Approximating Quantum Thermodynamic Properties using Density Functional Theory

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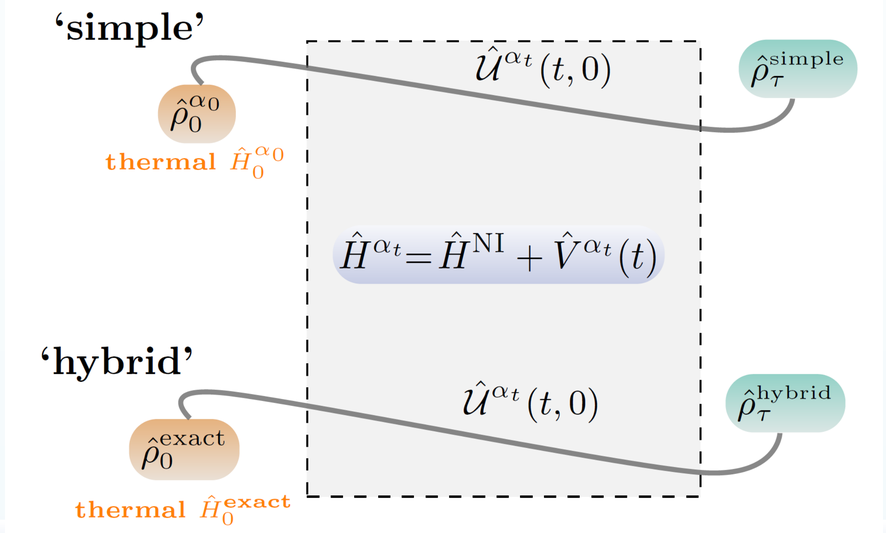
ABSTRACT

The fabrication, utilisation, and efficiency of quantum devices rely on a good understanding of quantum thermodynamic properties. This understanding is crucial for applications' limits, but also for device fabrication and efficiency. Many-body systems are often proposed as hardware for these quantum devices, but interactions between particles make the complexity of related calculations grow exponentially with the system size. In this respect, while Density Functional Theory (DFT) is one of the most successful methods to derive properties of complex many-body systems and materials [1], its extension to finite temperature problems, especially for out-of-equilibrium systems, is still in its infancy [2]. Here [3], we explore and systematically compare a set of approximations for the average work and entropy variation and which are built on static density functional theory concepts. We divide them in two classes, 'simple' and 'hybrid'. These approximations are computationally cheap and could be applied to large many-body systems. We demonstrate them by considering driven one-dimensional Hubbard chains and show that, for 'simple' approximations and low to medium temperatures, it pays to consider a good Kohn-Sham Hamiltonian to approximate the driving Hamiltonian. Our results confirm that a 'hybrid' approach, requiring a very good approximation of the initial and, for the entropy, final states of the system, provides great improvements. The 'hybrid' approach should be particularly efficient when many-body effects are not increased by the driving Hamiltonian.

'SIMPLE' AND 'HYBRID' APPROXIMATIONS

$$\hat{H} = \hat{H}^{\mathrm{NI}} + \hat{U} + \hat{V}(t)$$

dynamics: $\hat{H}(t) \approx \hat{H}^{\alpha_t}(t)$



Non-interacting: $V^{\alpha(t)} = V(t)$; Kohn-Sham: $V^{\alpha(t)} = V_{KS}(t)$

DENSITY FUNCTIONAL THEORY RELEVANT CONCEPTS

Kohn-Sham Hamiltonian ficticious non-interacting system

$$\hat{H}_{\mathsf{KS}} = \hat{T} + \hat{V}_{\mathsf{KS}} \qquad \hat{V}_{\mathsf{KS}}[n] = V[n] + V_H[n] + V_{\mathsf{xc}}[n]$$

external Hartree exchange correlation

H_{KS} : reproduces local density of the interacting system

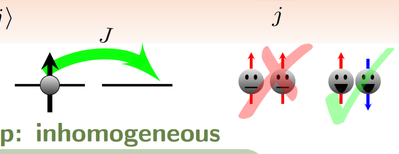
V_{xc} : needs approximating: BALDA and GSKS

BALDA: Bethe Ansatz Local Density Approximation

GSKS: reverse-engineering the exchange-correlation potential

APPLICATION: DRIVEN IONIC HUBBARD MODEL

$$H = -J\sum_{\langle i,j\rangle}(c_j^\dagger c_i + \mathrm{H.c.}) + U\sum_j n_{j\uparrow}n_{j\downarrow} + V\sum_j (-1)^j n_j$$

