Full Quantum Work Statistics for Non-Homogeneous Many-Body Systems

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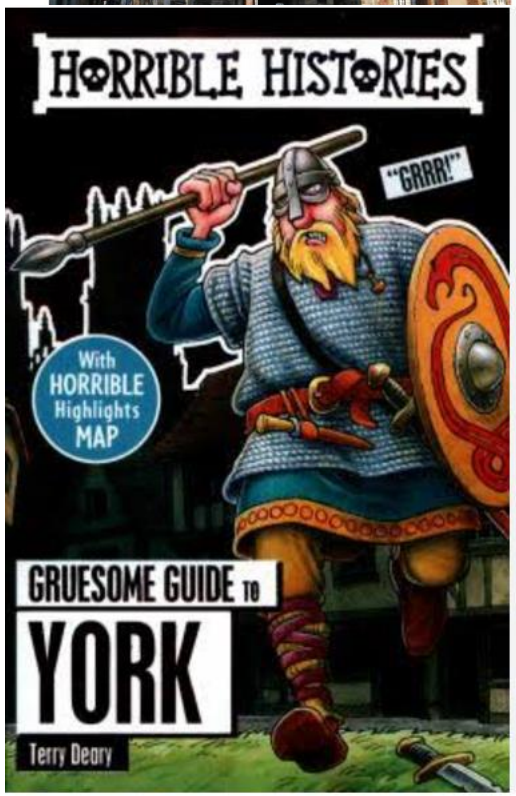
Pies and Ales!

Come and visit!



wikipedia

Ghosts and Hunted Pubs!

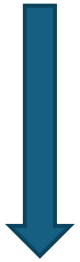
Vikings, Brrrrrrr!

Motivations

- Emergence of irreversibility at the quantum scale
- Effects of quantum fluctuations on thermodynamic quantities/processes
- Related effects on *performance and energetics* of quantum (thermal) machines/technologies
- Improve methods to study many-body quantum systems (relevant to actual experimental set-ups and devices)

Motivations

- Improve methods to study many-body quantum systems (relevant to actual experimental set-ups and devices)
  - interactions
  - + non-homogeneous
  - + finite temperature
  - + non-equilibrium
  - + finite-time dynamics



increased complexity

+open system dynamics

you must be joking!!

but: which quantities are we really interested in?
wave function/full system state? can we get away with less?

Today's focus:

- Irreversibility and quantum fluctuations in the context of dissipative quantum work statistics
- Development of first-principle method for many-body quantum systems
  - interactions
  - + finite temperature
  - + non-equilibrium
  - + finite-time dynamics: linear response
- Method based on density functional theory (DFT)

Outline

- Linear response for dissipated-work probability distribution: connection to relaxation function
- Microscopic approach to the relaxation function:
  - Briefest introduction to Density Functional Theory (DFT) concepts
  - Some considerations on open quantum systems and DFT
  - Relaxation function from Linear-Response Thermal Time-dependent Density Functional Theory (LR-thTDDFT)
- Application to the ionic Hubbard model: phase diagram, quantum and thermal fluctuations
- Some conclusions & future work…

Linear response for dissipated-work probability distribution: connection to relaxation function

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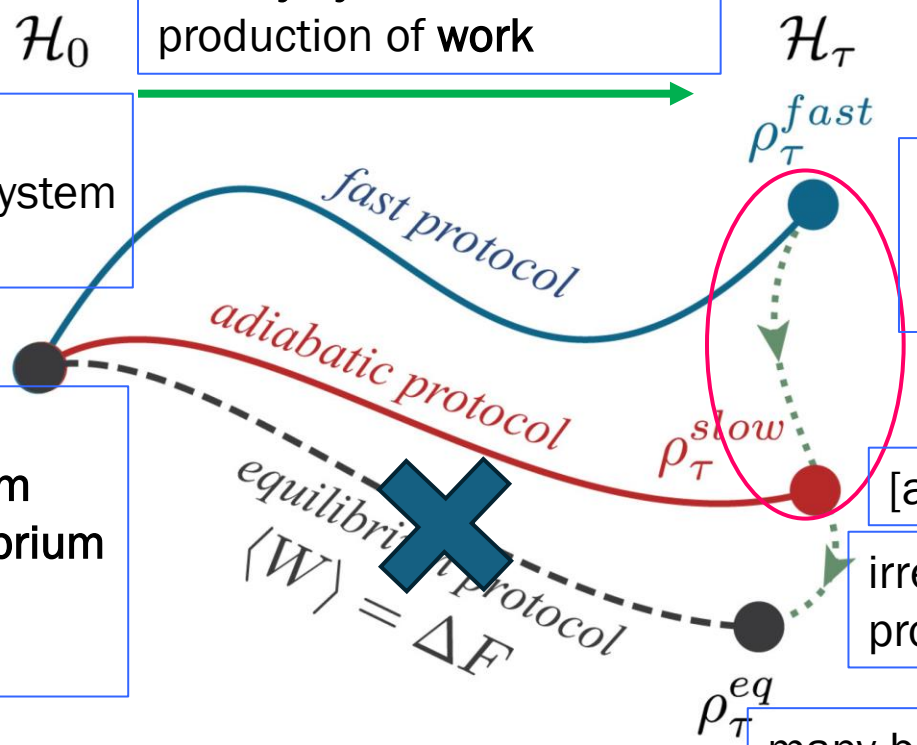
QTD protocol



drive many-body system as **closed** system: **unitary dynamics**; production of **work**

