LOW-TEMPERATURE HYBRID MONTE CARLO FOR PERYLENE AND CORANNULENE

Stabilizing Determinant and Force

28 JULY 2026 I PETAR SINILKOV I NRW-FAIR

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arXiv:
2604.00815

NRW-FAIR Netzwerk

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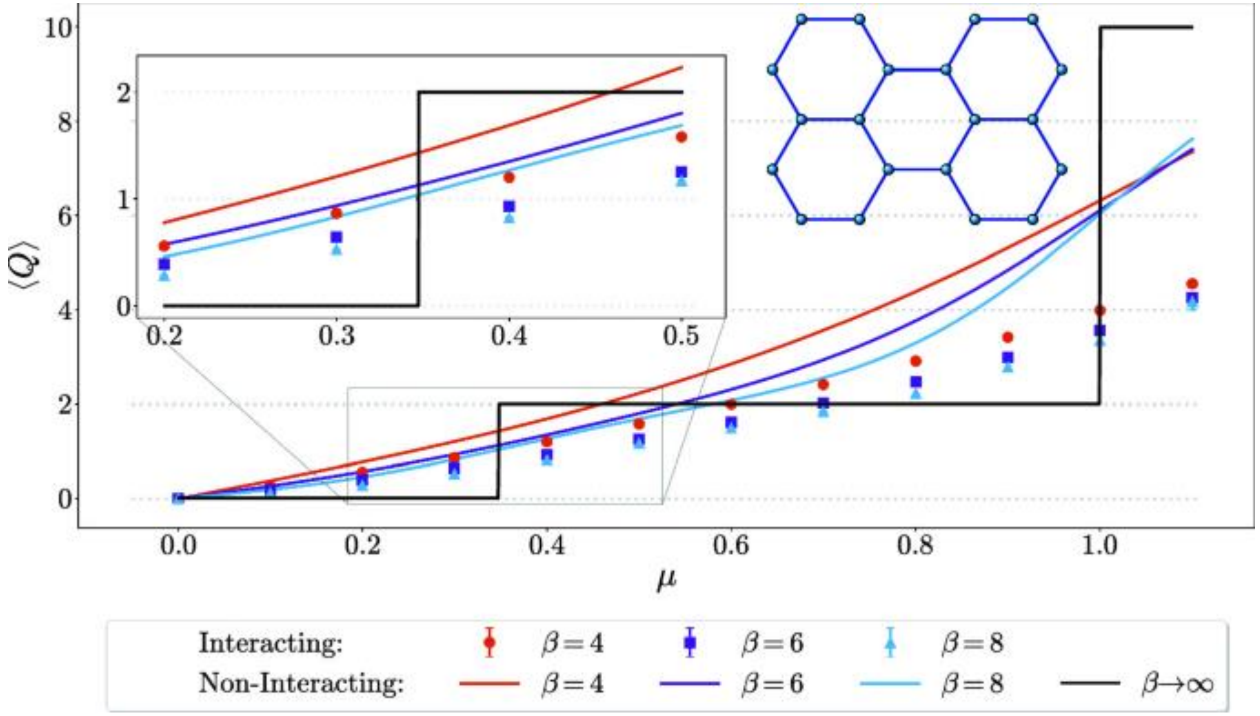
WHY DO WE CARE ABOUT LOW-TEMPERATURE

- Real experiments are performed usually at room temperature or as cold as possible
- Better zero temperature extrapolation
- Clean isolation of the low-energy states



M. Rodekamp et al., arXiv:2406.06711

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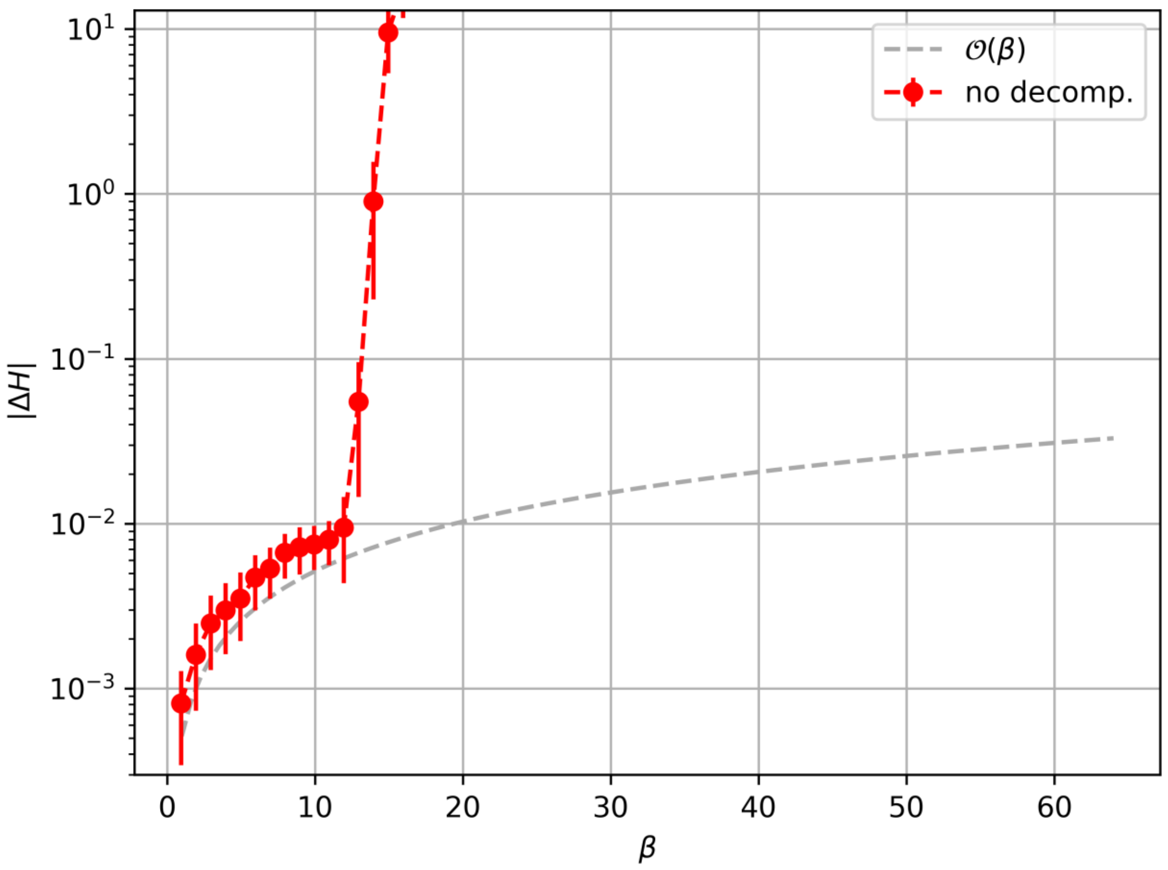

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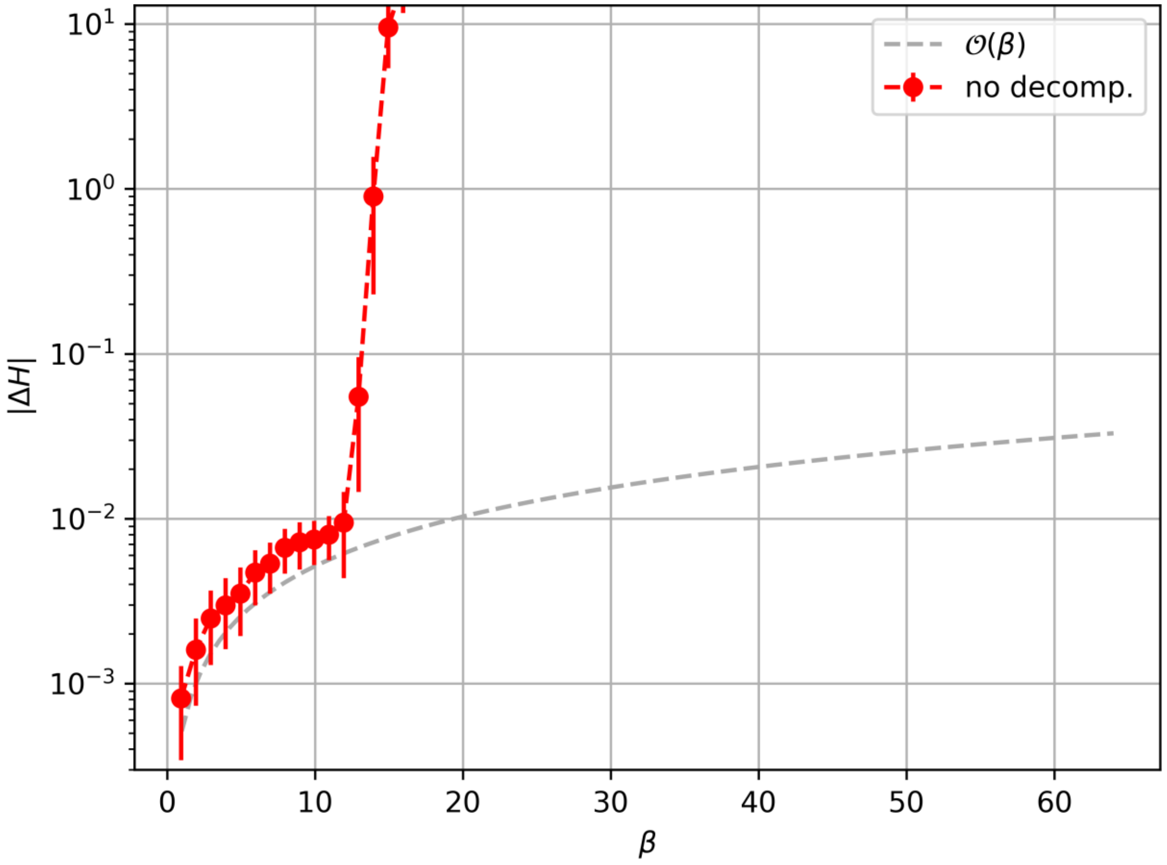
WHY DO WE CARE ABOUT LOW-TEMPERATURE



Why does this happen?