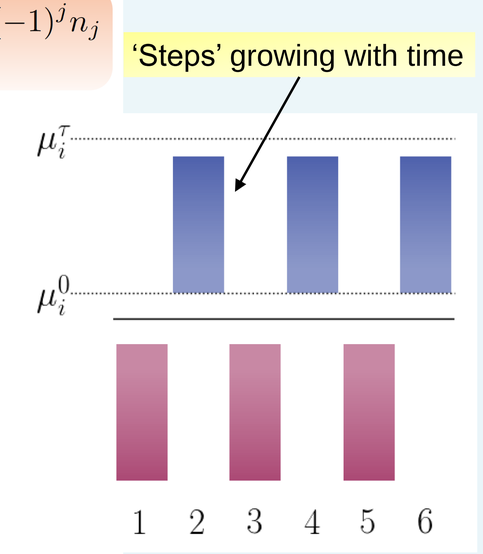


linear ramp: inhomogeneous

$$\hat{V}_j(t) = (-1)^j\left(\mu_0 + \mu_\tau \frac{t}{\tau}\right)\hat{n}_j$$

half filling $n = 1$

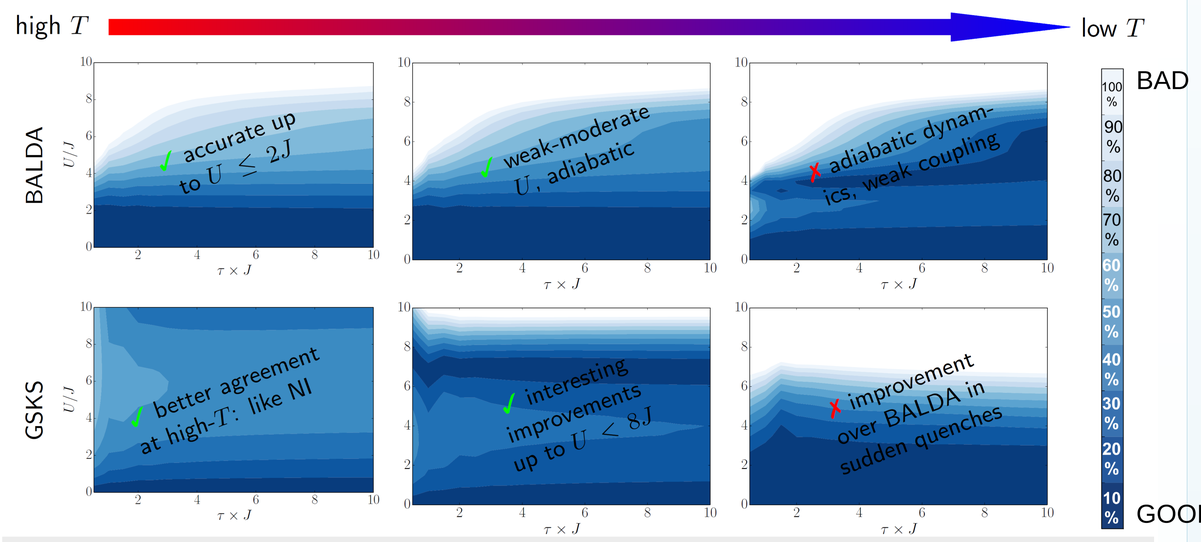
- $U = 0, \mu_0 = 0$: metal
- $U > J$: Mott insulator
- $\mu_0, \mu_\tau \gg U, J$: band insulator
- $U, \mu_0, \mu_\tau \gg J$: localization