[detach many-body system from bath]

stop of external drive: many-body system **OUT** of equilibrium

start: **many-body system** at **thermal equilibrium** with Hamiltonian H0

[attach many-body system to bath]

irreversibility: **dissipation** of energy to the bath; production of **heat**

many-body system **at thermal** equilibrium with Hamiltonian Hτ

irreversible entropy or dissipated work $\beta\langle W_{diss}\rangle$

finite kT;

Dissipated (or irreversible) work

S. Deffner and E. Lutz, PRL 107, 140404 (2011)

- measures the irreversibility of the thermodynamic process and is non-zero even for an adiabatic process, for close initially thermal systems:

$$\langle \Sigma \rangle = \beta(\langle W \rangle - \Delta F) = \beta \langle W_{\mathrm{ir}} \rangle$$

- given by the relative entropy

$$\beta \langle W_{\mathrm{diss}} \rangle = S\left(\hat{\rho}_\tau \,\|\, \hat{\rho}_\tau^{\mathrm{th}}\right)$$

- where

$$S(\rho_1 \,\|\, \rho_2) = \mathrm{tr}\{\rho_1 \ln \rho_1 - \rho_1 \ln \rho_2\}$$

- defined via a two-point measurement scheme, it is a stochastic quantity with an associated probability distribution $P(W_{diss})$

Dissipative work and relaxation function

G. Guarnieri, J. Eisert, and H. J. D. Miller, Phys. Rev. Lett. **133**, 070405 (2024).

- Given the Hamiltonian $\hat{H}(t) = \hat{H}_0 + \lambda(t)\,\hat{V}$
- with the system relaxation function R. Kubo J Phys Soc Jpn 12, 570 (1957)

$$\psi(t) = \beta \int_0^\beta ds\, \langle \hat{V}(-is)\,\hat{V}(t)\rangle_0 - \beta^2 \langle \hat{V}\rangle_0^2 \qquad \text{with} \qquad \hat{V}(t) = e^{i\hat{H}_0 t}\,\hat{V}\,e^{-i\hat{H}_0 t}$$

- under linear response (small perturbation) cumulants of $P(W_{diss})$

$$\beta^n k_{\mathrm{w}}^n = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, \tilde{\psi}(\omega)\, \gamma_n(\omega) \left| \int_0^\tau dt\, \dot{\lambda}(t)\, e^{i\omega t} \right|^2 \qquad \gamma_n(\omega) = \frac{1}{2}(\beta\omega)^{n-1} \begin{cases} \coth(\beta\omega/2), & \text{for even } n, \\ 1, & \text{for odd } n. \end{cases}$$

$$\beta\langle W_{\mathrm{diss}}\rangle = \frac{1}{2}\int_0^\tau dt \int_0^\tau dt'\, \psi(t-t')\,\dot{\lambda}(t)\,\dot{\lambda}(t') \qquad \text{for n=1}$$

Relaxation function: adiabatic and non-adiabatic

A. Palamara, F. Plastina, A. Sindona, Irene D'Amico arXiv:2512.18338
to be published in QST

- consider:

$$\psi(t) = \psi_{\mathrm{NA}}(t) + \psi_{\mathrm{AD}}$$

dynamical contributions arising from transitions between different energy levels

independent of the driving rate, reflects only the difference between the instantaneous spectra of initial and final Hamiltonians

Relaxation function: adiabatic and non-adiabatic

A. Palamara, F. Plastina, A. Sindona, Irene D'Amico arXiv:2512.18338
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ψ_{AD} :

- consider adiabatic process from $\lambda \to \lambda + \delta\lambda$ for $\tau \to \infty$
- calculate $\beta \langle W_{diss} \rangle = \beta \langle W_{diss} \rangle_{\mathrm{AD}}$ from $\beta \langle W_{\mathrm{diss}} \rangle = S\left(\hat{\rho}_\tau \,\|\, \hat{\rho}_\tau^{\mathrm{th}}\right)$
- expand to leading order in $\delta\lambda$ to obtain linear response expression

$$\beta \langle W_{\mathrm{diss}} \rangle_{\mathrm{AD}} = \frac{\delta\lambda^2 \beta^2}{2} \left(\sum_n p_n^0 |V_{nn}|^2 - \langle \hat{V} \rangle_0^2 \right)$$

