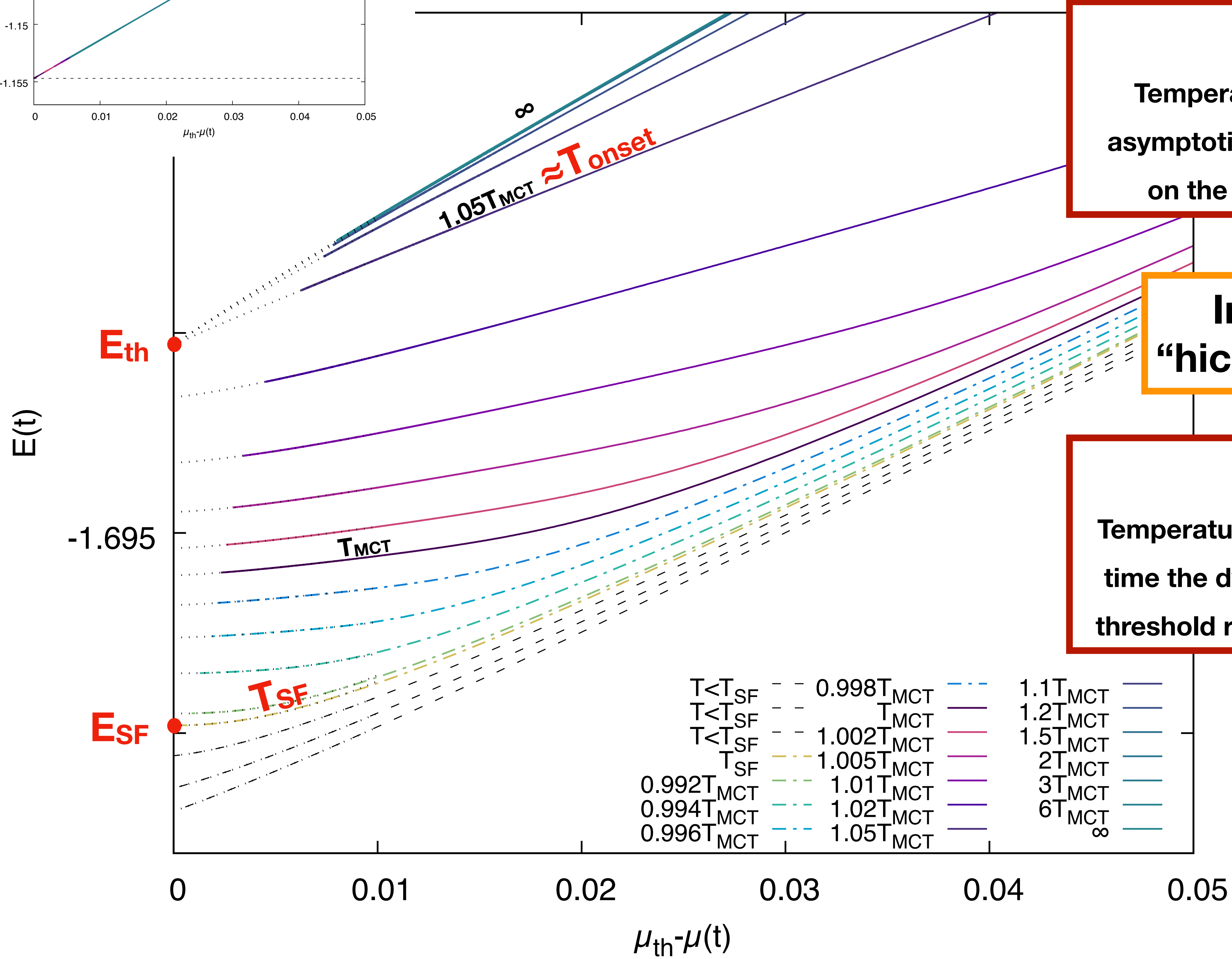
Temperature below which in a finite time the dynamics goes above the threshold radial reaction ($\mu > \mu_{th}$)

Energy vs radial reaction





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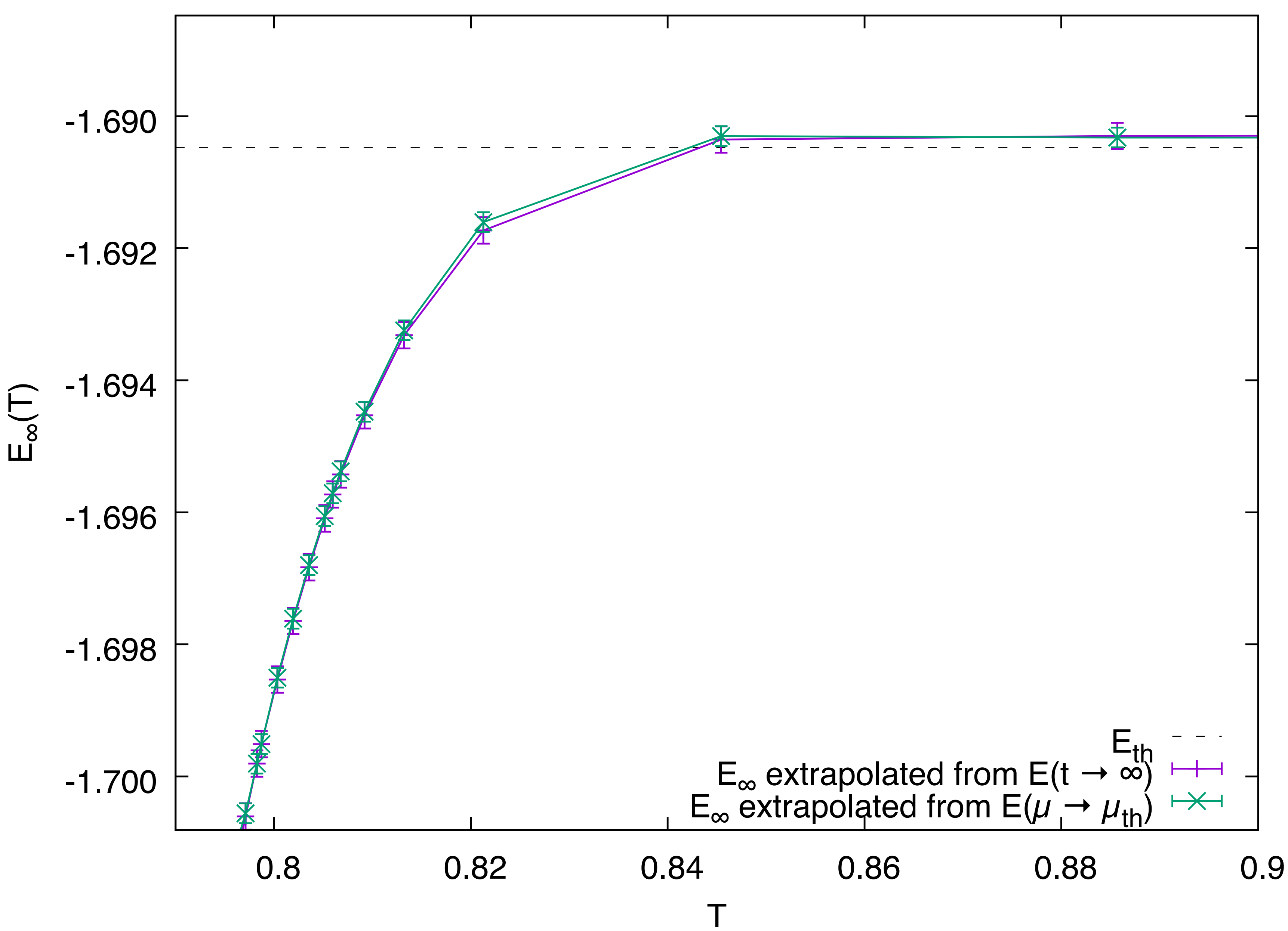
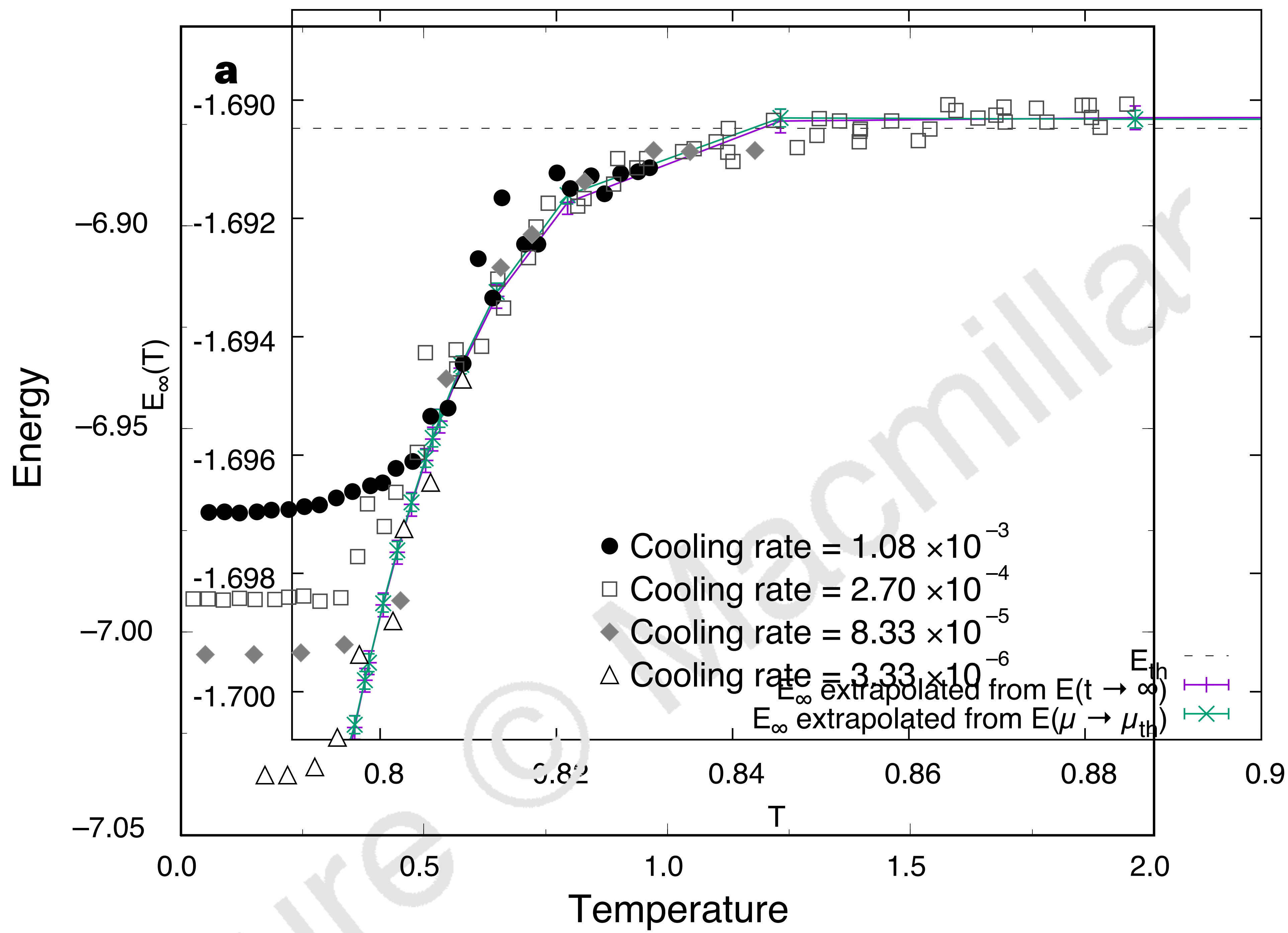
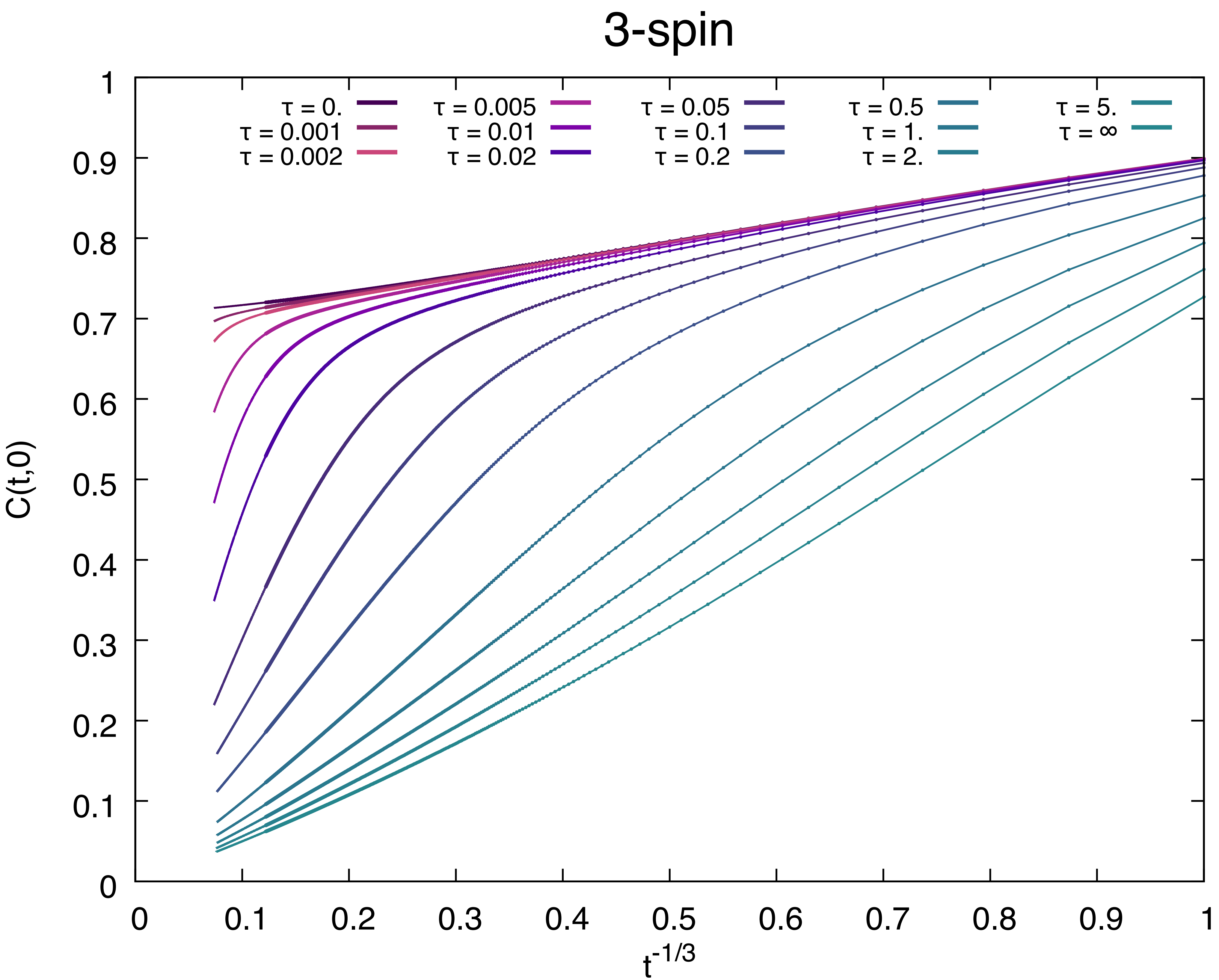
Asymptotic energy