LOW-TEMPERATURE HMC

Action

$$Z = \int \mathcal{D}[\phi] \left(\prod_{f=1,2} \det M^{(f)}[\phi] \right) e^{-S[\phi]} = \int \mathcal{D}[\phi] e^{-S[\phi] + \sum_{f=1,2} \log\det M^{(f)}[\phi]} \equiv \int \mathcal{D}[\phi] e^{-S_{\text{eff}}[\phi]}$$

$$M = \begin{pmatrix} \mathbb{1} & 0 & \cdots & 0 & M_{N_t-1} \\ -M_0 & \mathbb{1} & 0 & \cdots & 0 \\ 0 & -M_1 & \mathbb{1} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -M_{N_t-2} & \mathbb{1} \end{pmatrix}$$

$$M_t \equiv \exp(\delta\kappa) \cdot \text{diag}\left(e^{i\phi_{0,t}}, e^{i\phi_{1,t}}, \ldots, e^{i\phi_{x,t}}, \ldots, e^{i\phi_{N_x-1,t}}\right)$$

LOW-TEMPERATURE HMC

The Problem

$$\det(M) = \det\left(\mathbb{1} + M_0 M_1 \ldots M_{N_t - 1}\right)$$

$$\det(M)\big|_{U=0} = \prod_i \left(1 + e^{\beta\lambda_i}\right) \qquad\qquad -K \leq \lambda_i \leq K$$

$$\mathrm{cond}(M) = e^{2\beta K}$$

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Exponential Temperature Dependence!

LOW-TEMPERATURE HMC

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$e^{\delta\kappa} e^{i\phi_0}$ → $e^{\delta\kappa} e^{i\phi_1}$ → $e^{\delta\kappa} e^{i\phi_2}$ → … → $e^{\delta\kappa} e^{i\phi_{Nt-1}}$

LOW-TEMPERATURE HMC

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We get round-off errors while accumulating the matrix

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We get round-off errors while accumulating the matrix

The determinant has been stabilized in other works

$$M_0 M_1 \ldots M_{N_t-1} = U_0 \underbrace{D_0((T_0 U_1) D_1)}_{=UDT} T_1 \ldots U_{N_t-1} D_{N_t-1} T_{N_t-1}$$

J. Kreit et al. arXiv:2601.18273 (2026)

C. Bauer SciPost Phys. Core 2, 011 (2020)

E. Y. Loh et. al. International Journal of Modern Physics C 16, 1319 (2005).

F. Assaad et. al. John von Neumann Institute for Computing, ISBN 3000090576 (2002)

LOW-TEMPERATURE HMC

Stable Force

Unstable way $$\begin{bmatrix} s & s & s & s \\ s & s & s & s \\ s & s & s & s \\ s & s & s & s \end{bmatrix} \begin{bmatrix} s & & & \\ & s & & \\ & & S & \\ & & & S \end{bmatrix} \begin{bmatrix} s & s & s & s \\ s & s & s & s \\ s & s & s & s \\ s & s & s & s \end{bmatrix} \begin{bmatrix} s & s & s & s \\ s & s & s & s \\ s & s & s & s \\ s & s & s & s \end{bmatrix} \begin{bmatrix} S & & & \\ & S & & \\ & & s & \\ & & & s \end{bmatrix} \begin{bmatrix} s & s & s & s \\ s & s & s & s \\ s & s & s & s \\ s & s & s & s \end{bmatrix}$$

C. Bauer SciPost Phys. Core 2, 011 (2020)

Stable Method

$$\dot{\pi}_x(t) \equiv \partial_{\phi_{x,t}} \log\det(M)$$

$$\dot{\pi}_x(t) \equiv \mathrm{tr}\left(\left(\mathbb{1} + M_0 \dots M_{N_t-1}\right)^{-1} \partial_{\phi_{x,t}} M_0 \dots M_{N_t-1}\right)$$

$$\mathcal{N}(t) \equiv \left(\mathbb{1} + \underbrace{M_{t-1}^{-1} \dots M_0^{-1} M_{N_t-1}^{-1} \dots M_t^{-1}}_{N_t \text{ terms}}\right)^{-1}$$

$$\dot{\pi}(t) = \mathcal{N}(t)$$

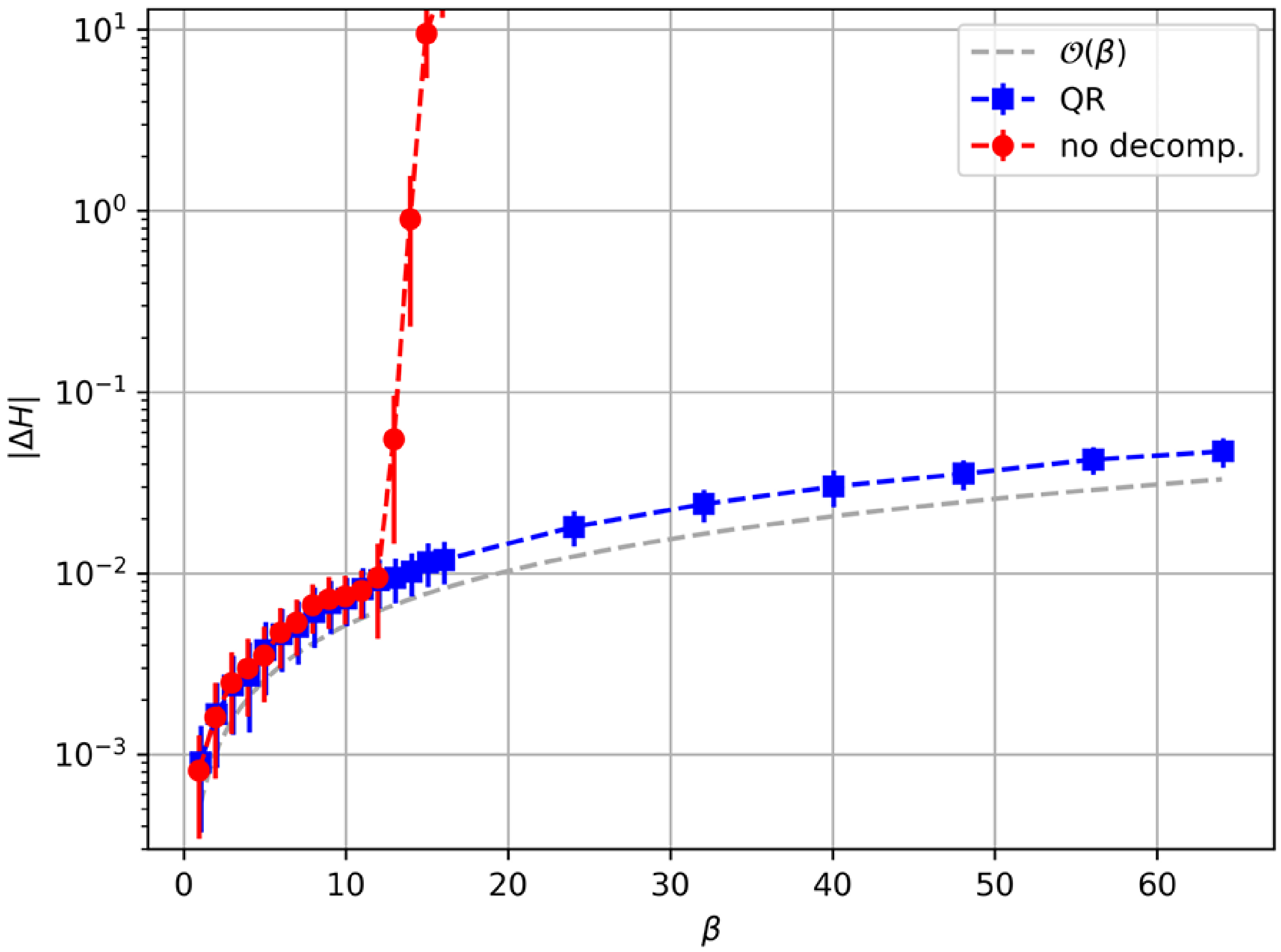
$$\Pi(t) \equiv M_t^{-1} M_{t-1}^{-1} \dots M_0^{-1} = U_\pi(t) D_\pi(t) T_\pi(t)$$

$$\Sigma(t) \equiv M_{N_t-1}^{-1} M_{N_t-2}^{-1} \dots M_t^{-1} = U_\sigma(t) D_\sigma(t) T_\sigma(t)$$

$$\mathcal{N}(t) = \left(\mathbb{1} + \Pi(t-1)\Sigma(t)\right)^{-1}$$

LOW-TEMPERATURE HMC

arXiv:
2604.00815



N-BODY 2-POINT CORRELATION FUNCTIONS

Propagator

$$\mathcal{M}(t',t) = \begin{cases} M_{t'}^{-1} M_{t'-1}^{-1} \dots M_{t+1}^{-1} M_t^{-1} & \forall t' \geq t \\ M_{(t'+N_t)\%N_t}^{-1} M_{(t'+N_t-1)\%N_t}^{-1} \dots M_{(t+1)\%N_t}^{-1} M_t^{-1} & \forall t' < t \end{cases}$$

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Columns of the Propagator

$$G(t,0) = \left[\mathcal{M}^{-1}(t-1,0) + \mathcal{M}(-1,t)\right]^{-1} = \left[\Pi^{-1}(t-1) + \Sigma(t)\right]^{-1}$$