- identify ψ_{AD} by comparing to corresponding linear response expression

$$\beta \langle W_{\mathrm{diss}} \rangle = \frac{1}{2} \int_0^\tau dt \int_0^\tau dt' \, \psi(t - t') \, \dot{\lambda}(t) \, \dot{\lambda}(t')$$

- $\psi_{NA} = \psi(t) - \psi_{AD}$

Relaxation function: adiabatic and non-adiabatic

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- consider $\psi(t) = \psi_{\mathrm{NA}}(t) + \psi_{\mathrm{AD}}$

dynamical contributions arising from transitions between different energy levels

independent of the driving rate, reflects only the difference between the instantaneous spectra of initial and final Hamiltonians

- using perturbation theory up to second order in $\delta\lambda$ we obtain

$$\psi_{\mathrm{NA}}(t) = \beta \int_0^\beta ds \left\langle \hat{V}(-is)\, \hat{V}(t) \right\rangle_0 - \beta^2 \sum_n p_n^0 |V_{nn}|^2 \qquad \psi_{\mathrm{AD}} = \beta^2 \left(\sum_n p_n^0 |V_{nn}|^2 - \langle \hat{V} \rangle_0^2 \right)$$

- from which

$$\tilde{\psi}(\omega) = \tilde{\psi}_{\mathrm{NA}}(\omega) + \sqrt{2\pi}\, \delta(\omega)\, \psi_{\mathrm{AD}}$$

time independent

also: Ma, Mitchell and Sela PRL 135, 130402 (2025)

Dissipated Work Distribution: adiabatic and non-adiabatic

A. Palamara, F. Plastina, A. Sindona, Irene D'Amico arXiv:2512.18338
to be published in QST

- consider

$$\beta^n k_{\mathrm{w}}^n = \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}}\, \tilde{\psi}(\omega)\, \gamma_n(\omega) \left| \int_0^{\tau} dt\, \dot{\lambda}(t)\, e^{i\omega t} \right|^2 \qquad \gamma_n(\omega) = \frac{1}{2}(\beta\omega)^{n-1} \begin{cases} \coth(\beta\omega/2), & \text{for even } n, \\ 1, & \text{for odd } n. \end{cases}$$

- from $\tilde{\psi}(\omega) = \tilde{\psi}_{\mathrm{NA}}(\omega) + \sqrt{2\pi}\,\delta(\omega)\,\psi_{\mathrm{AD}}$
- we get adiabatic and non adiabatic contributions to $P(W_{diss})$
- from structure of $\gamma_n(\omega)$:
  adiabatic components only for first two moments
  $P(W_{diss})$ is Gaussian in the adiabatic limit

- How to calculate the relaxation function from microscopic first principles?
- For a generic many-body interacting system?
- Let’s go the Density Functional Theory way…

Briefest introduction to Density Functional Theory (DFT) concepts

Irene D'Amico, University of York

Density Functional Theory (DFT)

- widely used for calculating energies of complex many-body systems and materials (‘T=0’)

Could help with

- many-body quantities (energy, entanglement, work…) from **local** properties (no need of wave function/system state)
- (good) approximation to many-body wave-function/system state
- expressions for non-local or ‘non-observable’ quantities in terms of local properties measurable in experiment

DFT: extensions and reach

?QOpen?

- ground state
- spin-dependent systems
- time-dependent systems (adiabatic regime) C. A. Ullrich's book on TDDFT (2012)
- lattice Hamiltonians (Hubbard, Heisenberg, XXZ...) Capelle and Campo Phys Rep 91, 528 (2013)
- thermal systems (in infancy) A. Pribram-Jones et al. (2014) https://doi.org/10.1007/978-3-319-04912-0_2
- ensembles (in infancy) T. Gould et al. J. Chem. Phys. 164, 040901 (2026)

- open systems:
  - Markovian Lindblad equation K. Burke et al. PRL 94, 146803 (2005)
  - General master equation (including memory) J. Yuen-Zhou et al. PRL 104, 043001 (2010)

DFT: extensions and reach

- GS energy, band structure calculations; properties of materials (predictions and/or analysis from experiments); optical, opto-electronic and magnetic properties of nanomaterials; graphene…

RSC Adv., 2021, 11, 27897

- well established (public) codes: new functionals could be embedded in well-oiled machinery

- **ability of tackling very large many-body systems** (even millions of atoms)

J. Phys.: Condens. Matter **22** 074207 (2010);
Chemical Physics Letters 475 (2009) 163–170

DFT, all flavours based on:

- Hohenberg-Kohn-like theorems [Runge-Gross; Mermin;...]
- Kohn-Sham-type equations