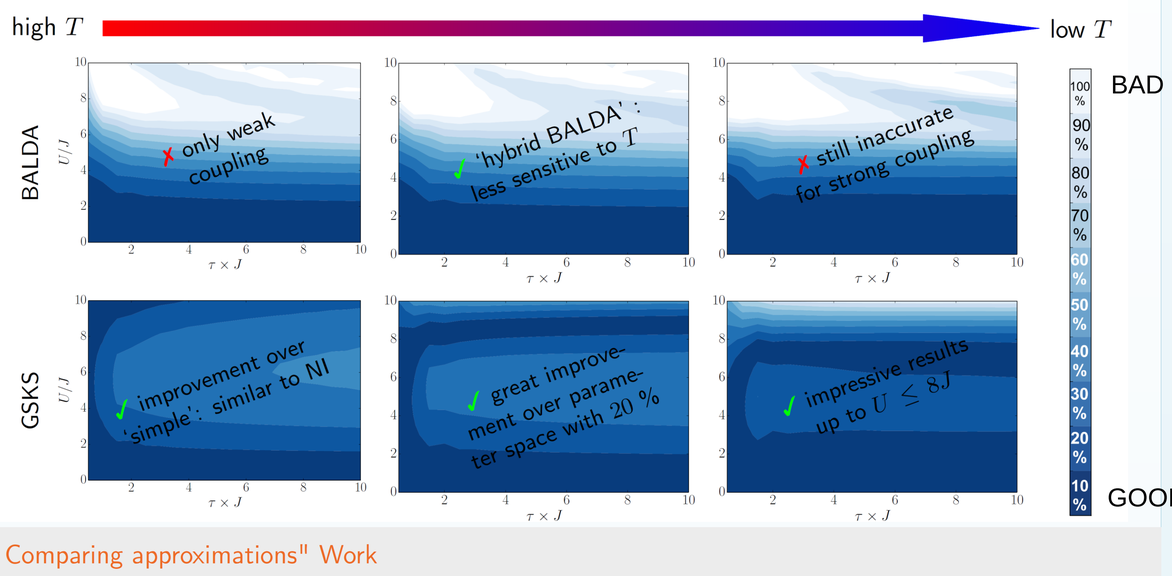
✓ benchmarks for a non-integrable correlated system
✓ beyond sudden quench: experimental protocols
✓ competition thermal vs energy scales

RESULTS FOR WORK (ENTROPY IN [3])

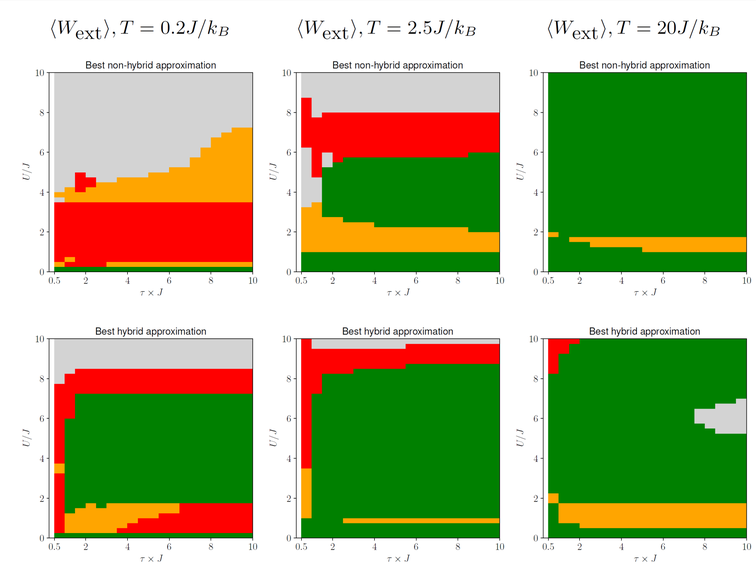
Work: BALDA and GSKS 'simple' approximations



Work: BALDA and GSKS 'hybrid approximations



Comparing approximations" Work



Green when the simple/hybrid NI approximation has the best accuracy;
Orange when the simple/hybrid BALDA has the best accuracy;
Crimson when the simple/hybrid GSKS approximation has the best accuracy;
Gray when the relative error for all approximation is over 20%;

CONCLUSIONS

Summary

- Recipes to approximate work and entropy in out-of-equilibrium strongly correlated systems
- Proposal of 'simple' and 'hybrid' approximations
- Comparison between NI, BALDA and GSKS approximations as a function of U, τ at T temperature

Main Findings

✓ Good approximation of initial state improves $\langle W\rangle$ even when the approximation for $\hat{H}(t)$ is poor

➤ Accuracy for $\langle\Sigma\rangle$ requires more than corrections on $\langle W\rangle$

✓ globally, NI is the cheapest, but DFT performs better as $T \to 0$

Future Perspectives

➢ Correct the time-dependent spectrum v_{xc} adding dependences in t and T and Perturbation Theory

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