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Rows of the Propagator

$$G(0,t) = -\left[\mathcal{M}^{-1}(-1,t) + \mathcal{M}(t-1,0)\right]^{-1} = -\left[\Sigma^{-1}(t) + \Pi(t-1)\right]^{-1}$$

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N-BODY 2-POINT CORRELATION FUNCTIONS

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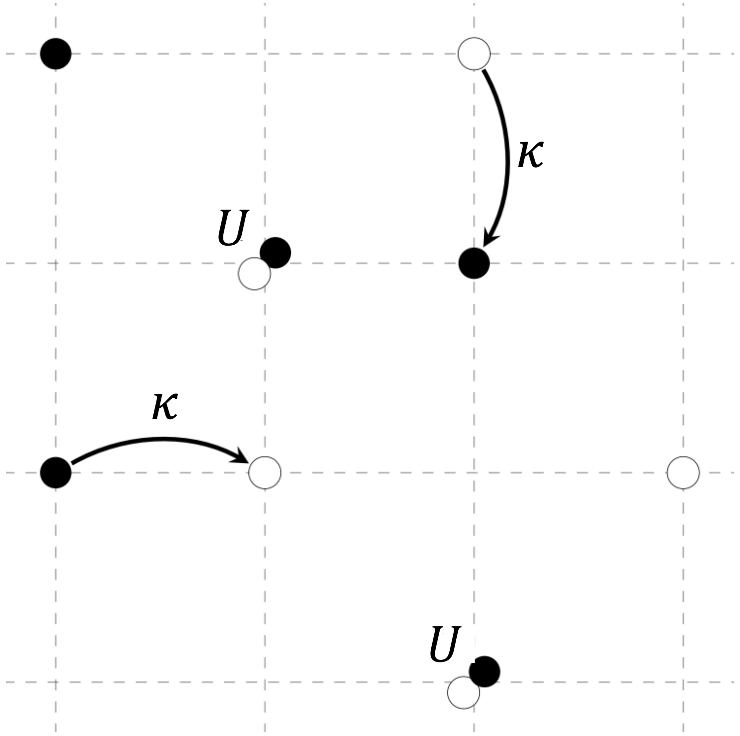
Diagonal of the Propagator

$$G(t,t) = \left[\mathbb{1} + \mathcal{M}(t-1,t)\right]^{-1} = \left[\mathbb{1} + \Pi(t-1)\Sigma(t)\right]^{-1} = \mathcal{N}(t)$$

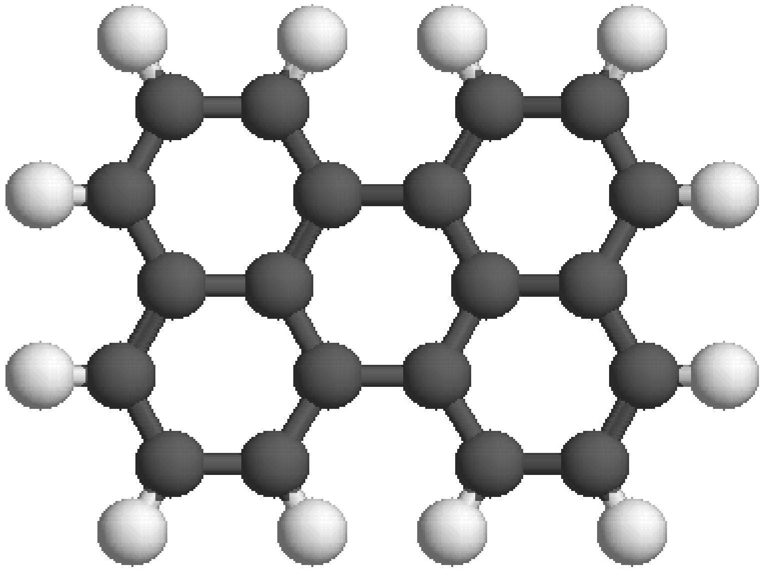
THE HUBBARD MODEL

$$H = -\kappa \sum_{\langle xy\rangle, f=1,2} c^\dagger_{xf} c_{yf} - \frac{U}{2} \sum_x \left(c^\dagger_{xf_1} c_{xf_1} - c^\dagger_{xf_2} c_{xf_2} \right)^2 - \mu \sum_x \left(c^\dagger_{xf_1} c_{xf_1} + c^\dagger_{xf_2} c_{xf_2} \right)$$

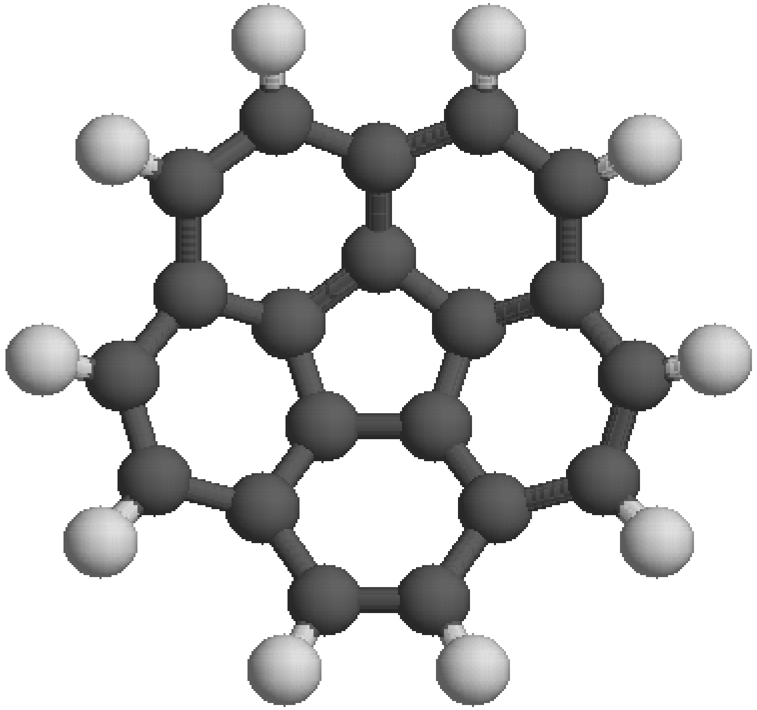
- $c^\dagger, c$: creation/annihilation operators
- κ : hopping parameter
- U : on-site interaction
- μ : chemical potential