Density Functional Theory: An Approach to the Quantum Many-Body Problem
Reiner M. Dreizler , Eberhard K. U. Gross, Springer 1990

A Bird's-Eye View of Density-Functional Theory
Klaus Capelle, Brazilian Journal of Physics, vol. 36, no. 4A (2006)

Time-Dependent Density-Functional Theory: Concepts and Applications
Carsten Ullrich, Oxford University Press (2012)

Density functionals and model Hamiltonians: Pillars of many-particle physics
K. Capelle and V. L. Campo Jr, Phys Rep 91, 528 (2013)

[.....] e.g. google DFT books or reviews

Hohenberg-Kohn (HK) theorem (Ground State, GS)

$$\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \left[\sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_{i=1}^{N} V(\mathbf{r}_i) + \sum_{i<j}^{N} U(\mathbf{r}_i, \mathbf{r}_j)\right]\Psi = E\Psi$$

kinetic term

external potential

two-body interactions

ground state local density $n_{GS}(r)$

many-body ground state and ground state local density contain the **same information**!

many-body ground state $\Psi_{GS}(r1,r2,....rN)$

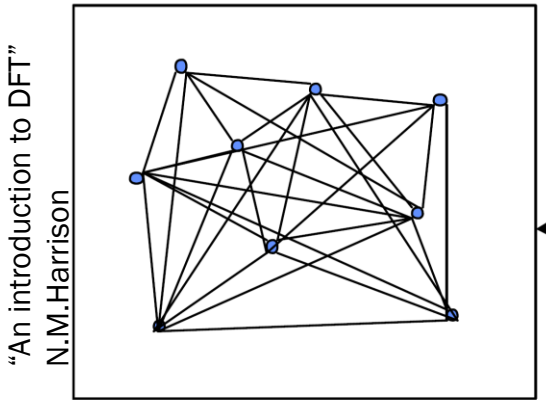
$$n(\mathbf{r}) = N\int \mathrm{d}^3\mathbf{r}_2 \cdots \int \mathrm{d}^3\mathbf{r}_N\, \Psi^*(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)\Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

implication: $O[\Psi] = \langle \Psi | \hat{O} | \Psi \rangle$ becomes: $O[n_{GS}] = \langle \Psi[n_{GS}] | \hat{O} | \Psi[n_{GS}] \rangle$

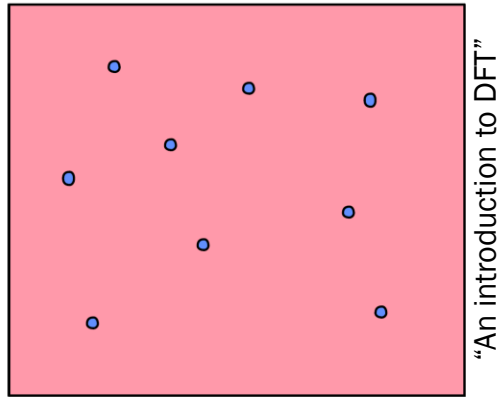
NB: existence of functional, but not its form!

Kohn-Sham (KS) system/scheme:

many-body (**interacting**) system, $n_{GS}(x)$



KS



Kohn-Sham system: **non-interacting** system, $n_{GS}(x)=n_{KS,GS}(x)$

Price:

- **exchange-correlation potential**, $v_{xc}([n_{GS}])$
- **unknown functional** of the density and must be **approximated**.

solve **many-body** Schroedinger equation;

$$O[\Psi] = \langle \Psi | \hat{O} | \Psi \rangle$$

$\Psi=\Psi$(**3N variables**)

solve **single-particle** KS-equations;

$$O[n_{GS}] = \langle \Psi[n_{GS}] | \hat{O} | \Psi[n_{GS}] \rangle$$

$n_{GS}=n_{GS}$(**3 variables**)

Two different types of density functionals to be found or approximated:

1. **exchange-correlation potential, $v_{xc}([n])$:**
   needed to solve the KS equations and find the local density n of the system

2. **functional dependence on the local density n of the quantity of interest,**
   i.e. usually the explicit dependence on n of

$$O[n] = \langle \Psi[n] | \hat{O} | \Psi[n] \rangle$$

QTD: Two **plus one** different types of density functionals to be found or approximated:

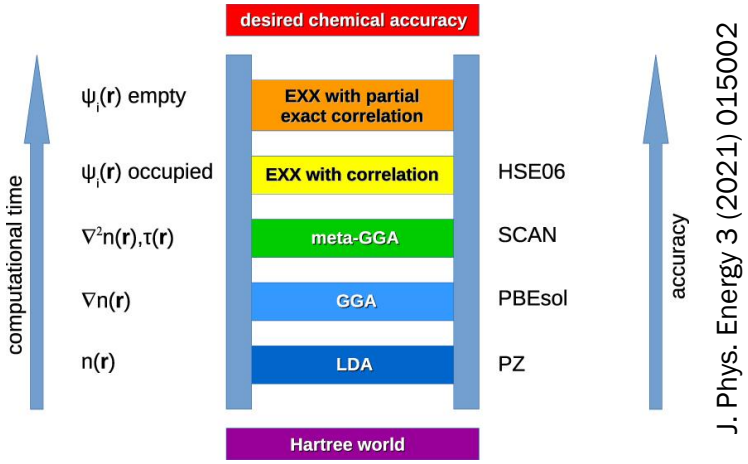
1. exchange-correlation potential, $v_{xc}([n])$:
   needed to solve the KS equations and find the local density n of the system
2. functional dependence on the local density n of the quantity of interest,
   i.e. usually the explicit dependence on n of $O[n] = \langle \Psi[n] | \hat{O} | \Psi[n] \rangle$

3. **QTD:**
   - I. **demonstrate that non-local, non-observable quantities are functionals of the densities** (and which densities) e.g. entanglement & P(W)
   - II. **find the functionals** and their viable approximation

A Palamara, F Plastina, A. Sindona and I. D'Amico PRA 110, 062203 (2024)

The exchange-correlation potential v_{xc}

- The exchange-correlation energy E_{xc} (and its functional derivative v_{xc}) contains information about the many-body interactions of the original interacting system.
- In general v_{xc} is an **unknown functional** of the density and must be approximated (Jacob ladder).



- Most used: local density approximation (LDA).
  LDA: at each point r, replace the exact xc energy density with that of the corresponding uniform, homogeneous system whose density has the same value as the local density n(**r**).

Uncharted territory

DFT: functionals?
dependency on which local densities?
dependency of density functionals?
workable approximations for v_xc?

- Demonstrate that QTD quantities are local-density functional
- Functionals of ***which*** local densities
- Find explicit expression for functionals
- Find workable approximations for functionals to apply KS scheme and/or time-dependent DFT
- Benchmark functionals and approximations to exact results
- (Find new results…)

P(W), P(W_{diss}), sudden quench:
A Palamara, F Plastina, A. Sindona and I. D'Amico PRA 110, 062203 (2024)

Relaxation function from Linear-Response Thermal Time-dependent Density Functional Theory (LR-thTDDFT)

Irene D'Amico, University of York

Relaxation function from Linear-Response

NA: Connection between relaxation function and response function (Kubo)

$$\frac{d\psi(t)}{dt} = \frac{d\psi_{\mathrm{NA}}(t)}{dt} = -i\beta \sum_{ij} g_i g_j \left\langle [\hat{A}_i(t), \hat{A}_j(0)] \right\rangle_0 . \qquad \lambda_i(t) = [\lambda_0 + \delta\lambda(t)]\, g_i$$

and density-density response function $\chi^{\beta}_{ij}(t) = -i\,\theta(t) \left\langle [\hat{A}_i(t), \hat{A}_j(0)] \right\rangle_0$

gives $$\tilde{\psi}_{\mathrm{NA}}(\omega) = 2\beta \sum_{ij} g_i g_j \frac{\mathrm{Im}\,\chi^{\beta}_{ij}(\omega)}{\omega}$$

$\mathrm{Im}\,\chi^{\beta}_{ij}(\omega)$: excitations between different energy levels, i.e. NA contributions

Relaxation function from Linear-Response

- AD: using expression for irreversible entropy from PRA 110, 062203 (2024)

$$\psi_{\mathrm{AD}} = -\frac{\beta^2\delta\lambda^2}{b(0)}\sum_{ij} g_i g_j \frac{\partial a_i^{\beta,0}}{\partial \lambda_j} - 2\beta \sum_{ij} g_i g_j \int \frac{d\omega}{\sqrt{2\pi}} \frac{\mathrm{Im}\,\chi_{ij}^{\beta}(\omega)}{\omega} \frac{b(\omega)}{b(0)},$$

with $b(\omega) = \lim_{\tau\to 0}\left|\int_0^{\tau} dt\, \dot{\lambda}(t)\, e^{i\omega t}\right|^2$ and $\lambda_i(t) = [\lambda_0 + \delta\lambda(t)]\, g_i$

- now $\mathrm{Im}\,\chi_{ij}^{\beta}(\omega)$ and $\frac{\partial a_i^{\beta,0}}{\partial \lambda_j}$ can be calculated with DFT methods

Equilibrium and KS quantities

- Many-body generalized time-dependent thermal densities $a_i^{\beta,0} = \mathrm{Tr}\left\{\hat{\rho}_\beta^{\mathrm{th}}[\{\lambda_i^0\}]\,\hat{A}_i\right\}$ can be obtained from the self-consistent non-interacting **KS Hamiltonian** $\hat{H}_{\mathrm{KS}}[\{\lambda_{i,\mathrm{KS}}(0)\}]$ with $\lambda_{i,\mathrm{KS}}[\{a_i(0)\}]$ from which $\dfrac{\partial a_i^{\beta,0}}{\partial \lambda_j}$