Asymptotic energy



Correlation with the initial configuration



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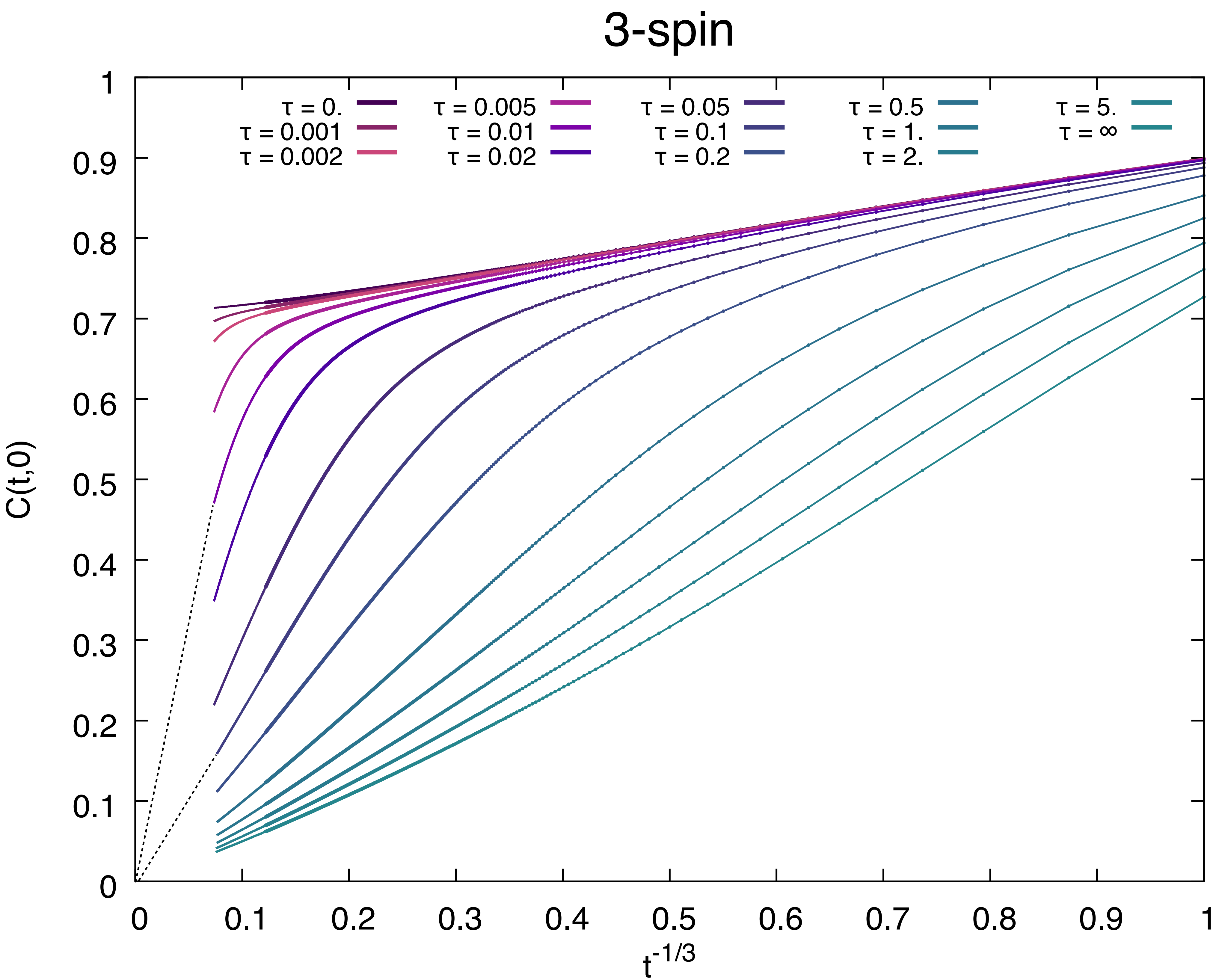

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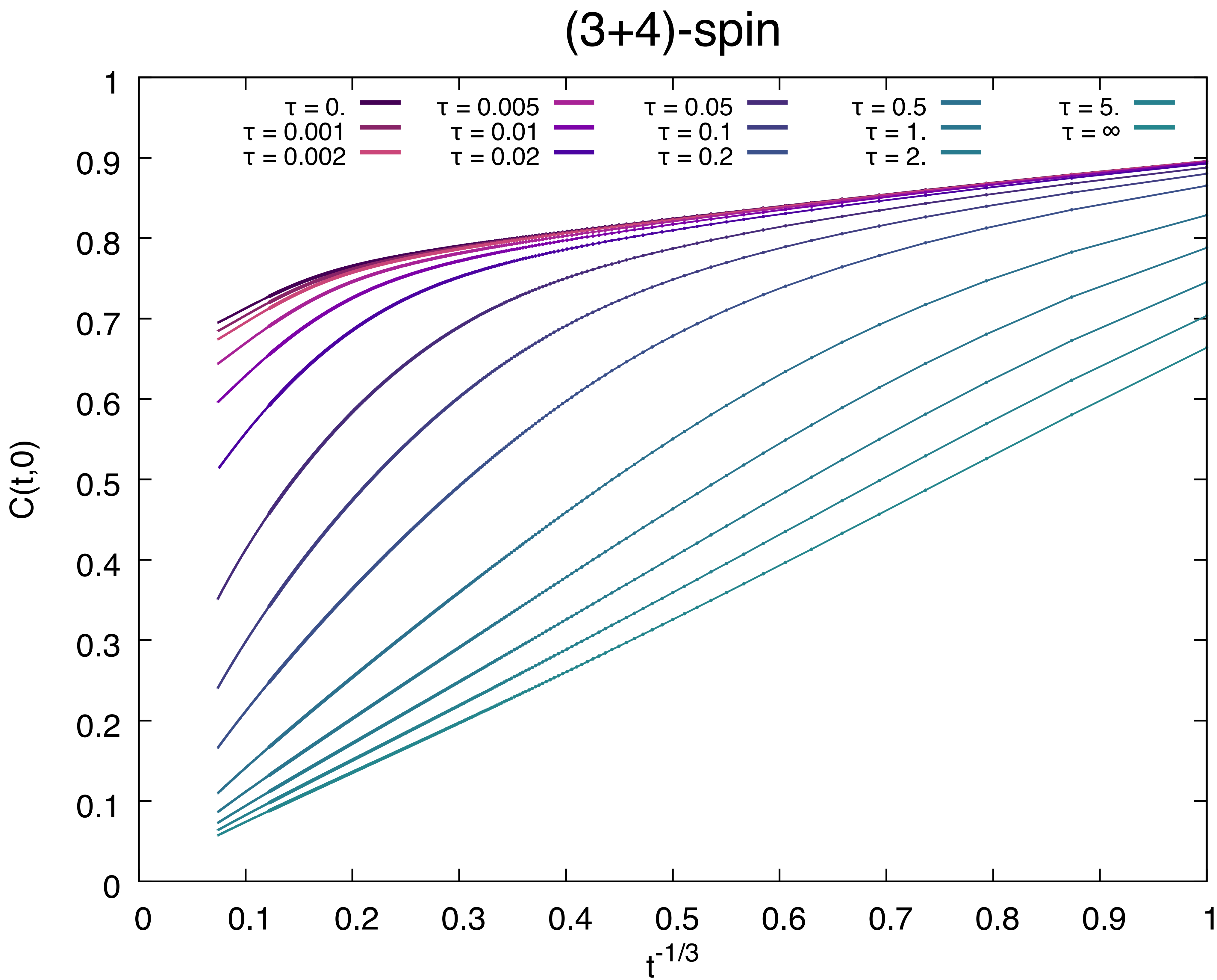

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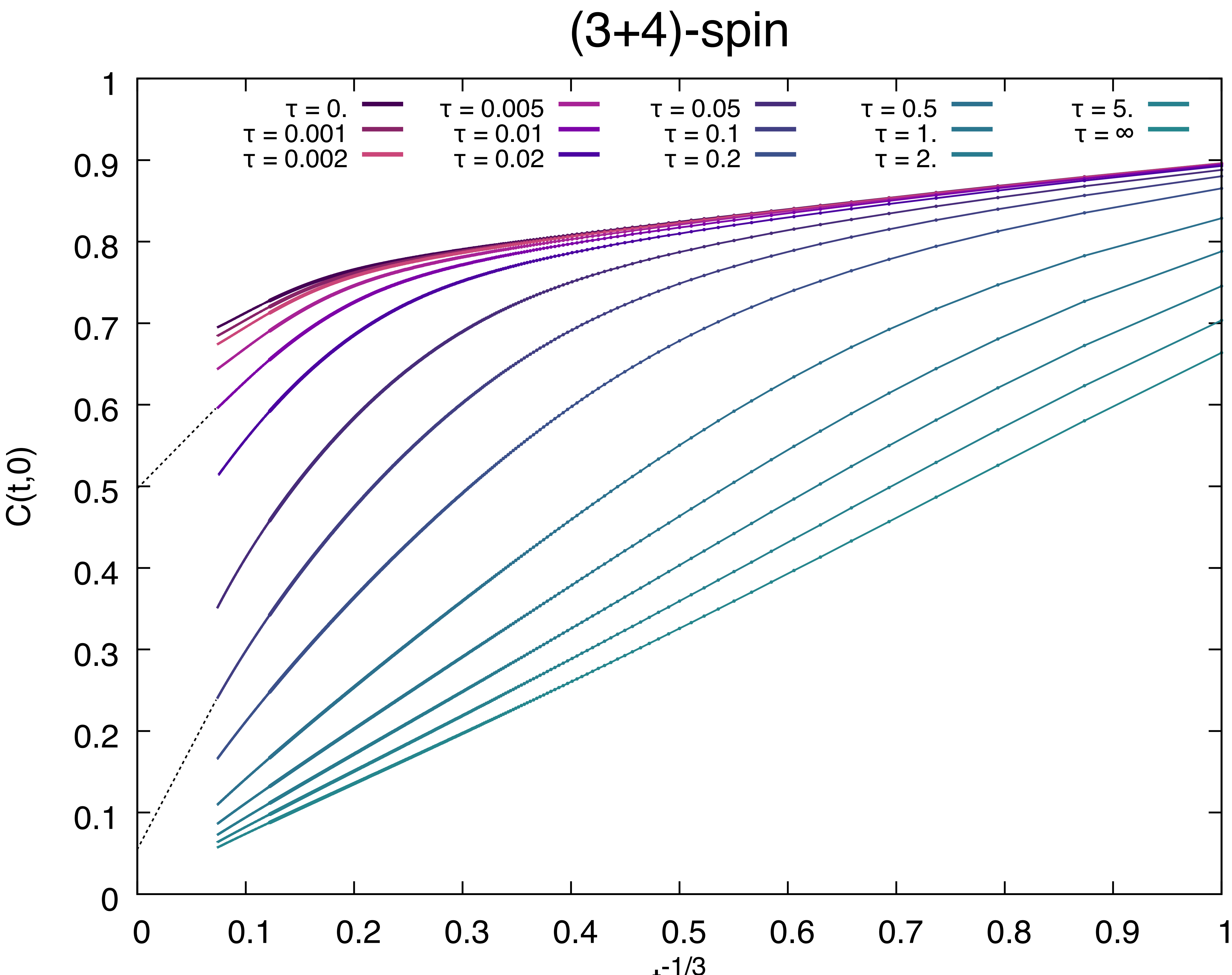
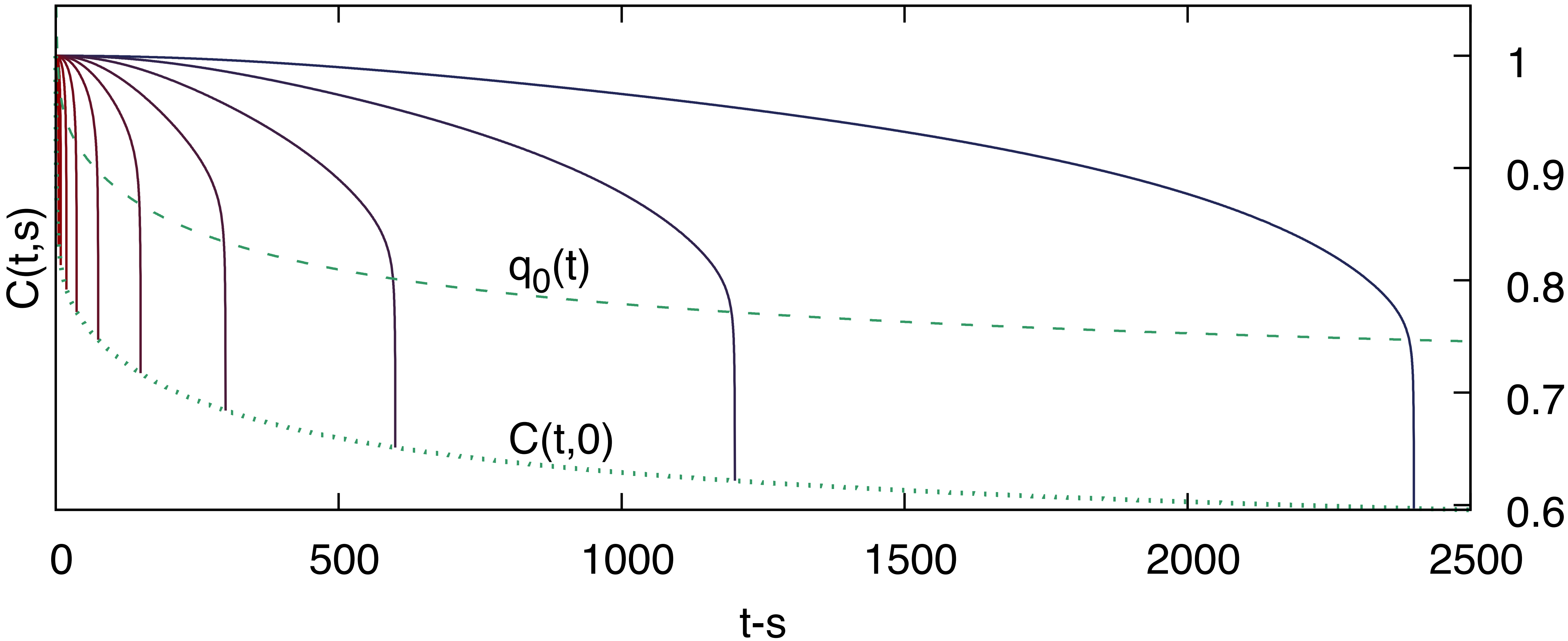