WARM MOLECULES



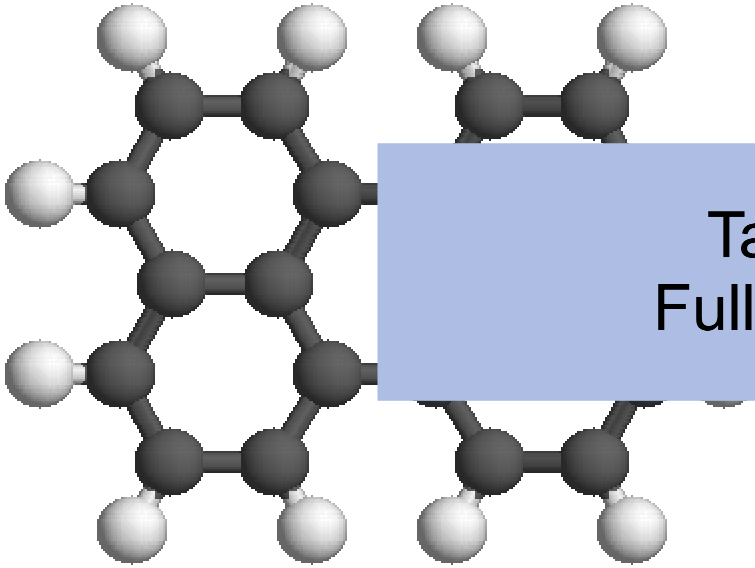
Perylene



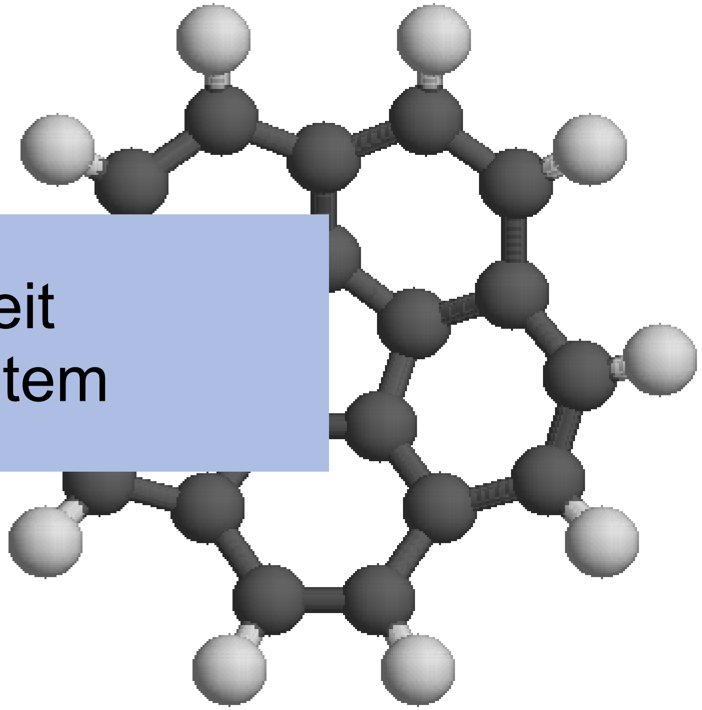
Corannulene

G. Malloci and M. A. L. Marques et al.
https://www.dsf.unica.it/~gmalloci/pahs/frames/citation.html

WARM MOLECULES



Talk by Janik Kreit
Fullerene C60 system



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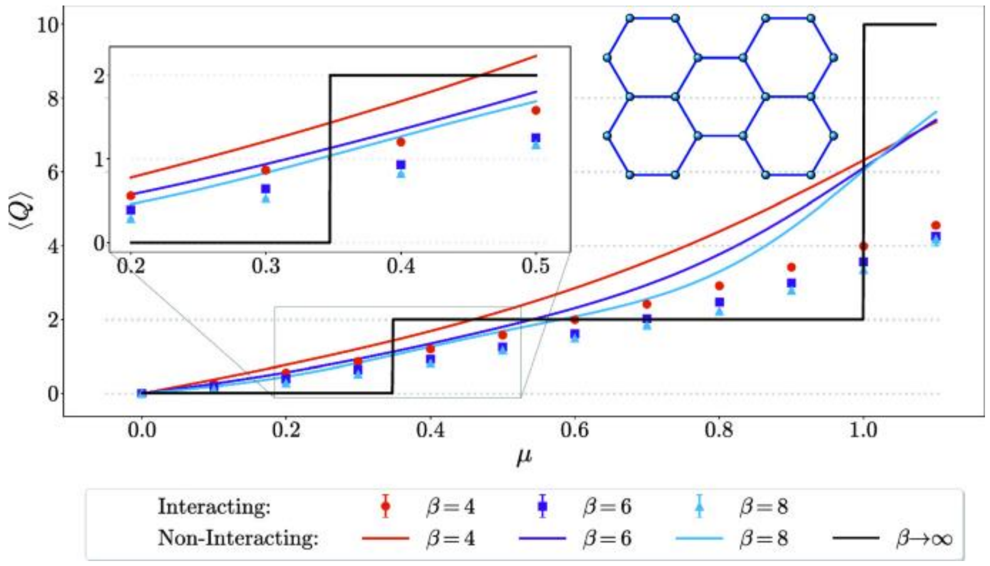

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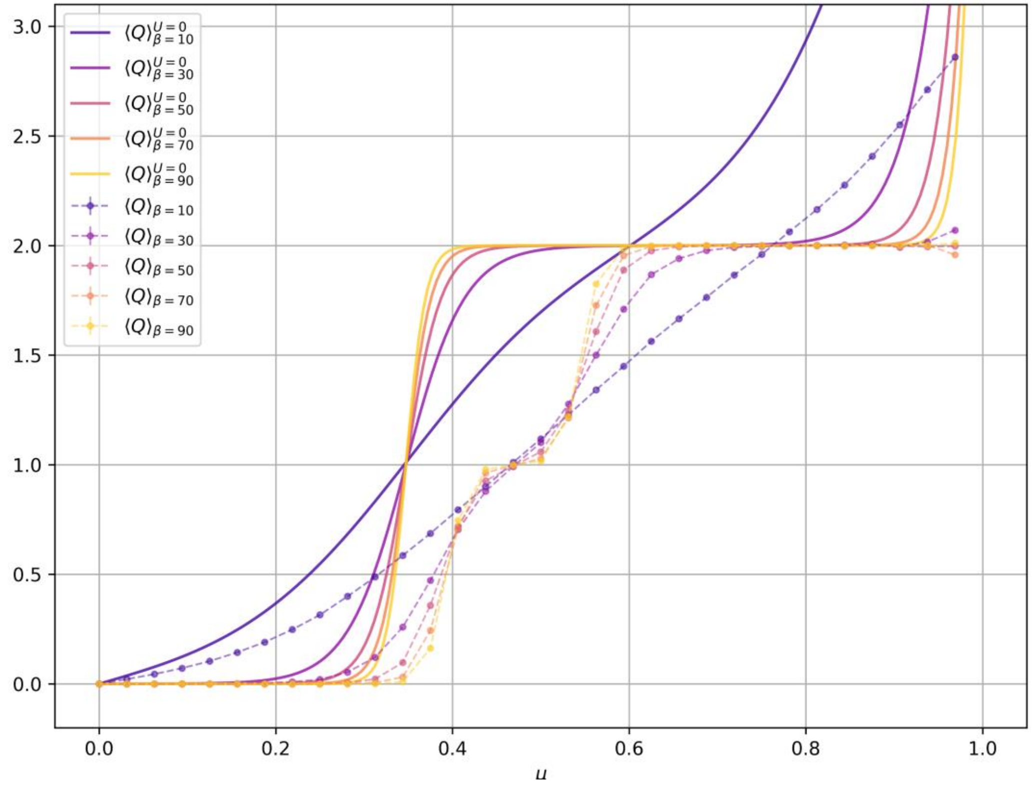
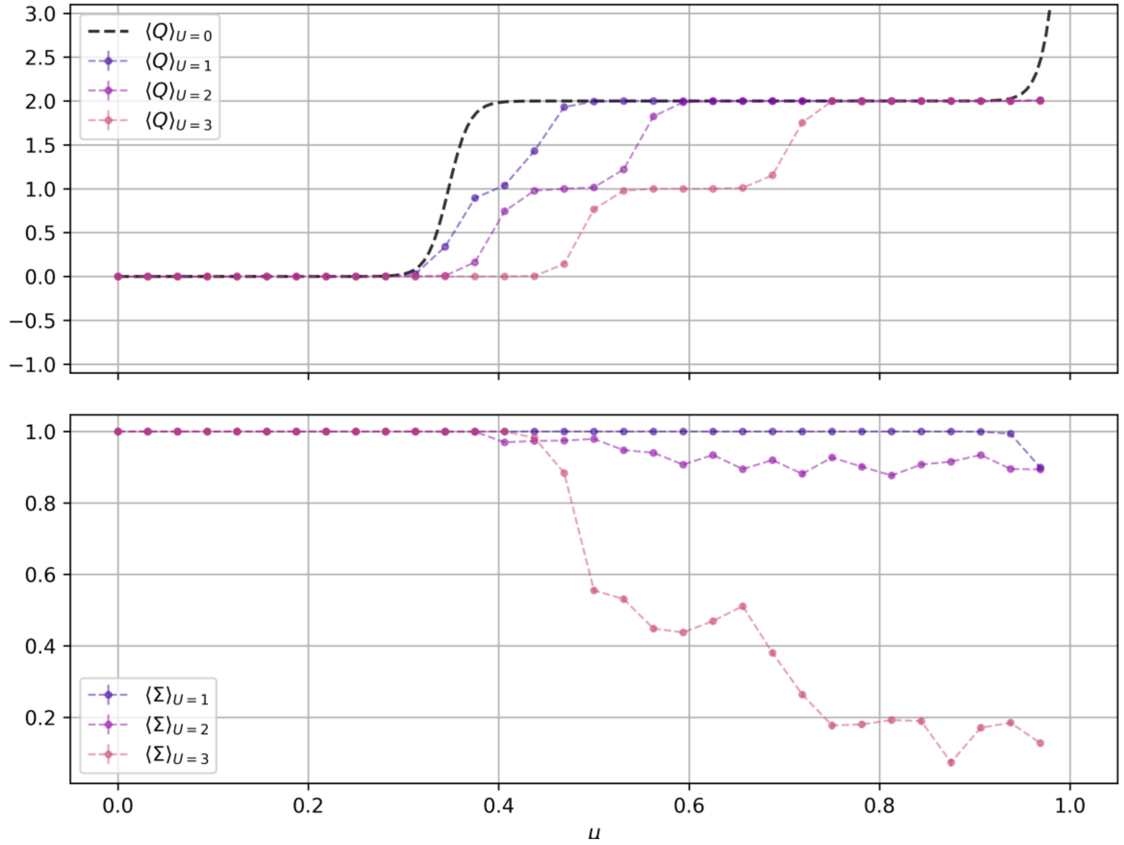


WARM MOLECULES

Perylene

- $\Delta Q = 1$ transition when $U > 0$
- Plateau increases with increasing of U
- Statistical power decreases



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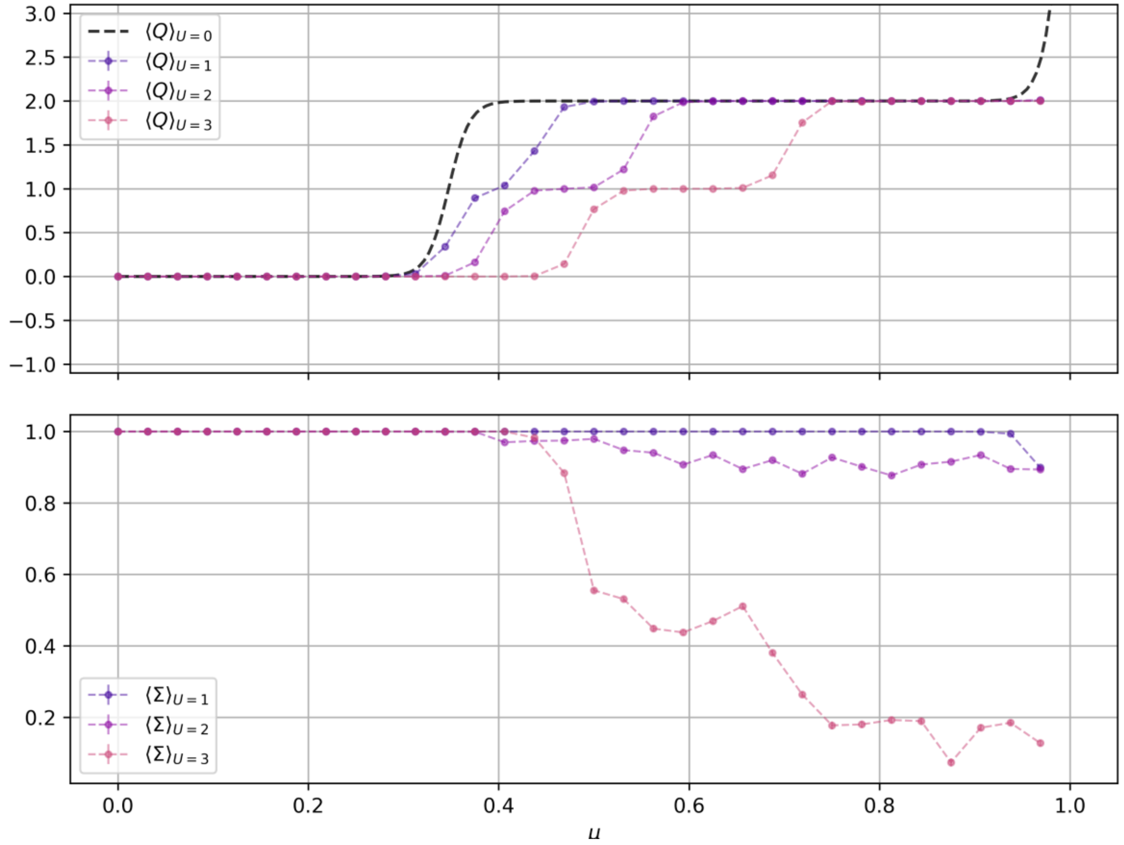