- KS density-density response function $\chi_{KS}^{\beta}(\omega)$ can be obtain from KS equations (Lehmann representation)

Linear Response – th -Time Dependent DFT formalism (LR-thTDDFT)

- Under weak-enough time-dependent perturbation (linear response), the density response to changes is given by the density-density response function

$$\chi_{ij}^{\beta}(t) = -i\,\theta(t)\left\langle [\hat{A}_i(t), \hat{A}_j(0)] \right\rangle_0$$

- which can be obtained from the KS dynamics as

$$\chi^{\beta}(\omega) = \chi_{\mathrm{KS}}^{\beta}(\omega) + \chi_{\mathrm{KS}}^{\beta}(\omega) * \mathbf{f}_{\mathrm{Hxc}}^{\beta}(\omega) * \chi^{\beta}(\omega)$$

- with Hxc kernel

$$f_{\mathrm{Hxc}}^{\beta}(\omega) = \left[\chi_{\beta}(\omega)\right]^{-1} - \left[\chi_{\beta}^{\mathrm{KS}}(\omega)\right]^{-1}$$

LR-th: A. Pribram-Jones et al. PRL 116, 233001 (2016)
LR: Gross and Kohn PRL 55, 2850 (1985)

Recap of method

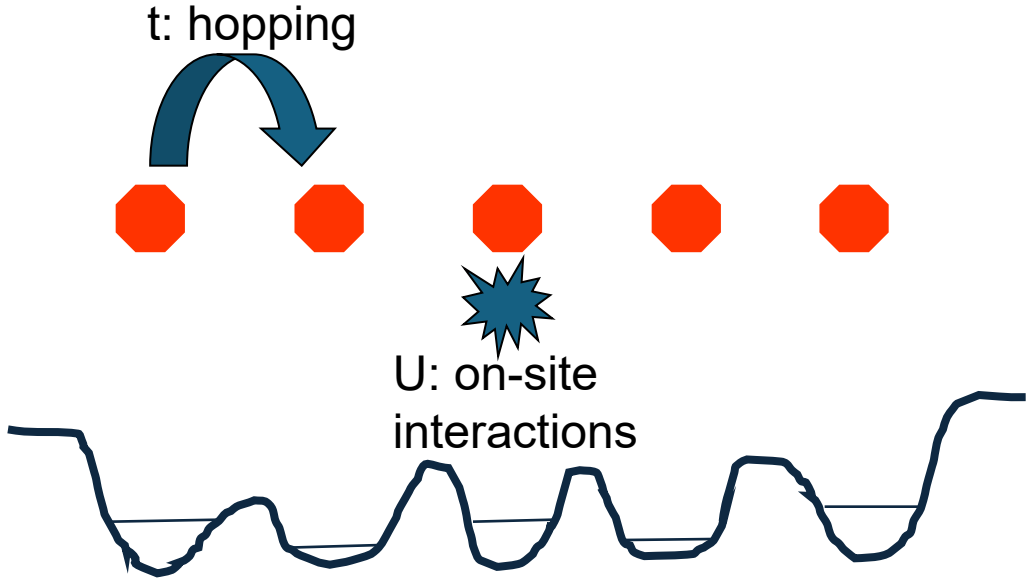
LR-thTDDFT provides the (in principle) exact relaxation function through the following steps:

1. computation of the KS response function from thDFT;
2. inclusion of interaction effects via the Hxc kernel to obtain the fully interacting response;
3. extraction of Im $\chi^{\beta}_{\mathrm{i}j}(\omega)$;
4. combination of the non-adiabatic contribution with the static adiabatic term to obtain the full relaxation function $\tilde{\psi}(\omega)$

Application to the ionic Hubbard model

1D Fermionic Hubbard model

- It allows for both itinerant electron spins (conduction band) and localized magnetic moments
- to describe ‘strongly correlated systems’; recently also cold atoms in an optical lattice, chains of trapped ions, excitons and electrons in coupled quantum dots, or small molecules
- half-filling, inhomogeneous chains with OBC



each site 4 states:
$|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$

2 sites: 16 states
10 sites: 1,048,576 states

e.g. each site a quantum dot with a single energy level

Driven 1D Fermionic Hubbard model

hopping

$$\hat{H}(t) = -J\sum_{i,\sigma}^{N}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma} + \hat{c}^{\dagger}_{i+1,\sigma}\hat{c}_{i,\sigma}\right)$$

$$+ U\sum_{i}^{N}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \sum_{i}^{N} v_i(t)\hat{n}_i,$$