Aging for $T>T_{SF}$



T=0 fluctuation-dissipation plot

- parametric plot in t′ at fixed t

$$\chi(t,t') = \int_{t'}^{t} R(t,s)ds \quad \text{vs.} \quad C(t,t')$$

- marginality at T=0

$$\chi_{th} = \lim_{T\to 0} \frac{1-q_m}{T} = \frac{1}{\sqrt{f''(1)}}$$

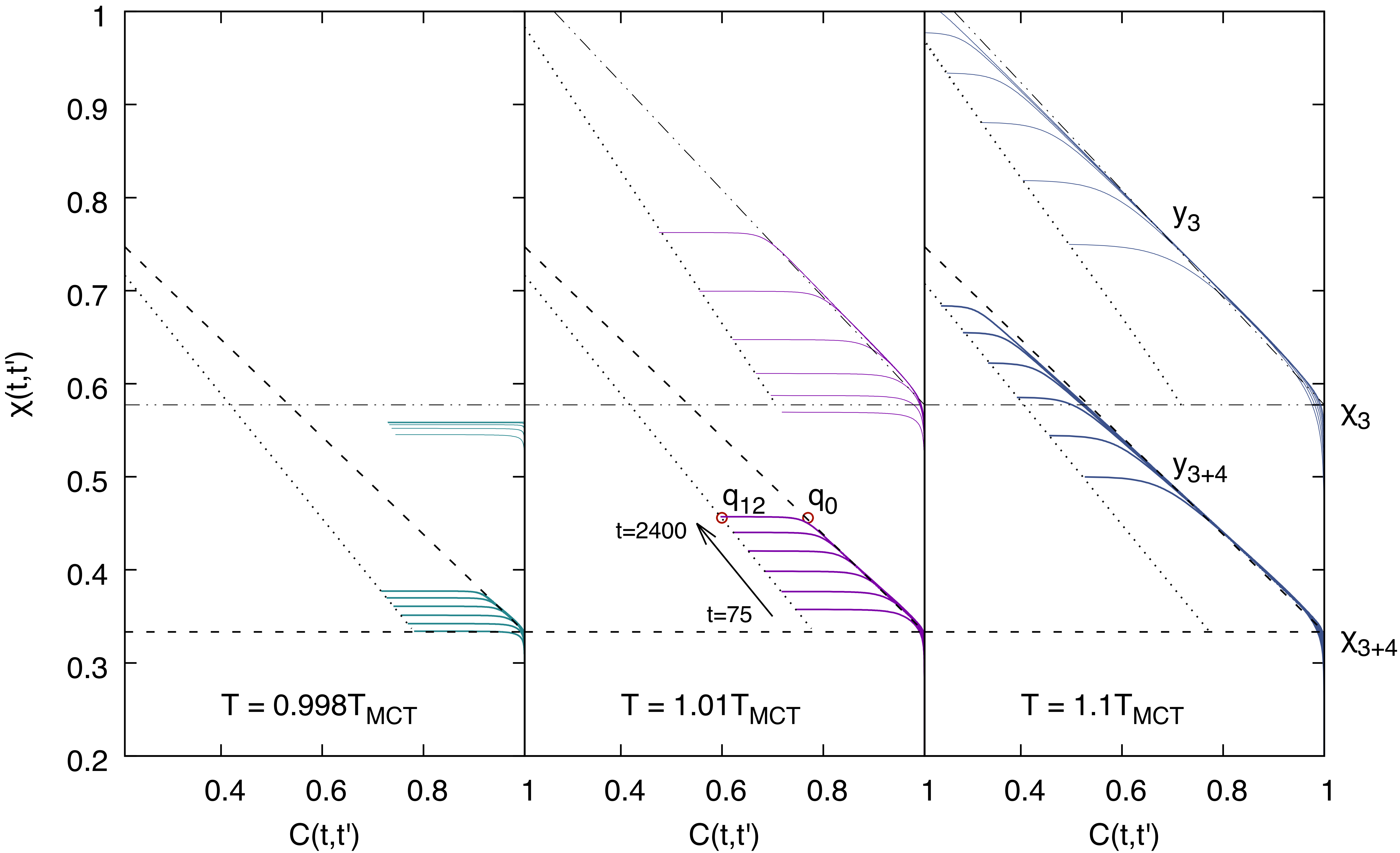
- memoryless solution has

$$q_0 = q_{12} = 0$$

$$y_0 = \lim_{T\to 0} \frac{x_0}{T} = \frac{\sqrt{f''(1)}}{f'(1)} - \frac{1}{\sqrt{f''(1)}}$$

$$x_0 = \partial_E \Sigma(E_{th})$$

T=0 fluctuation-dissipation plot

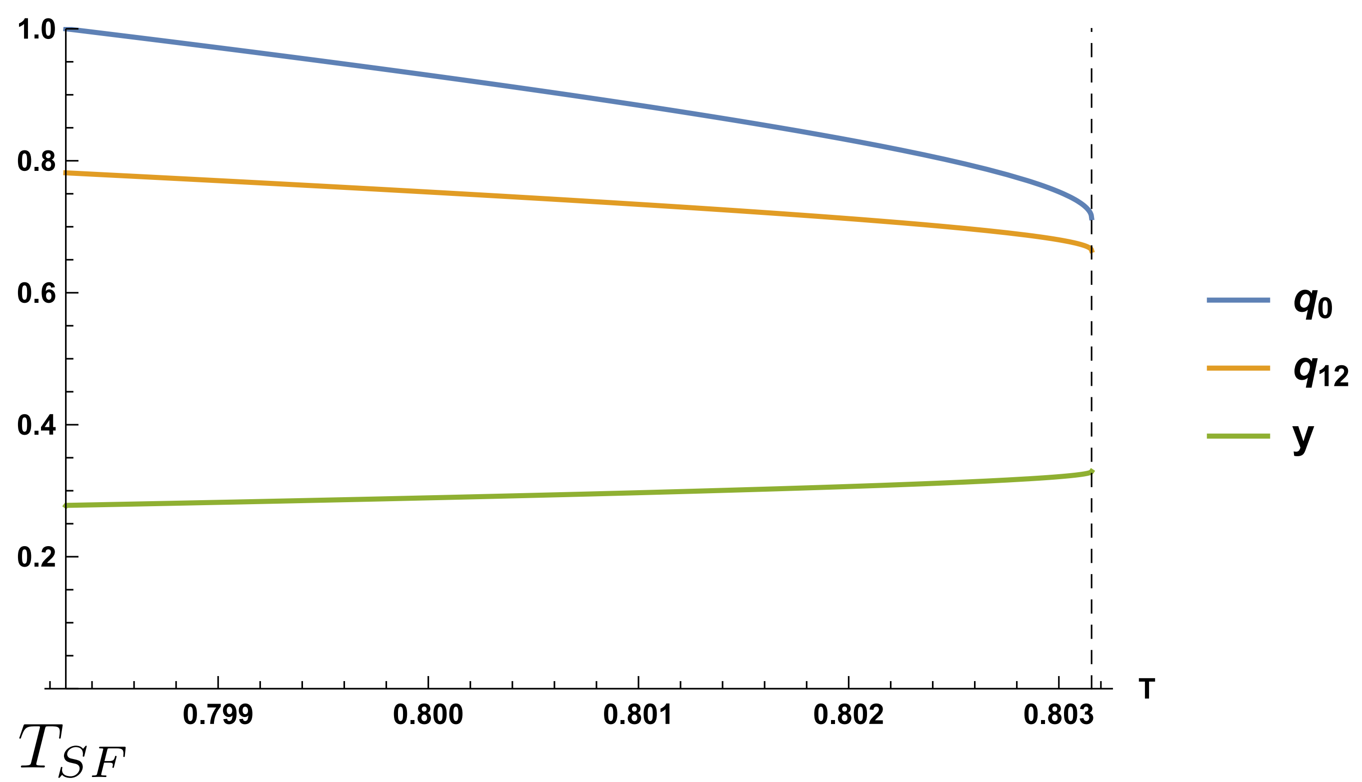


Search for the asymptotic solution

- Standard approach

$$-2V_{\mathrm{1RSB}}(q_{12},\chi,q_0,y)=\chi f'(1)+y(f(1)-f(q_0))+\frac{1}{y}\log\left(\frac{\chi+y(1-q_0)}{\chi}\right)+\frac{q_0-q_{12}^2}{\chi+y(1-q_0)}+2\beta f(q_{12})$$

$$\begin{cases}\partial_\chi V_{\mathrm{1RSB}}=0 & \Longrightarrow\ \chi(1-q_{12}^2)+y(1-q_0)^2-\chi(\chi+y(1-q_0))^2f'(1)=0\\ \partial_{q_0}V_{\mathrm{1RSB}}=0 & \Longrightarrow\ q_0-q_{12}^2-(\chi+y(1-q_0))^2f'(q_0)=0\\ \partial_{q_{12}}V_{\mathrm{1RSB}}=0 & \Longrightarrow\ q_{12}-\beta(\chi+y(1-q_0))f'(q_{12})=0\\ \text{marginality} & \Longrightarrow\ \chi^2f''(1)=1\end{cases}$$



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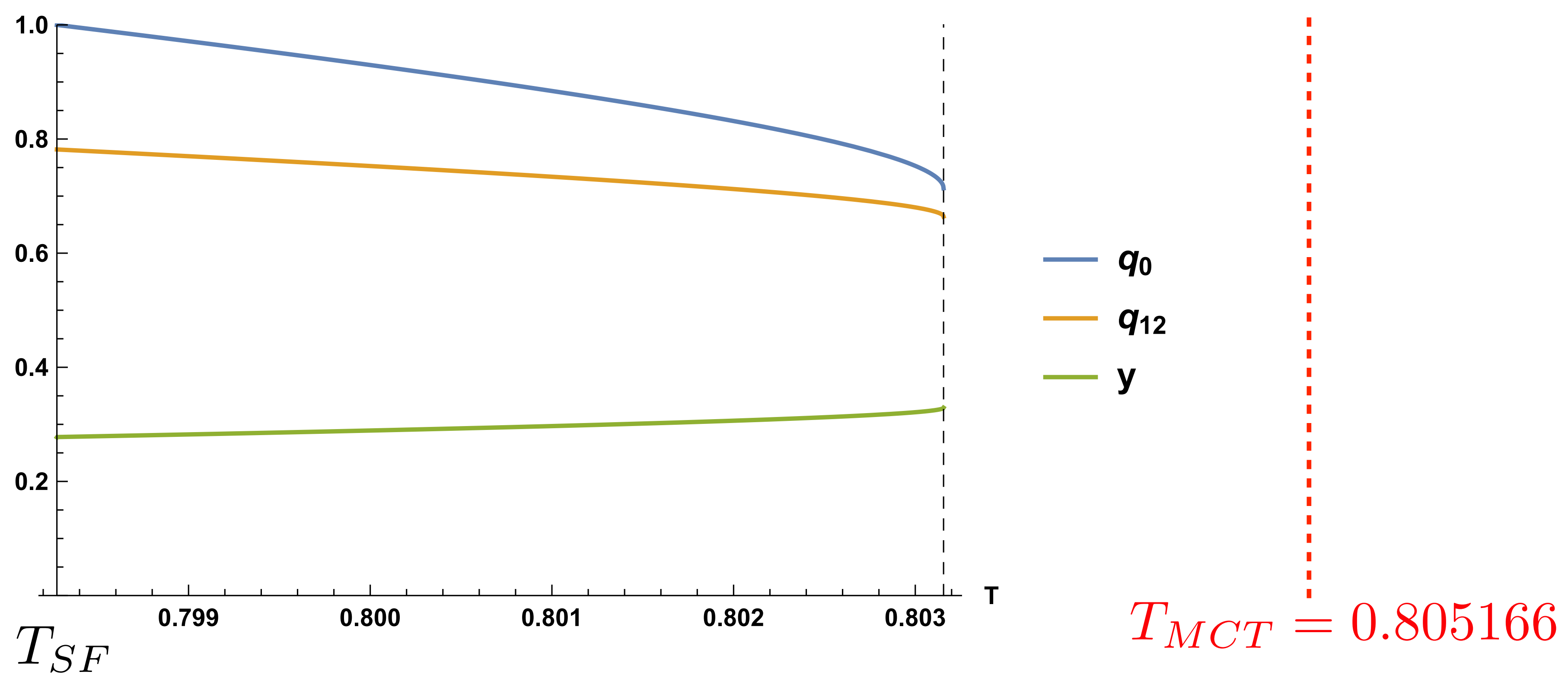