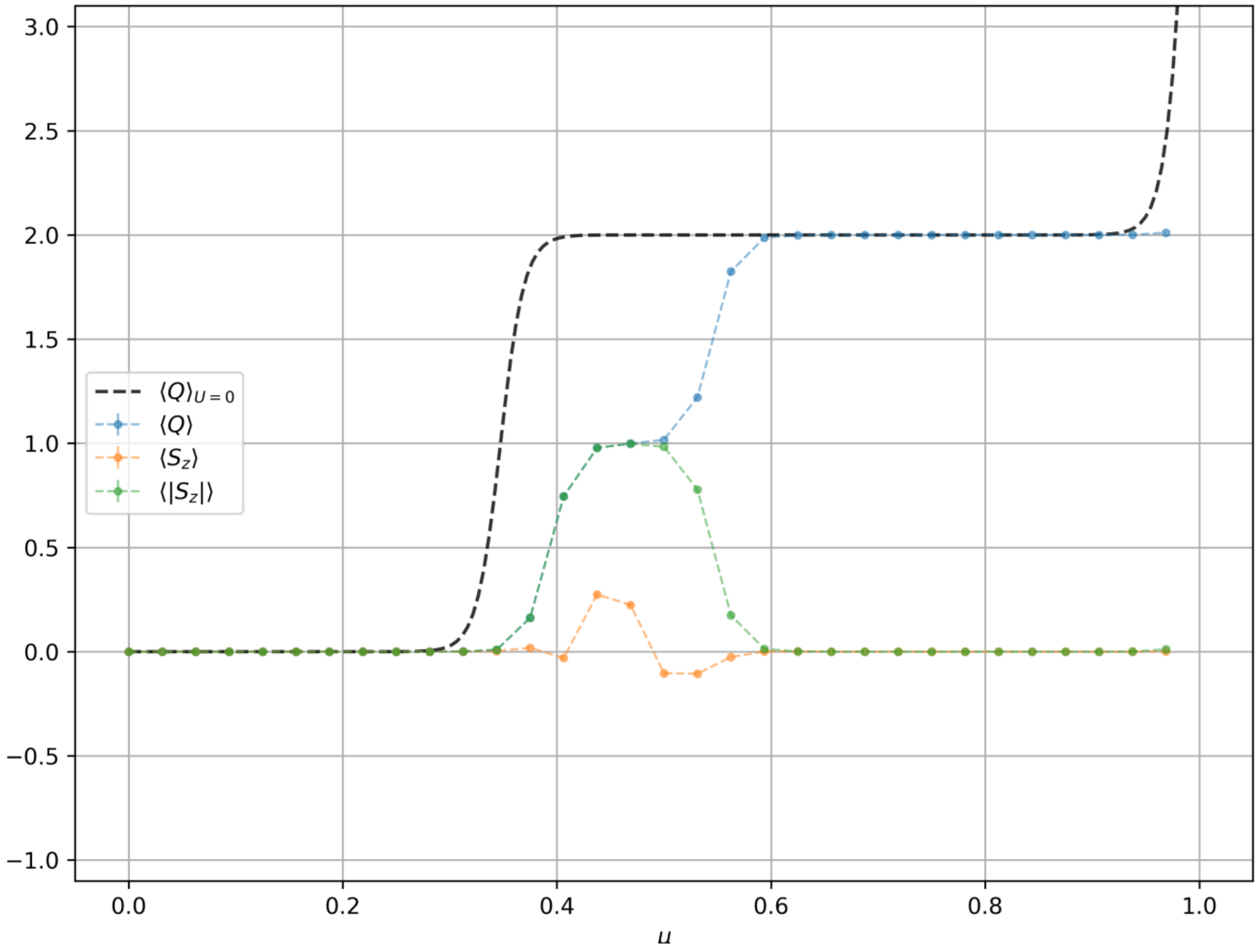
Why is there such a transition?

WARM MOLECULES

Perylene

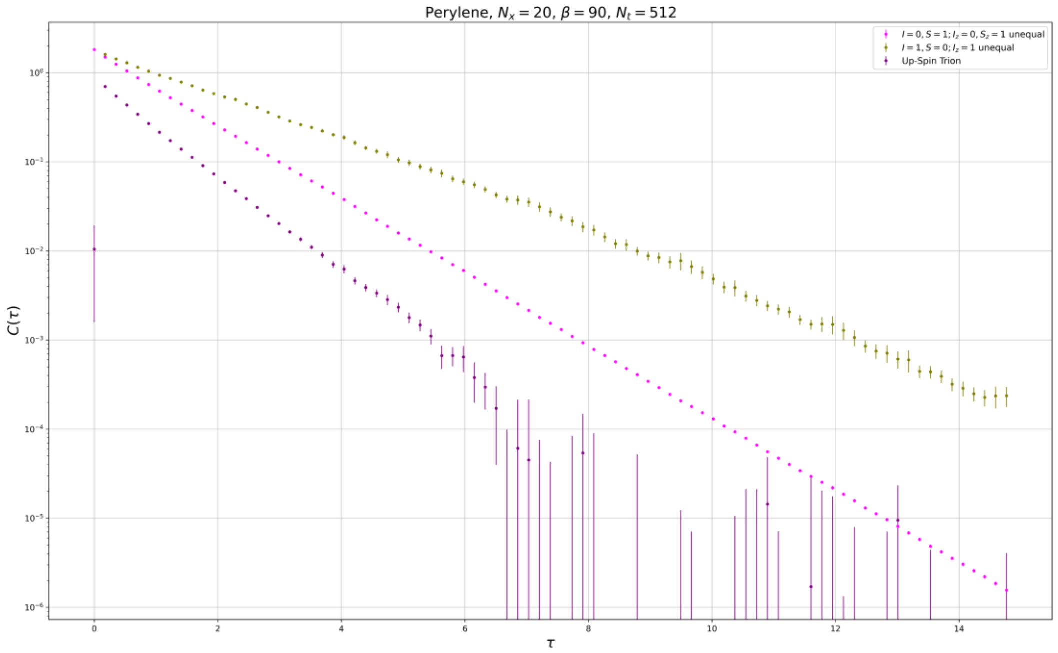
- Spin symmetry of the ground state is broken

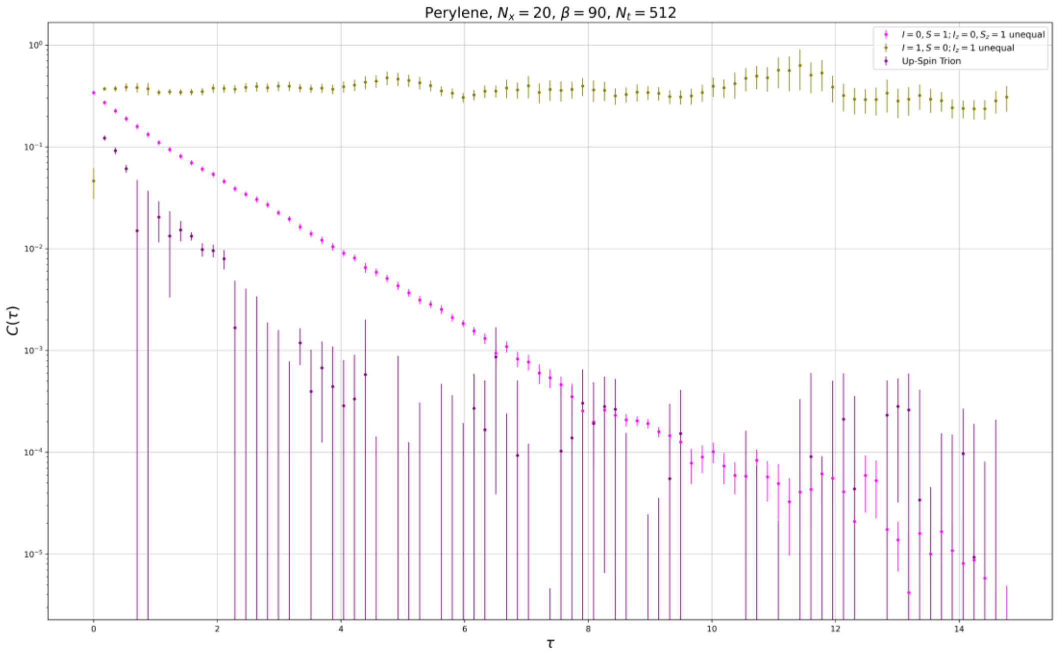
- Due to interactions, it is more energetically favorable in this region to have an odd number of electrons in the Dirac sea