many-body interactions

external drive

$$\hat{V}_{\mathrm{EXT}}(t) = \sum_{i=1}^{\mathcal{L}} v_i(t)\hat{n}_i,$$

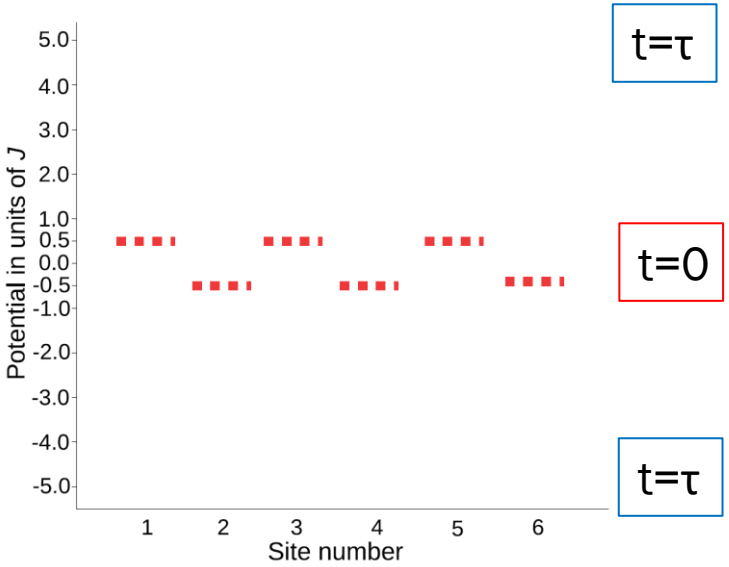
with:

$$v_i(t) = v(t)(-1)^i$$

$$v(t) = v_0 + \frac{\delta v\, t}{\tau}$$

$$\delta v \ll v_0$$

$$t \in [0, \tau]$$



t=τ

t=0

t=τ

- half-filling,
- Open BC

Phase Transitions:

- fermions
- U>0
- Metal to Mott Insulator (MIT) (driven by U)

Bond-order insulator

- Transition to Band-Insulator (driven by **external drive**)

[PRL 83, 2014 (1999)]

thALDA approximation for Hxc kernel

$$f_{\mathrm{Hxc}}^{\beta\, i\, j}[n_i^\beta] = \frac{\partial v_{\mathrm{Hxc}}^{\beta}[n_i^\beta]}{\partial n_j^\beta}\,\delta_{i\,j}$$

with

$$v_{\mathrm{Hxc}}^{\beta}[n_i^\beta] = U + \frac{1}{\beta}\ln\Gamma_U^\beta[n_i^\beta]$$

Single-site Hxc potential:
Hubbard chain is approximated to a collection of single sites coupled by the kinetic term

and

$$\Gamma_U^\beta[n_i^\beta] = \frac{(n_i^\beta - 1) + \sqrt{(n_i^\beta - 1)^2 + e^{-\beta U}\left[1 - (n_i^\beta - 1)^2\right]}}{n_i^\beta}$$