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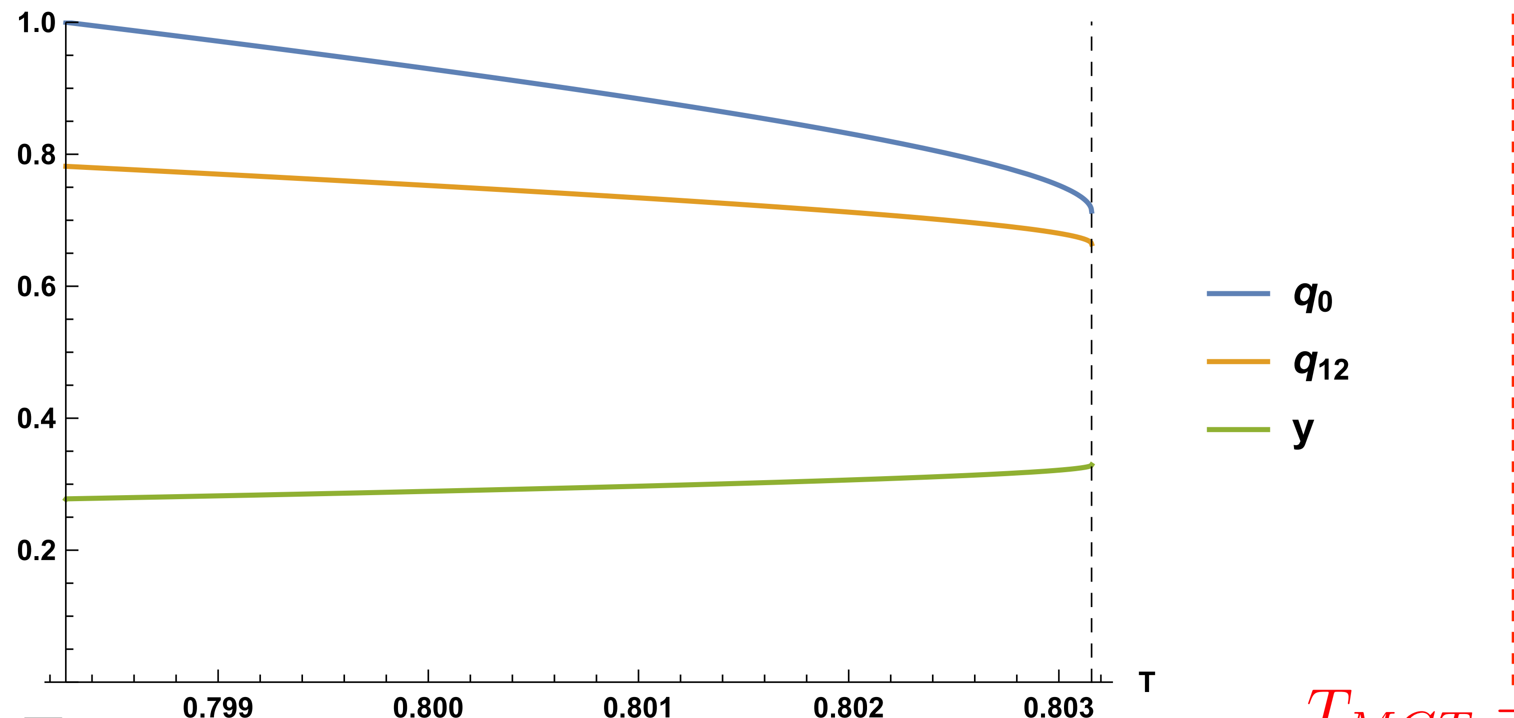
Too small y!!



T_{SF}

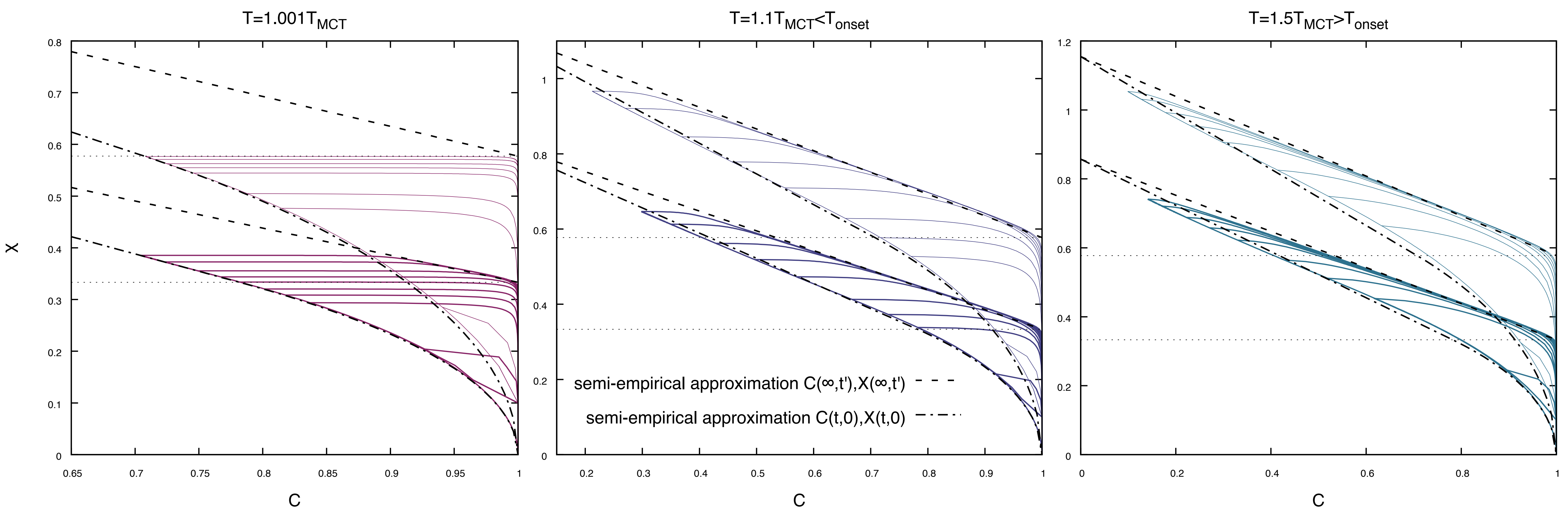
$T_{MCT}=0.805166$

Search for the asymptotic solution

- Our approximated ansatz

$$\mu = \mu_{th} \qquad \chi = \chi_{th} \qquad y = \begin{cases} 0 & q_{12} < C < q_0 \\ y_0 & q_0 < C < 1 \end{cases}$$

Linear relation between q_{12} and q_0



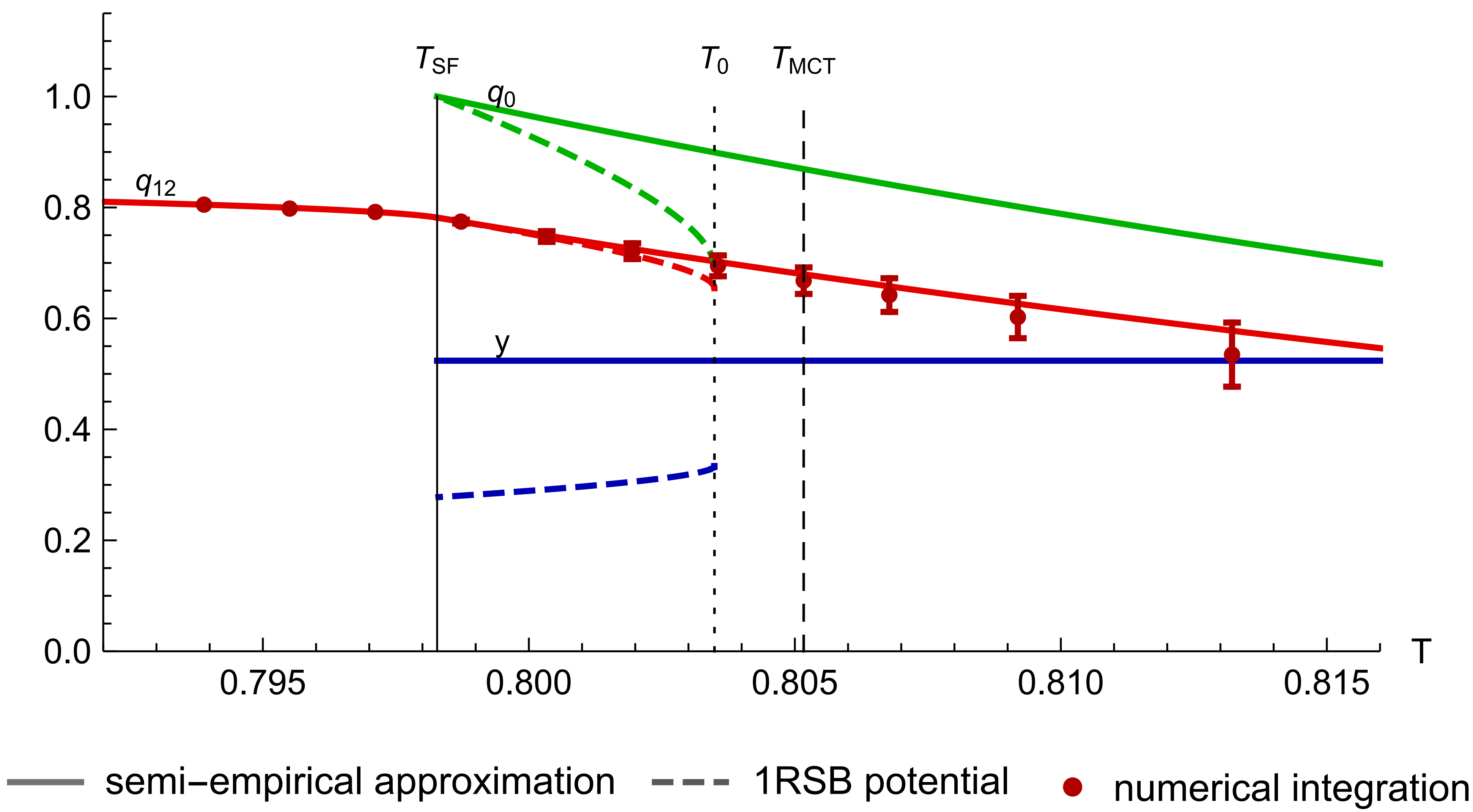
Dashed and dash-dotted lines are the same in all panels!

Search for the asymptotic solution

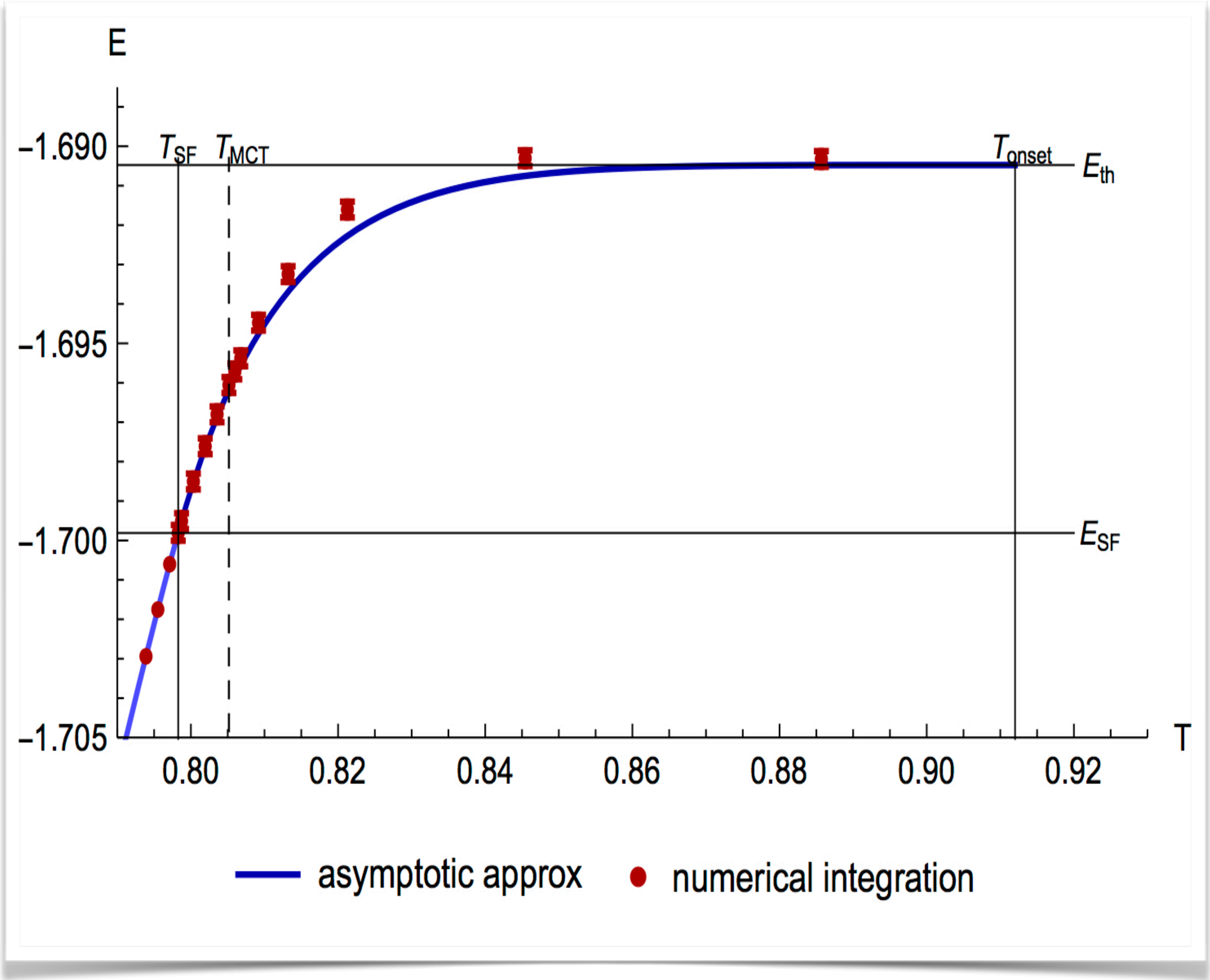
- Our approximated ansatz predicts a non-zero q_{12} for

$$T < T_{\mathrm{onset}} \equiv \frac{q_{12,\mathrm{SF}}^k}{y_0} = \frac{f'(1)[f''(1) - f'(1)]^{\frac{k}{2}-1}}{f''(1)^{\frac{k-1}{2}}}$$