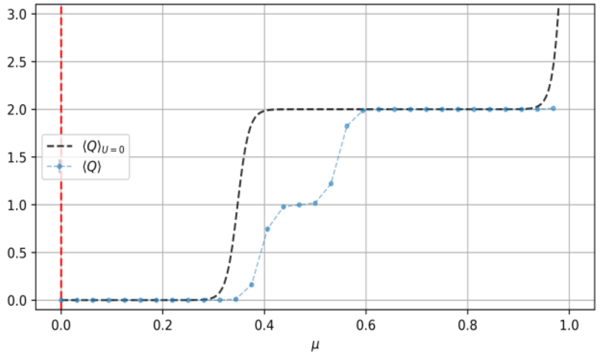


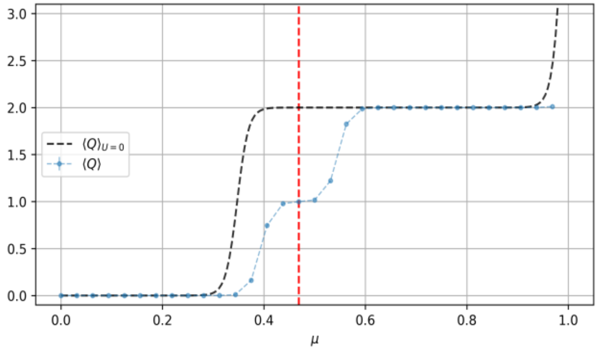
WARM MOLECULES

Perylene









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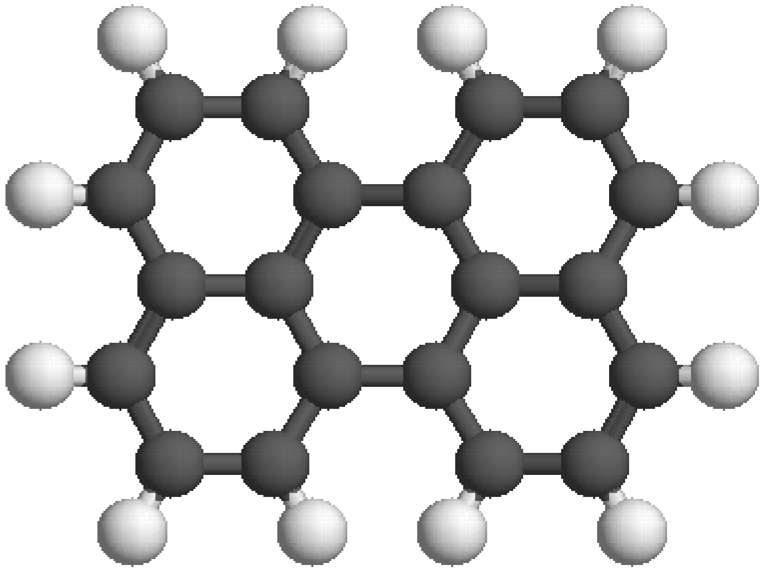

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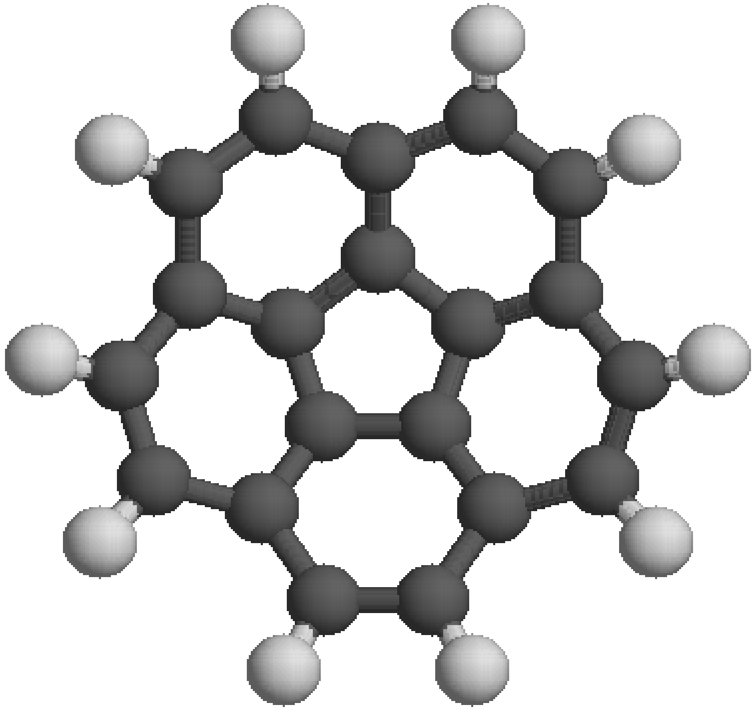


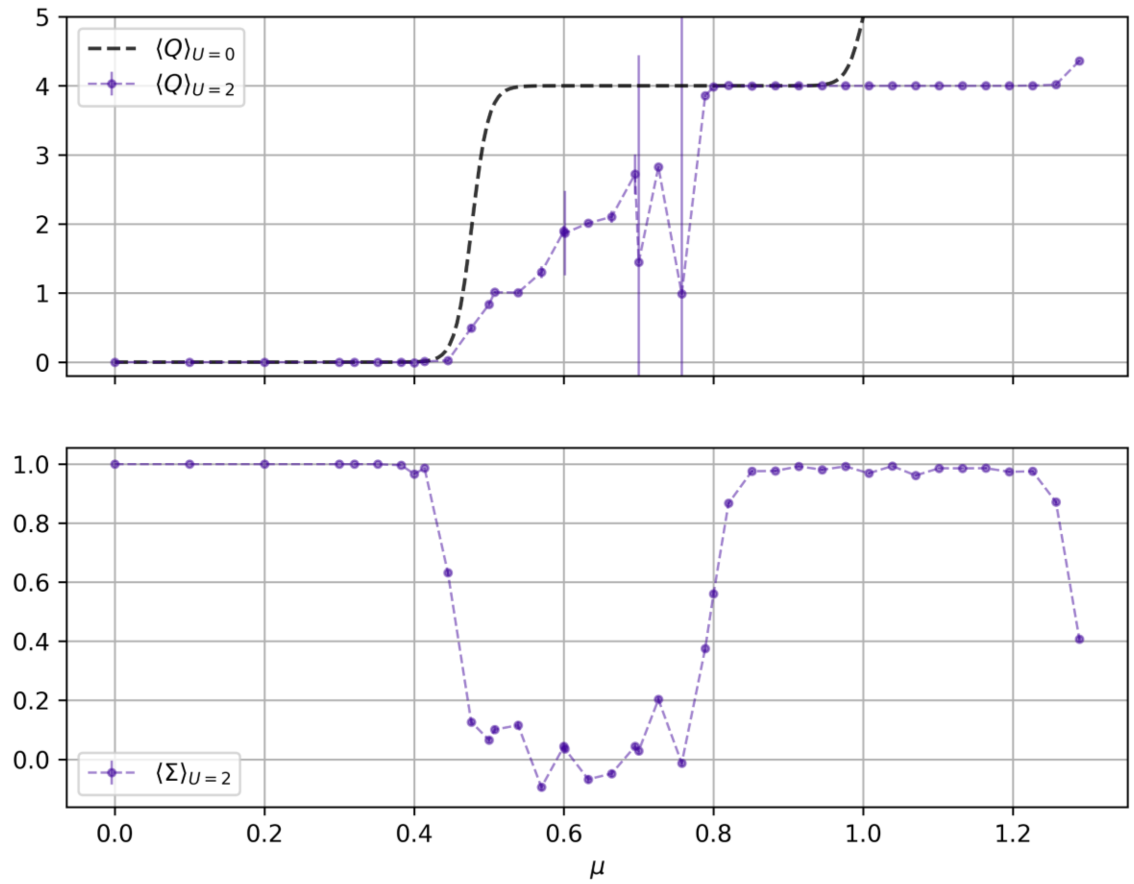
Corannulene

G. Malloci and M. A. L. Marques et al.
https://www.dsf.unica.it/~gmalloci/pahs/frames/citation.html

WARM MOLECULES

Corannulene

- It is difficult to see a plateau
- Statistical power plummets in the transition region