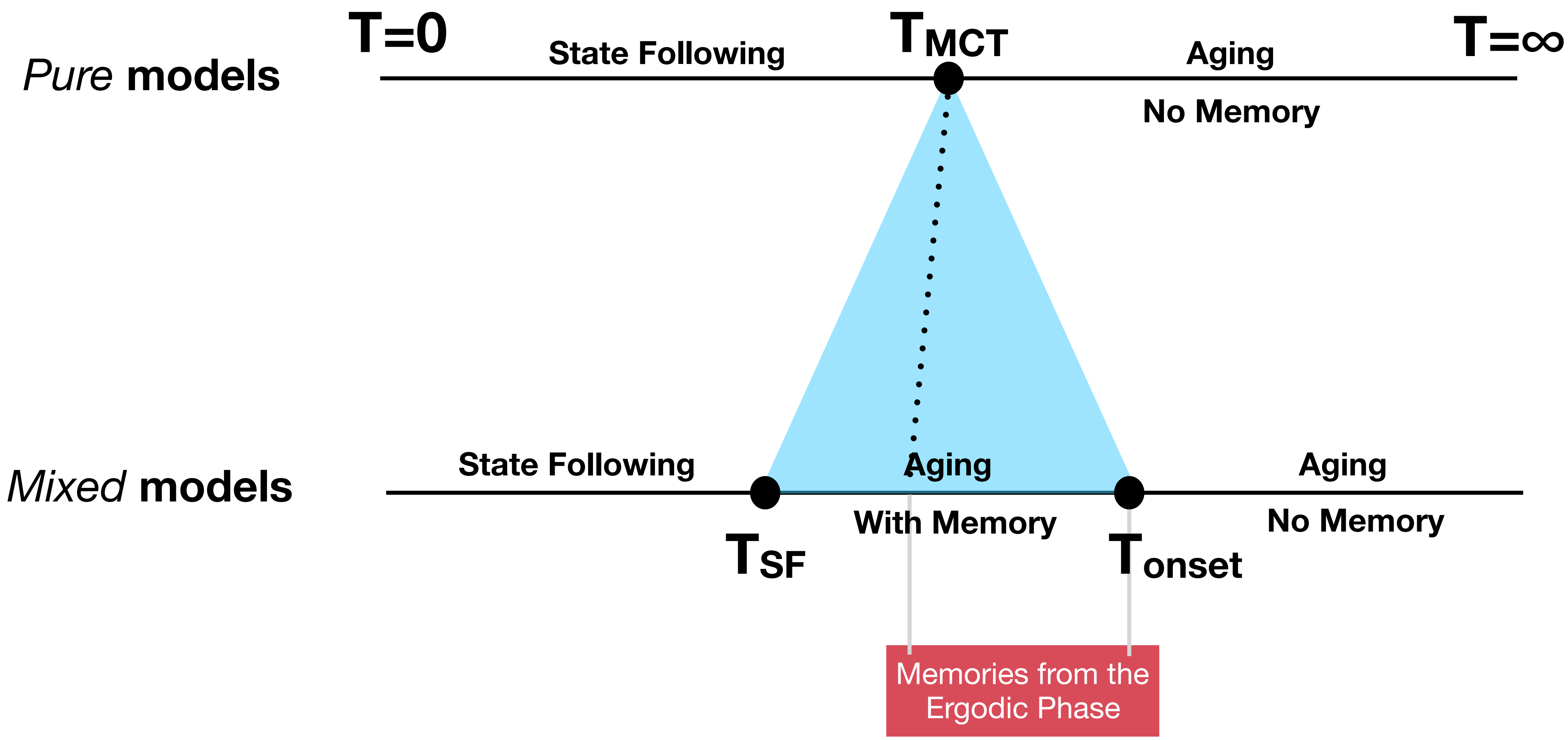
$$f(q) \propto q^k \text{ for } q \to 0$$



We can predict the asymptotic energy



A new phase in mixed models



Can we predict the dynamics asymptotic via a static complexity computation?

- Zero temperature relaxation dynamics goes to local minima
- Count the mean logarithm of the number of local minima at fixed overlap q_{12} to an equilibrium configuration at T

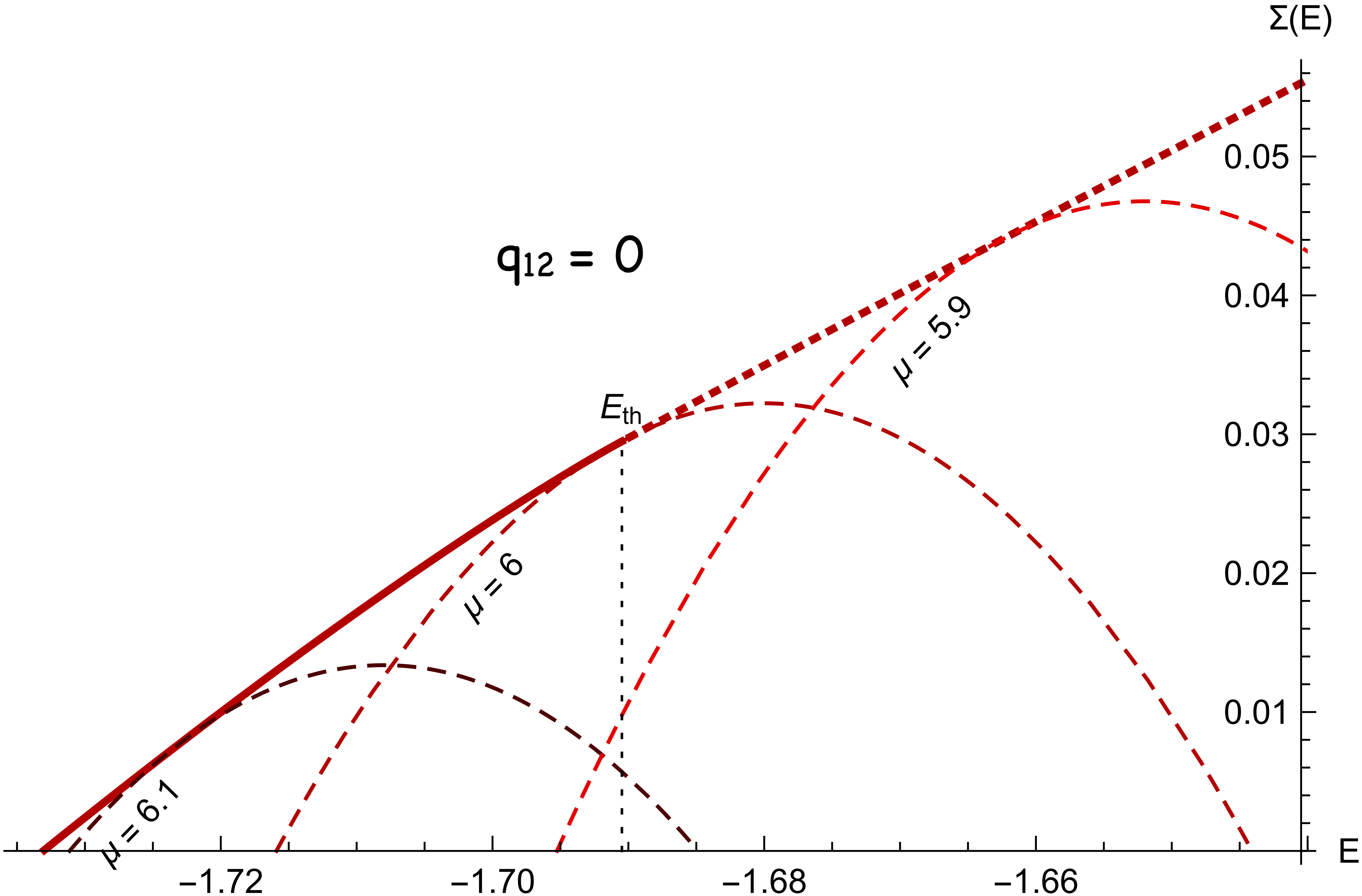
$$\Sigma(q_{12},T,E,\mu) = \mathbb{E}_J \int \mathcal{D}\underline{\sigma}^0 \, e^{-H_J(\underline{\sigma}^0)/T}$$

$$\log\left[\int \mathcal{D}\underline{\sigma}\, \delta\Big(\underline{\sigma}\cdot\underline{\sigma}^0 - q_{12}N\Big)\delta\Big(H_J(\underline{\sigma})-E\Big)\delta\Big(\nabla H_J(\underline{\sigma})+\mu\underline{\sigma}\Big)\Big|\det(\mathbb{H}(H_J(\underline{\sigma}))+\mu\mathbb{I})\Big|\right]$$

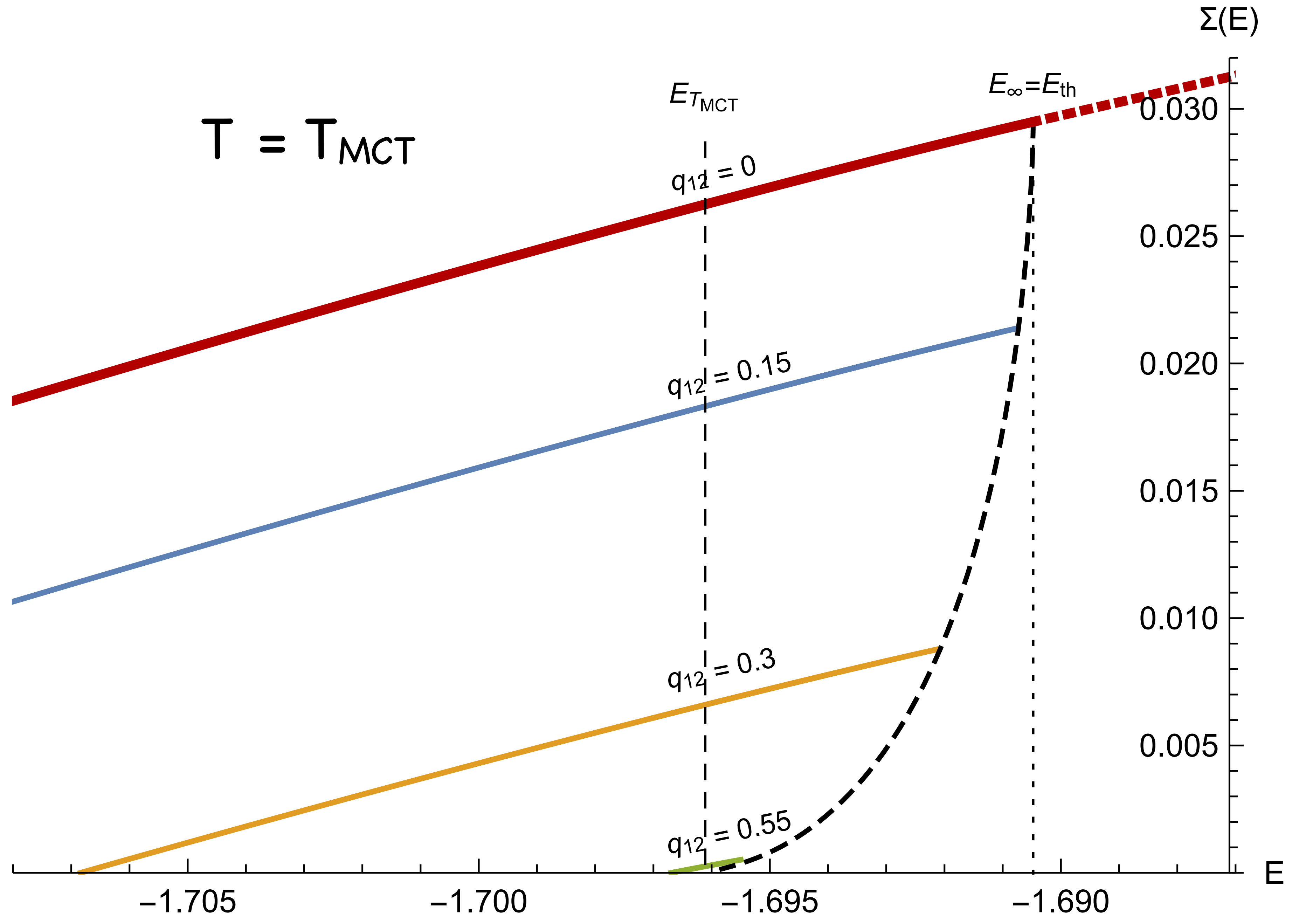
- Good candidates for describing the dynamics at large times are marginal stationary points of the energy function

Complexity in the mixed model

in the (3+4)-spin $\mu_{th} = 6$



Complexity in the mixed model



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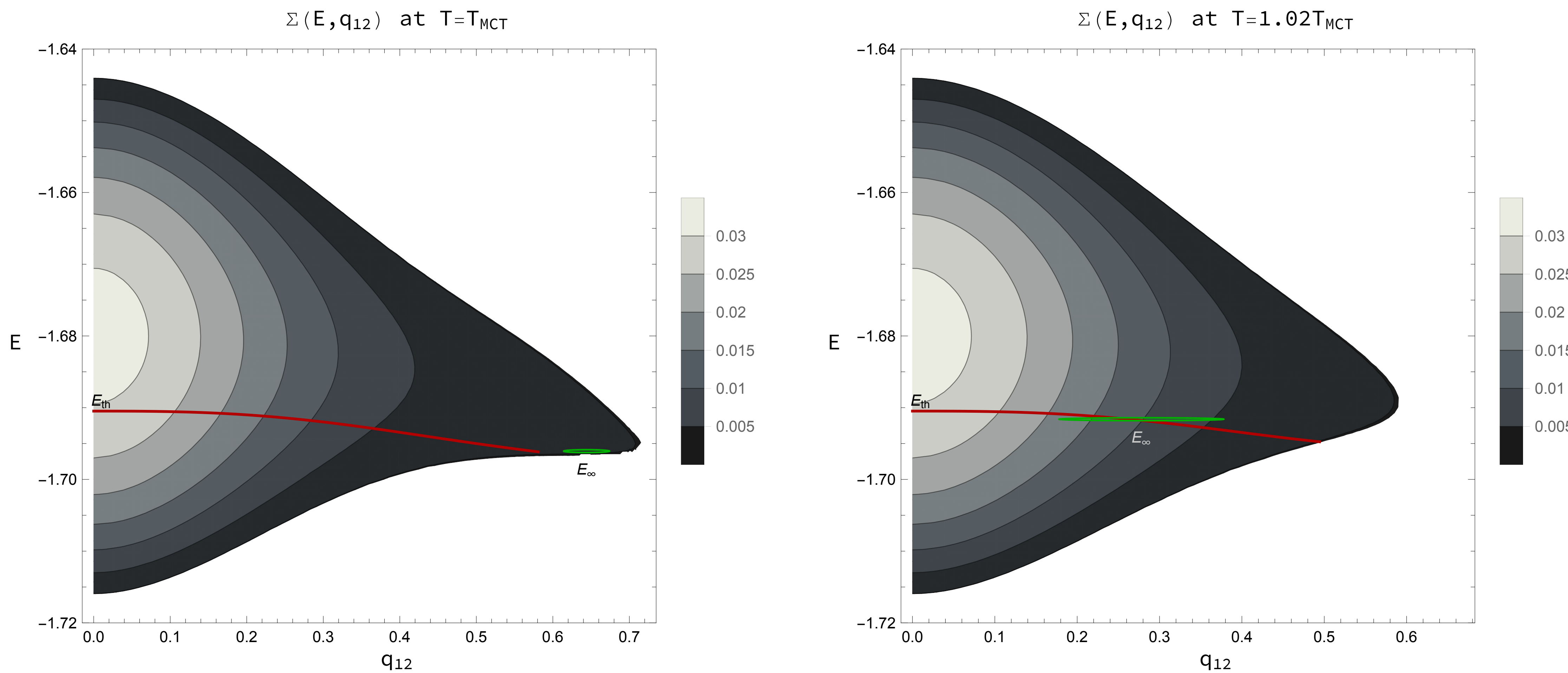

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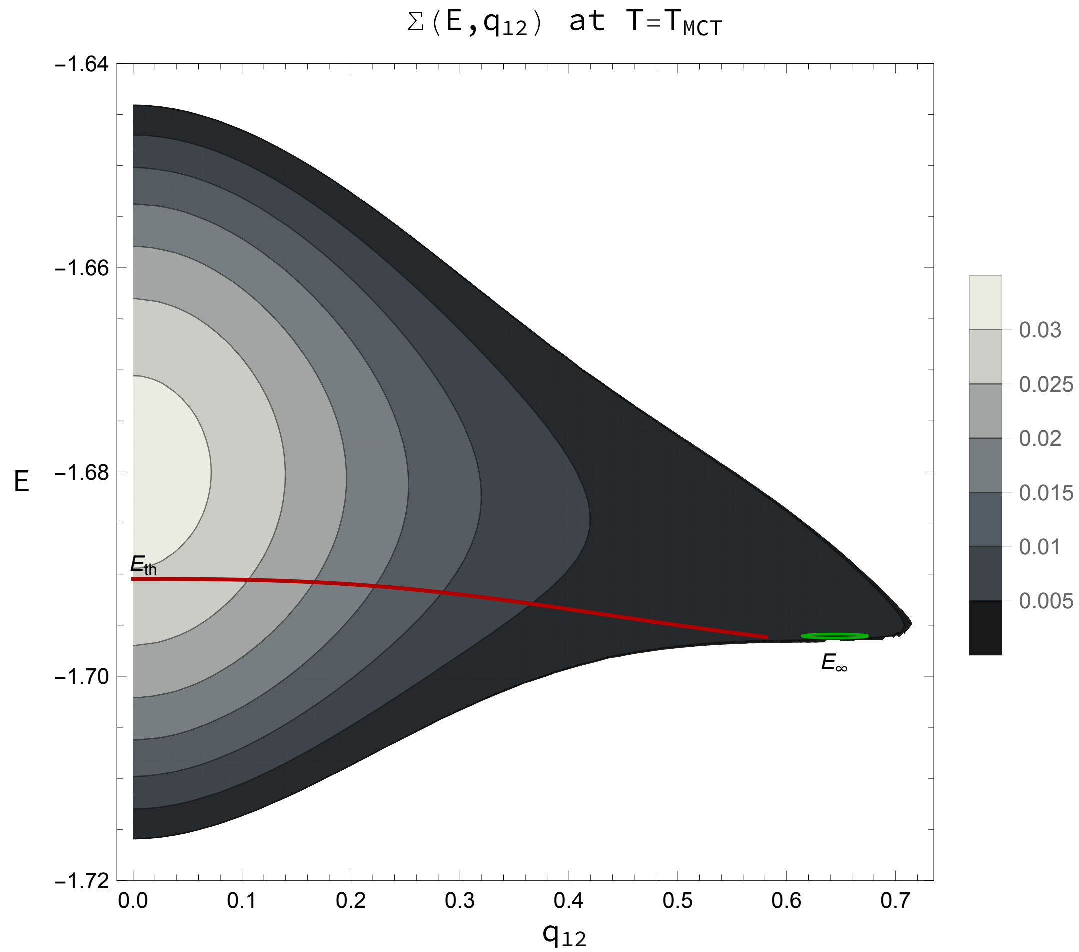

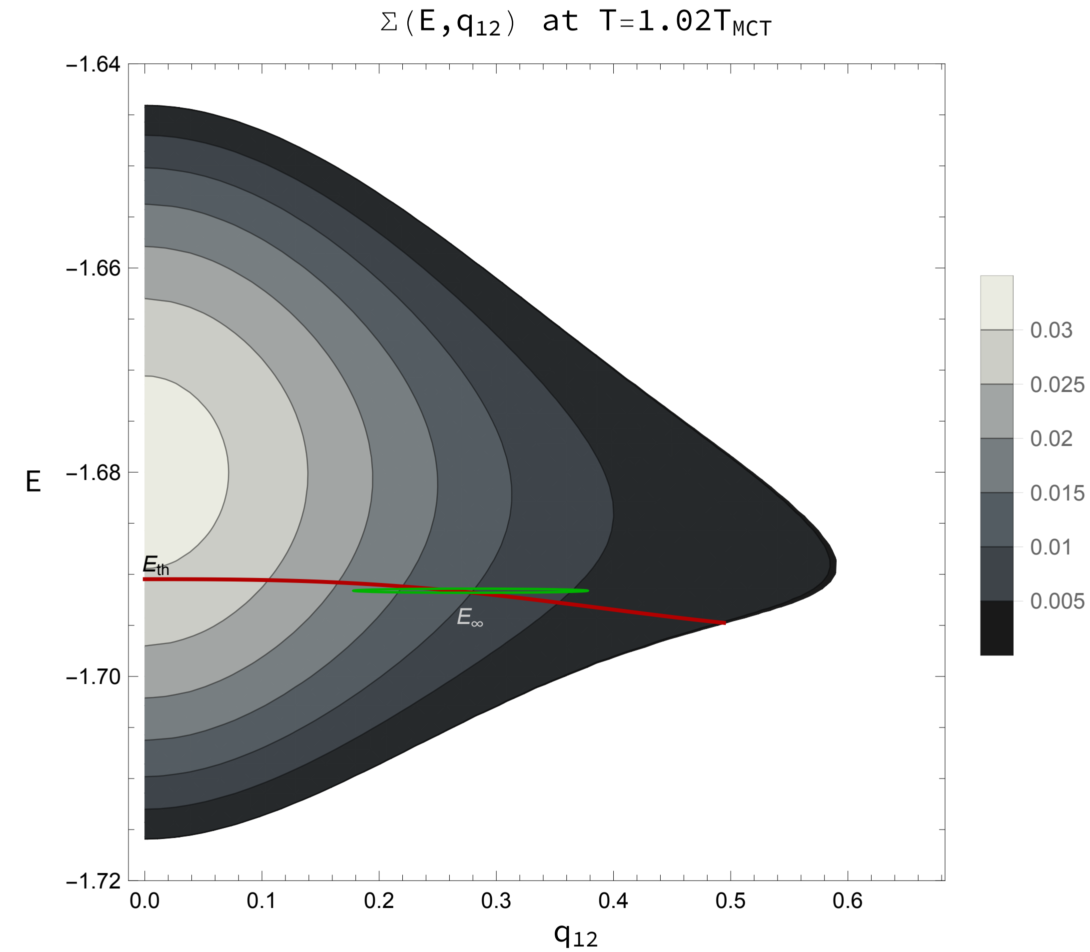

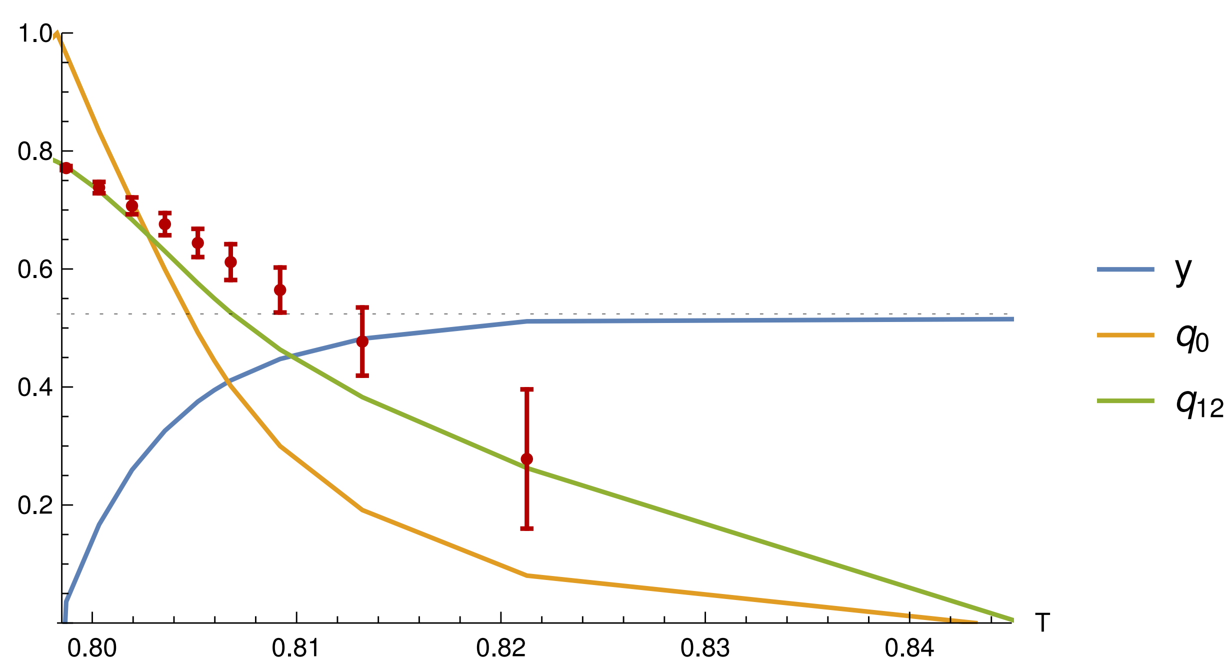

Satisfied with the constrained complexity?

- Explains well why marginals states closer to the initial configuration ($q_{12}>0$) have lower energies
- Predicts too low values for y and q_0

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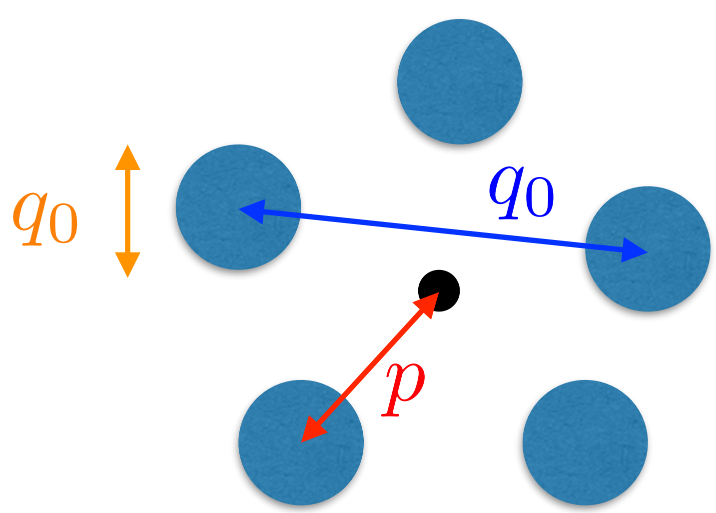
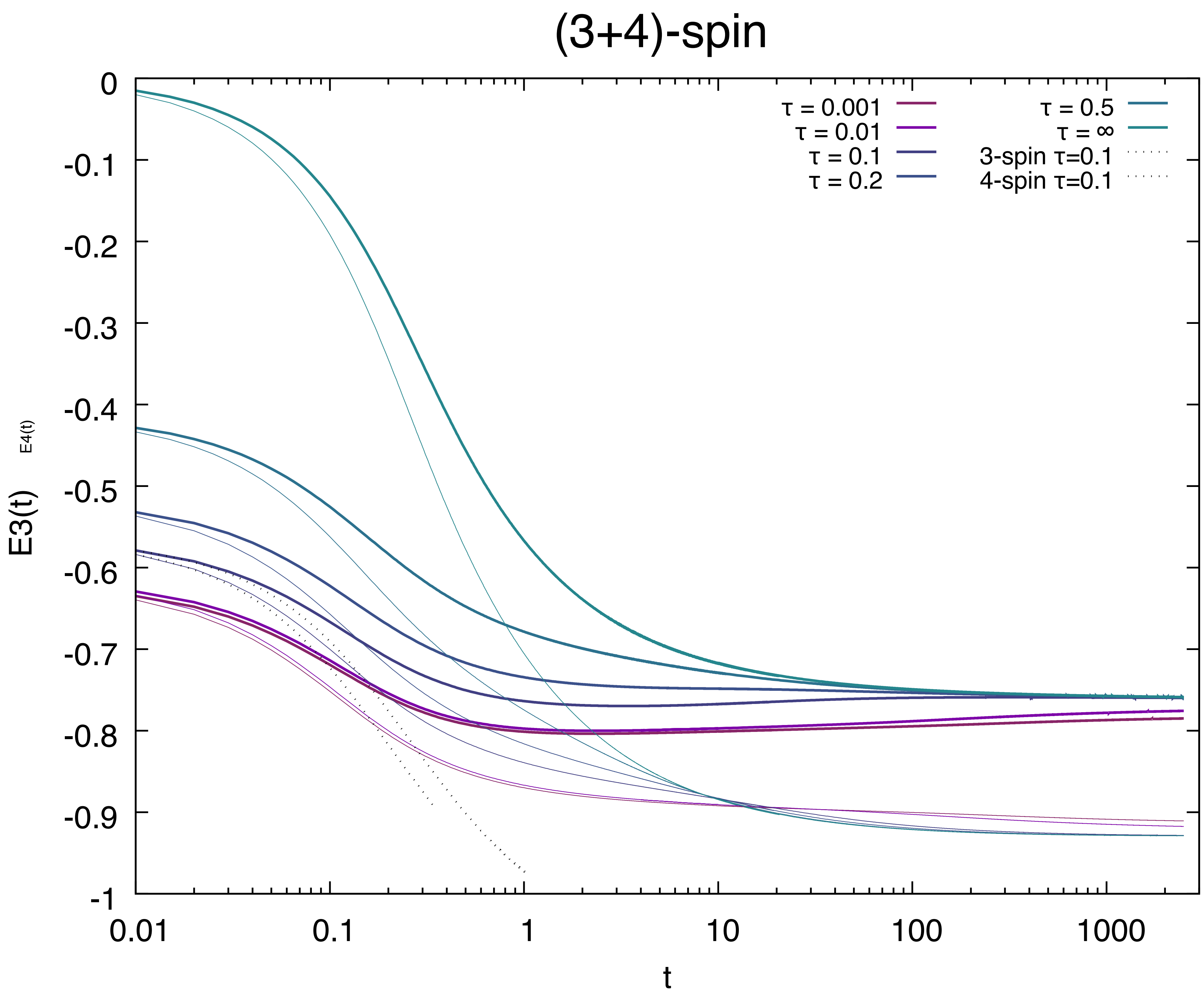