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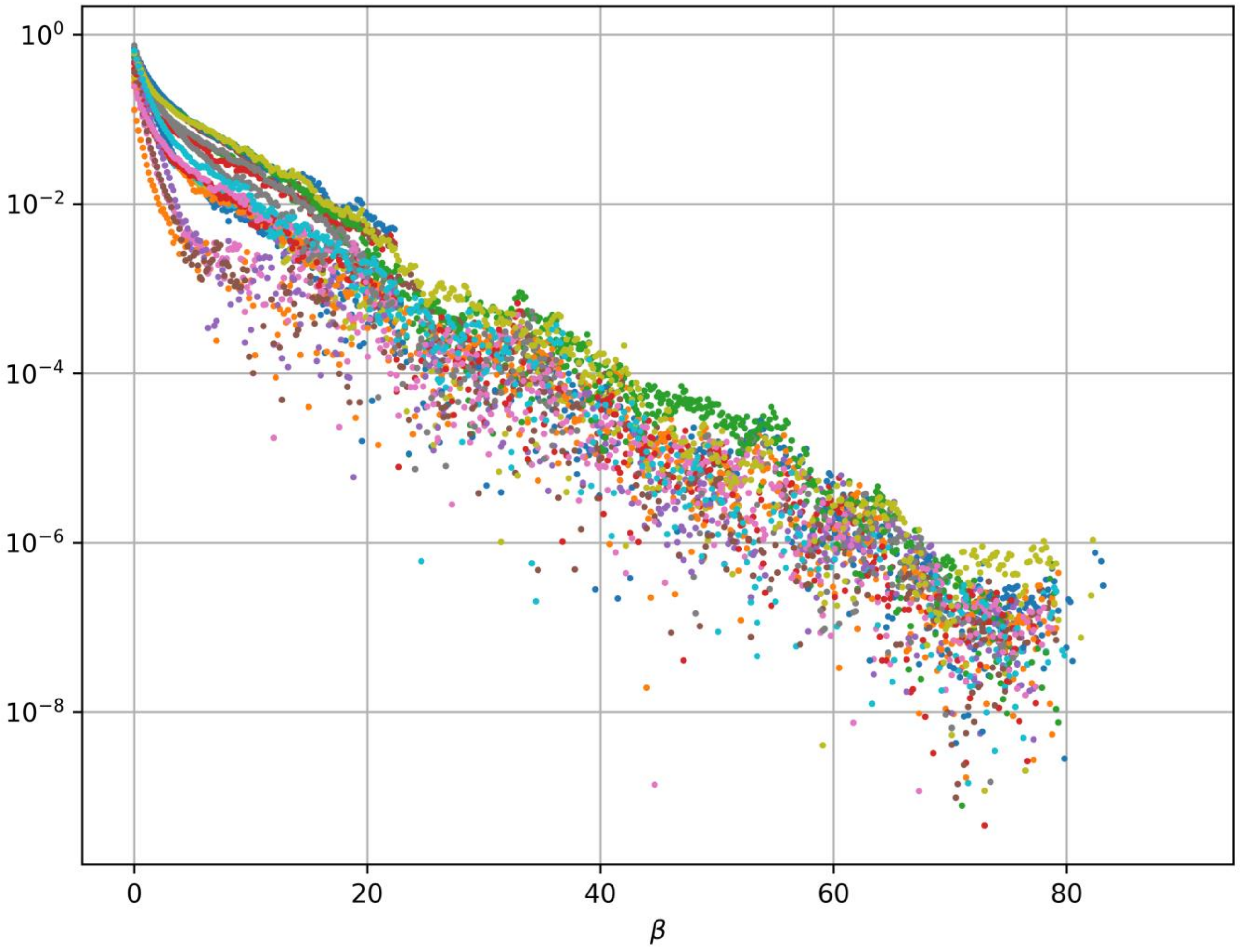
WARM MOLECULES

Corannulene

- 1-body correlators are noisy even at $\mu = 0$
- We need more configurations to clean up the signal



SUMMARY

Outlook

Stable Determinant and Force

- HMC simulations at large β or **Low-Temperature**
- Now the **zero-temperature** limit can be better estimated
- The **Full Propagator** is available – all n-body 2-point correlation functions

arXiv:
2604.00815

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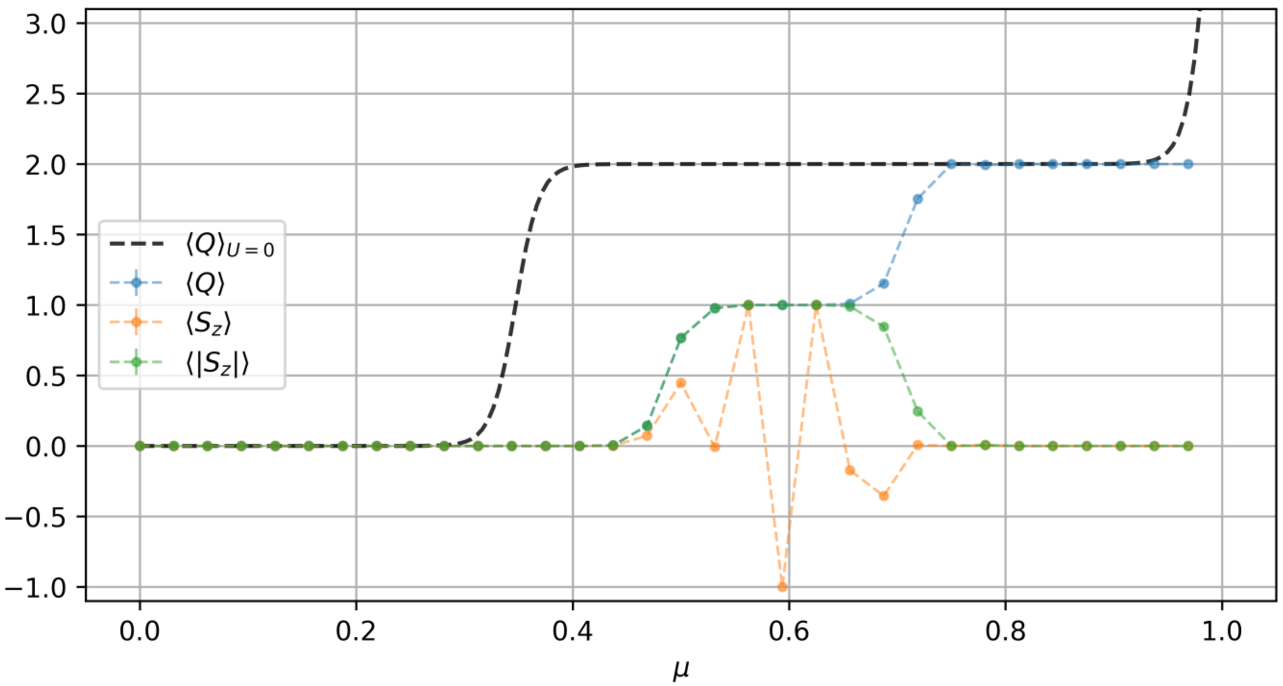
SUMMARY

Outlook

Stable Determinant and Force

Room Temperature Simulations

- **Spin symmetry breaking** in the presence of interactions
- $\boldsymbol{\Delta Q = 1}$ **transition** with an interaction strength dependence
- Showcase of **2-** and **3-body** correlation functions in the $\boldsymbol{Q = 0}$ and $\boldsymbol{Q = 1}$ regions (preliminary)



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SUMMARY

Outlook

Stable Determinant and Force

Room Temperature Simulations

What can we do next?

- Improve the signal by applying a Sign-Problem-Mitigation-Scheme
- Use a different model that accounts for neighbor interactions
  - Started investigating the Pariser-Parr-Pople model with a Mataga–Nishimoto potential at $\mathrm{U} = 4$

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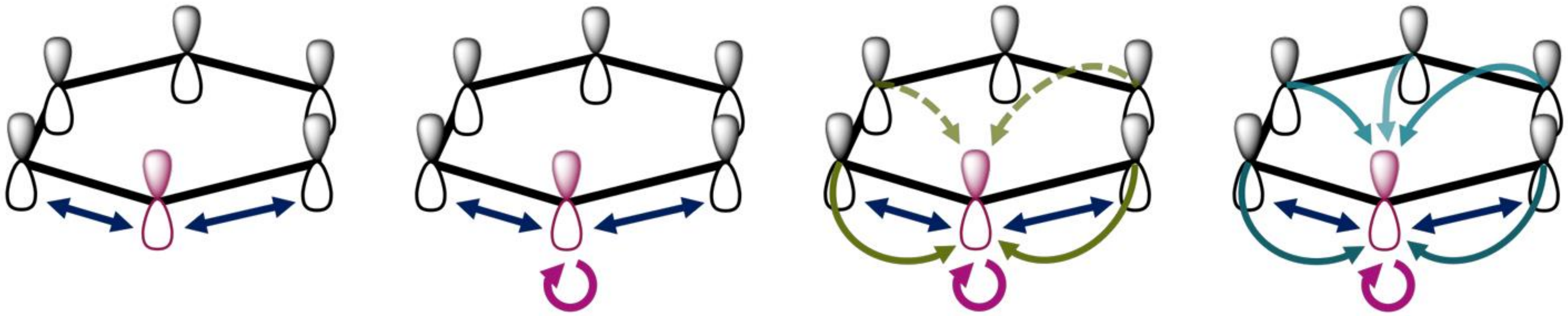
BACKUP

PARISER-PARR-POPLE

Model

M. Fabian et al. arXiv:2510.04632



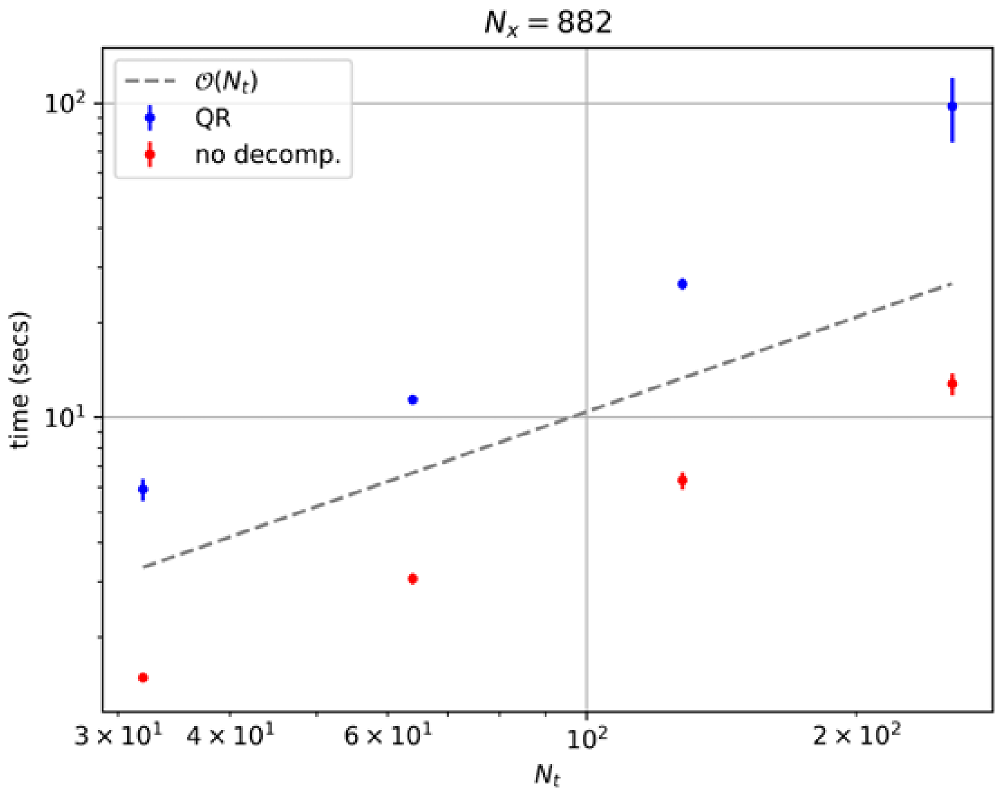
(a) Hückel (b) Hubbard (c) extended Hubbard (d) PPP