Possible explanation:
- dynamics gets trapped and makes aging in just one marginal manifold (large q_0)
- static complexity counts them all (small q_0)

Conclusions

- Unexpected new dynamical regime: **aging with memory**
  - the configuration at initial or short time is **not forgotten** (strong ergodicity breaking)
  - long time dynamics takes place in a **restricted marginal manifold**
  - in this regime the model reproduces important features of glass formers
- The statics-dynamics connection should be rethought: predicting the long time behavior of Langevin dynamics is an open problem for mixed (i.e. realistic) models
- More details can be found in arXiv:1903.01421

How it goes below the threshold?



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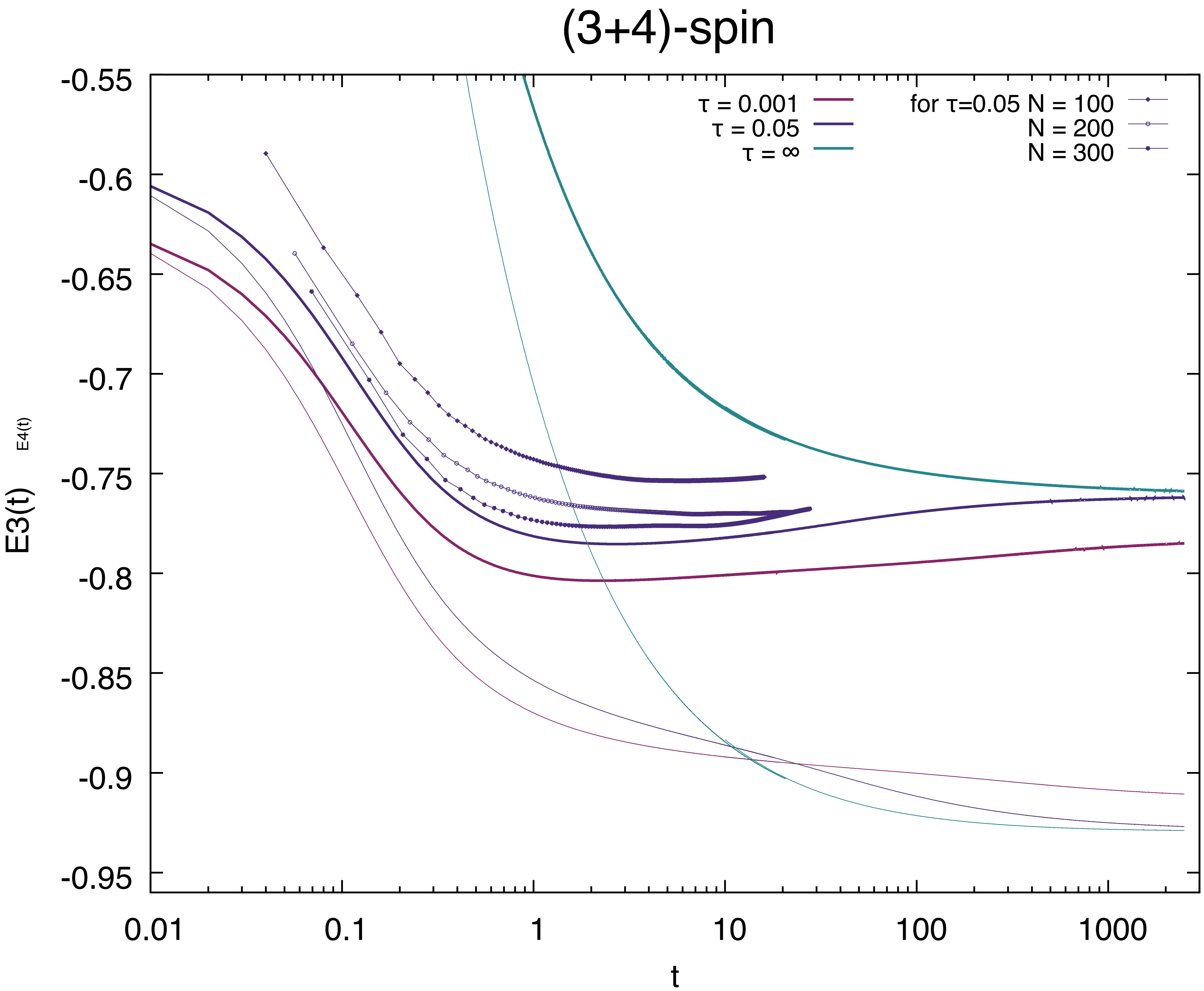

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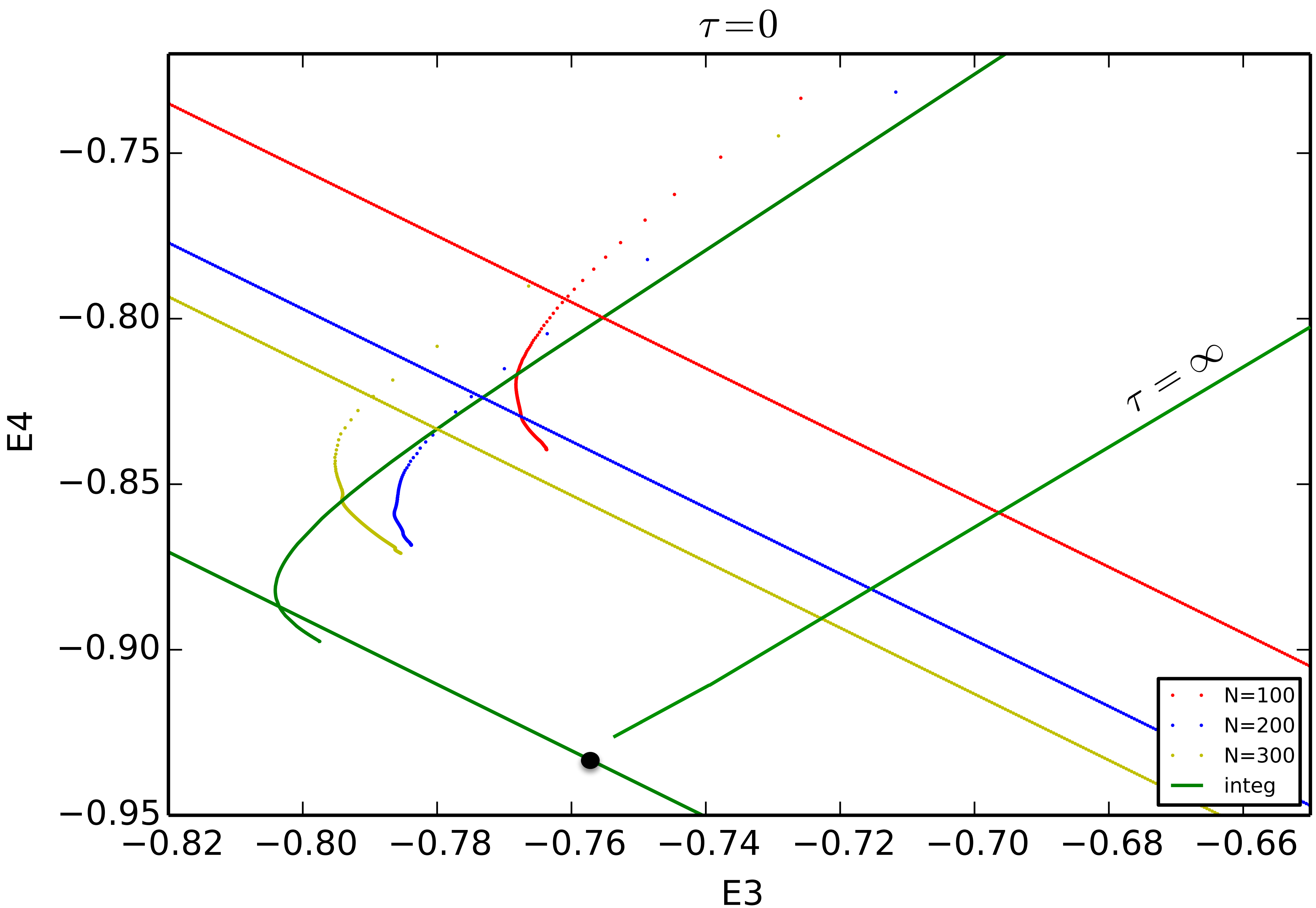
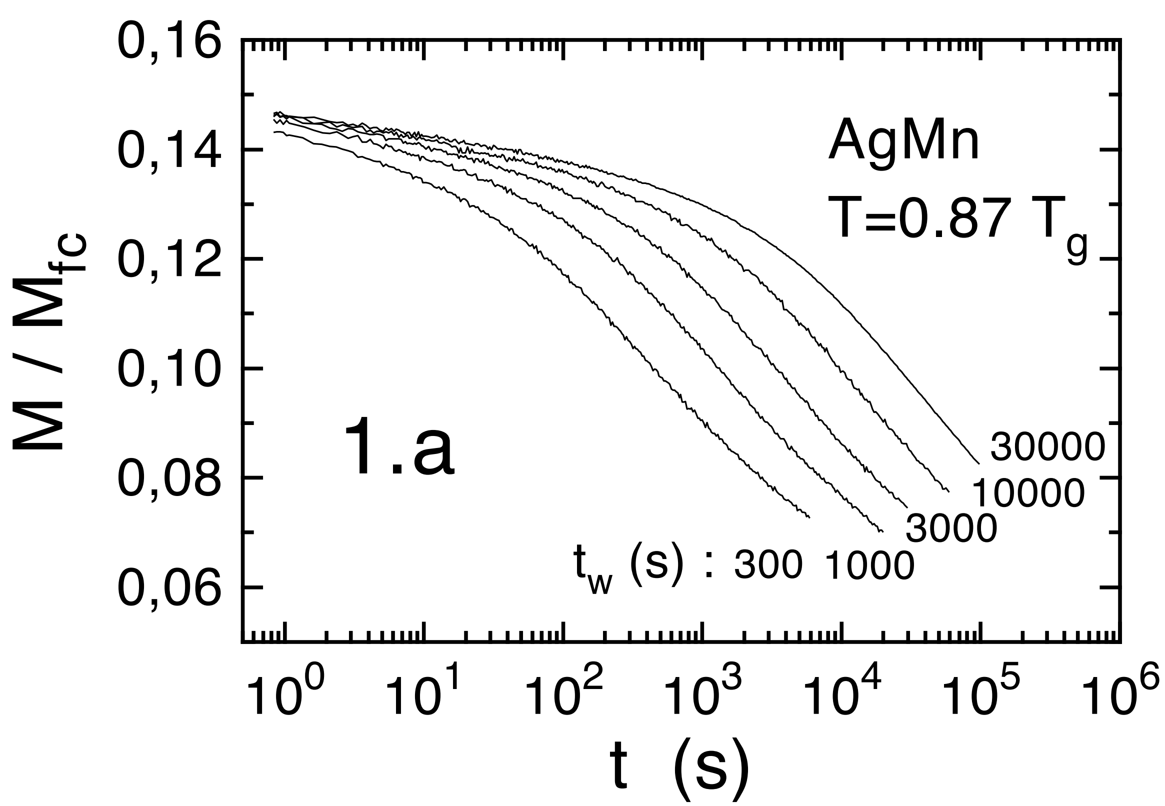
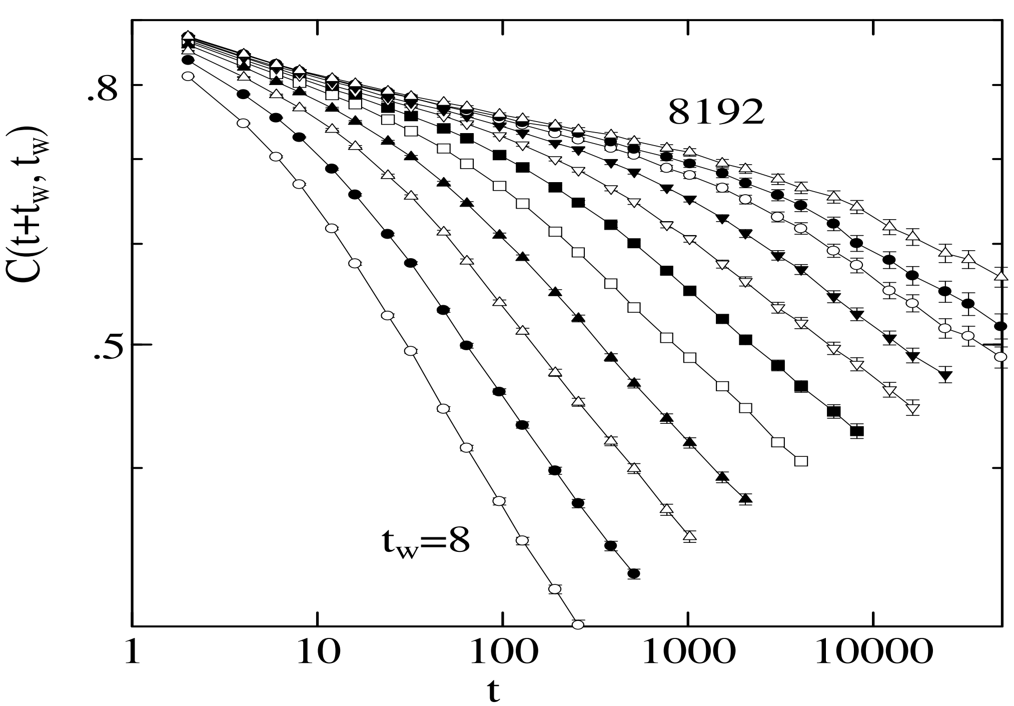