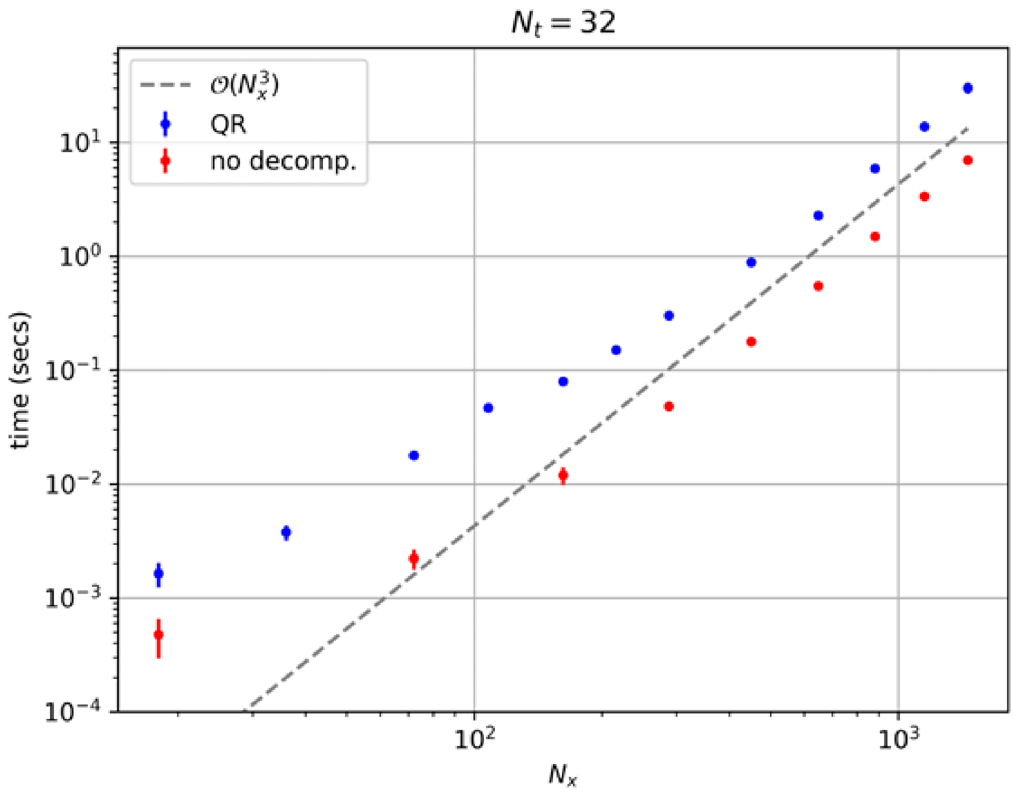
Mataga-Nishimoto potential

$$V_{ij} = \frac{U}{1 + U\epsilon_r r_{ij}/14.397}$$

LOW-TEMPERATURE HMC

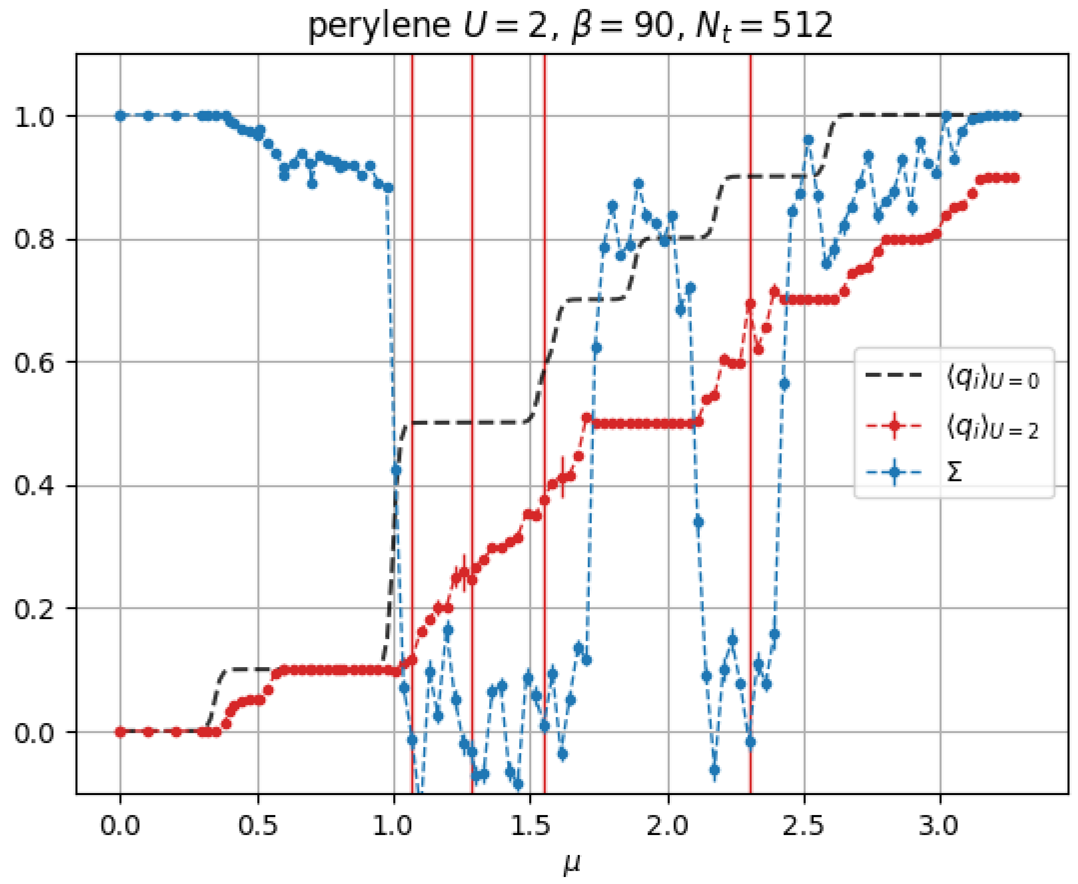
Stable Logarithmic Determinant Scaling

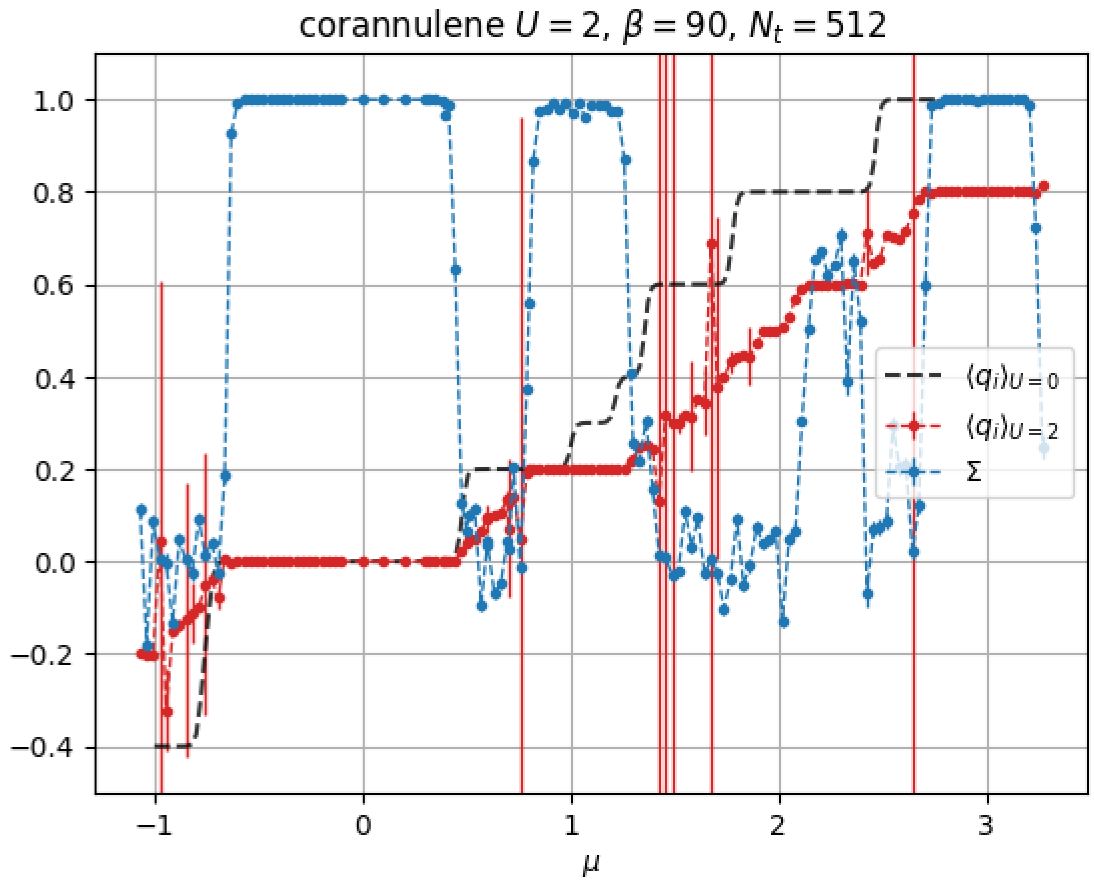




WARM MOLECULES

Extended Regions





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