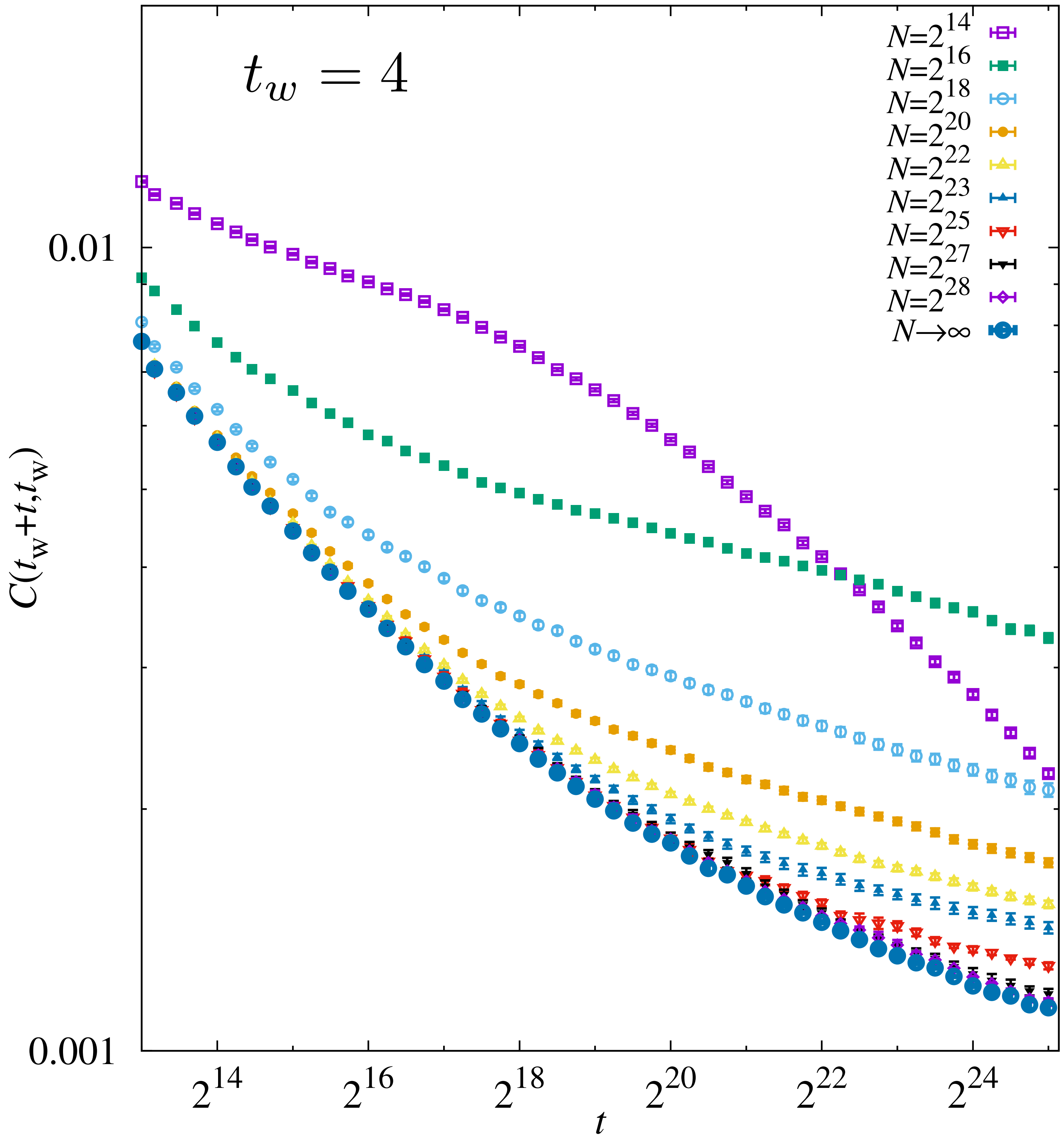
Ising SG on a sparse RRG

- Random 4-regular graph, $J_{ij} = \pm 1$
- Quench from $T_0=\infty$ to $T=0.8\ T_C$
- Expected aging behavior $\lim_{t\to\infty} C(t,t_w) = 0 \quad \forall t_w$
  based on previous experiments & numerics





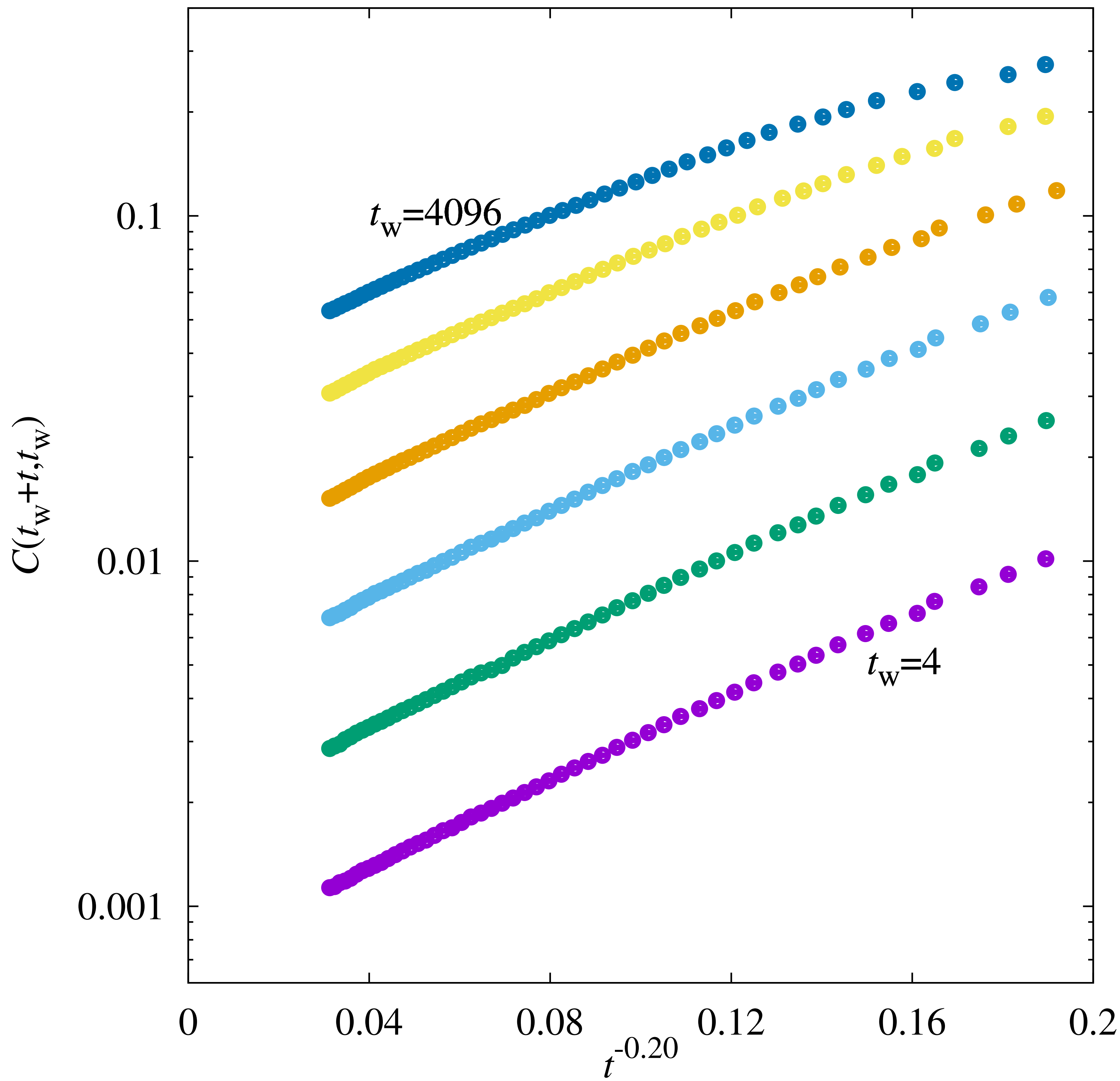
Finite size effects under control



Huge sizes!
Safe extrapolation to the large N limit

We work in the regime of very long times (t>>1) and very small correlations (C<<1)

Non-zero large times limit



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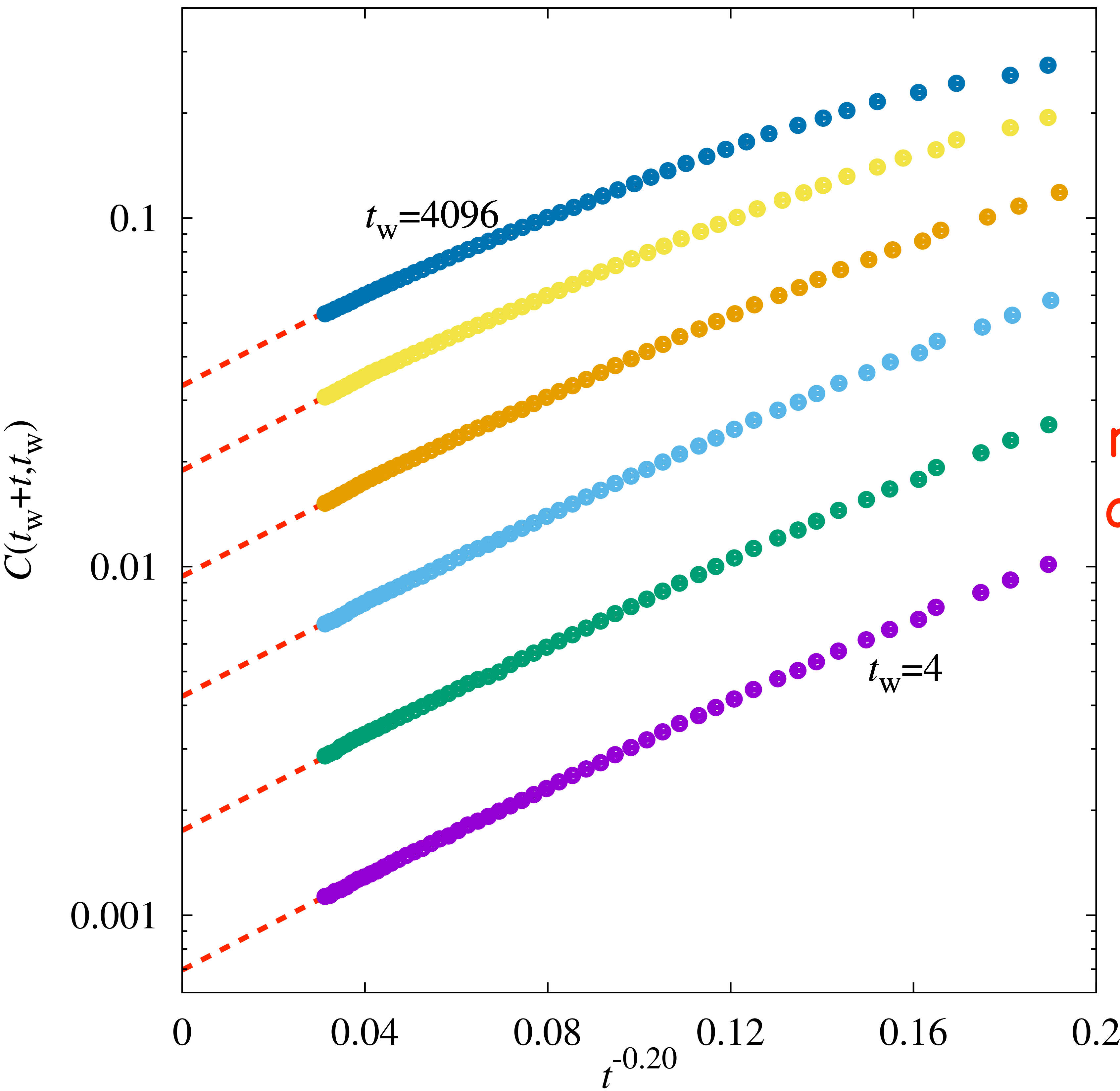

Aging in a
more and more
confined space?

Main (unexpected) results

- **Spherical mixed p-spin model**:
  - T=0 dynamics goes below the threshold energy!
  - positive correlation with the initial configuration
  - complexity gives only a qualitative explanation of the asymptotic dynamics

- **Viana-Bray model (SG on a RRG)**:
  the dynamics with $T<T_c$ does not decorrelate from the initial <u>random</u> configuration

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~~Weak ergodicity breaking~~

Strong ergodicity breaking