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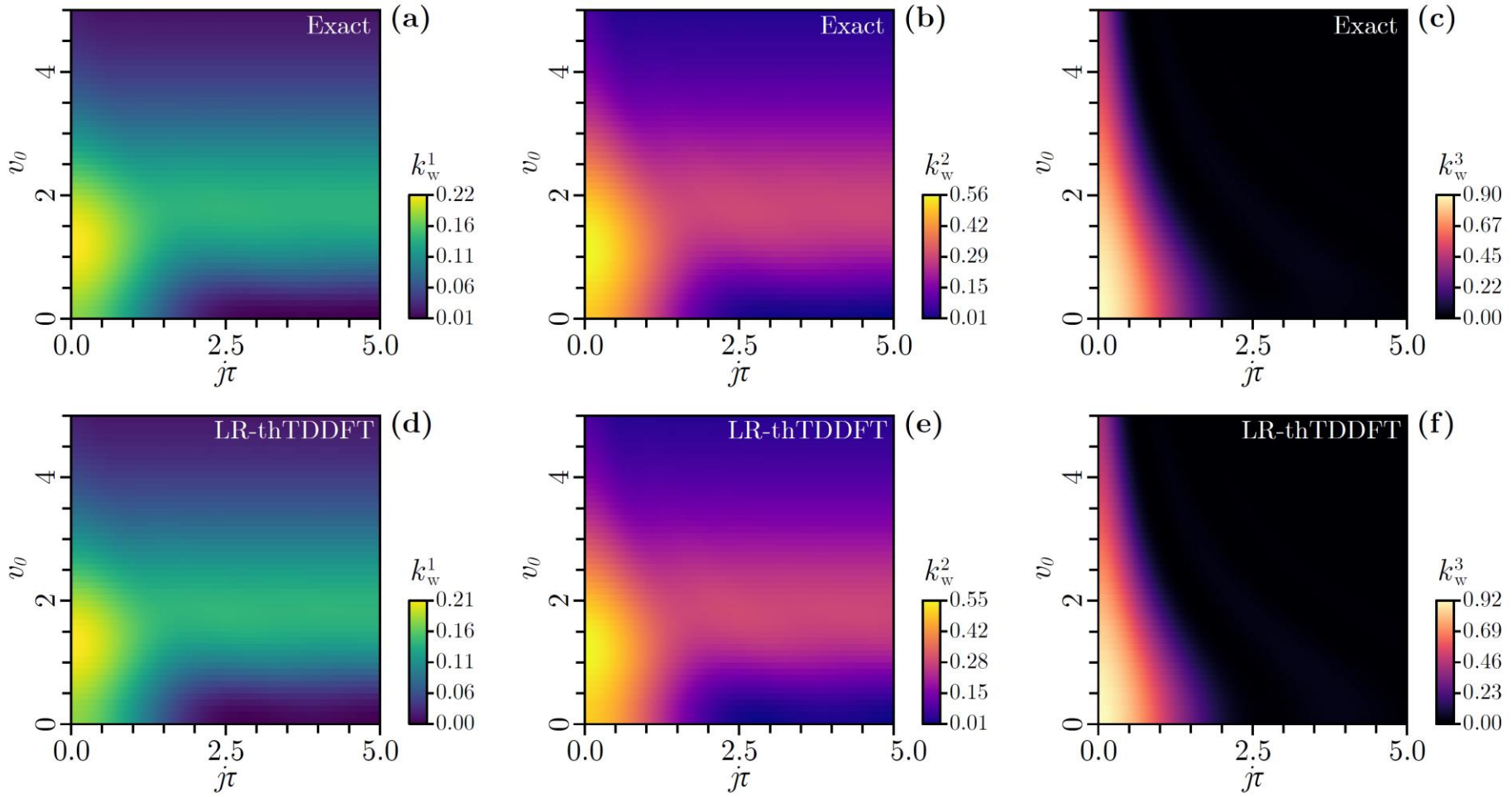
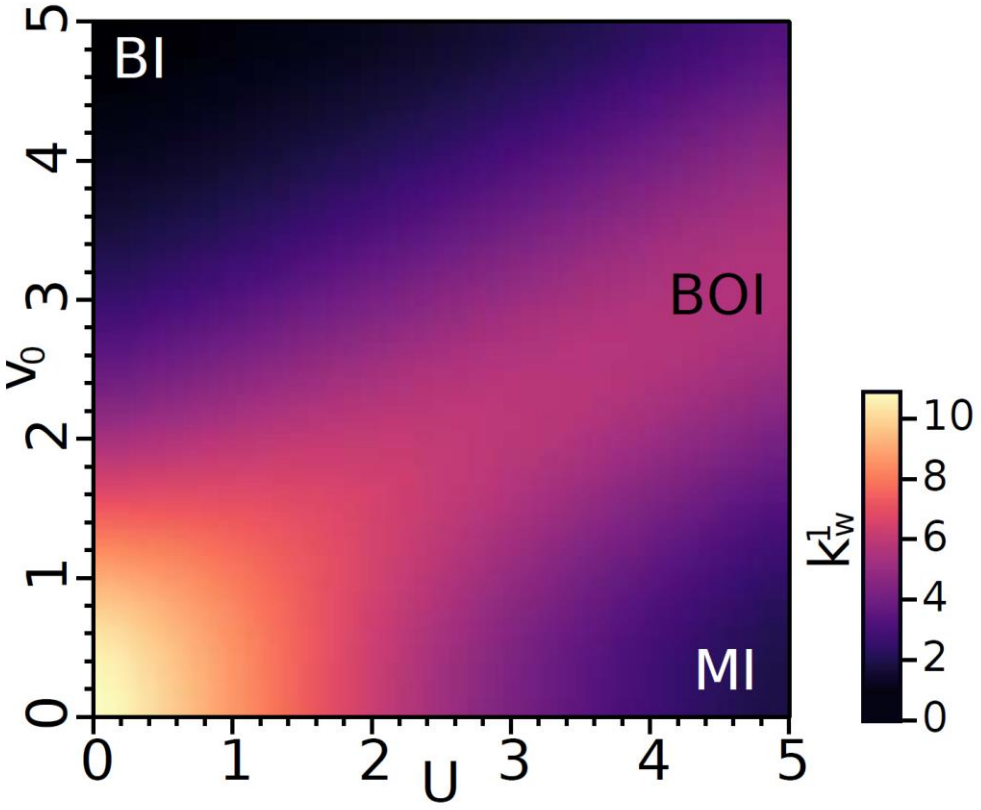
Benchmarking: Exact vs LR-TDDFT, dimer



U = 1 J

Dissipated Work: Finite Temperature Phase Diagram with Staggered Applied Field

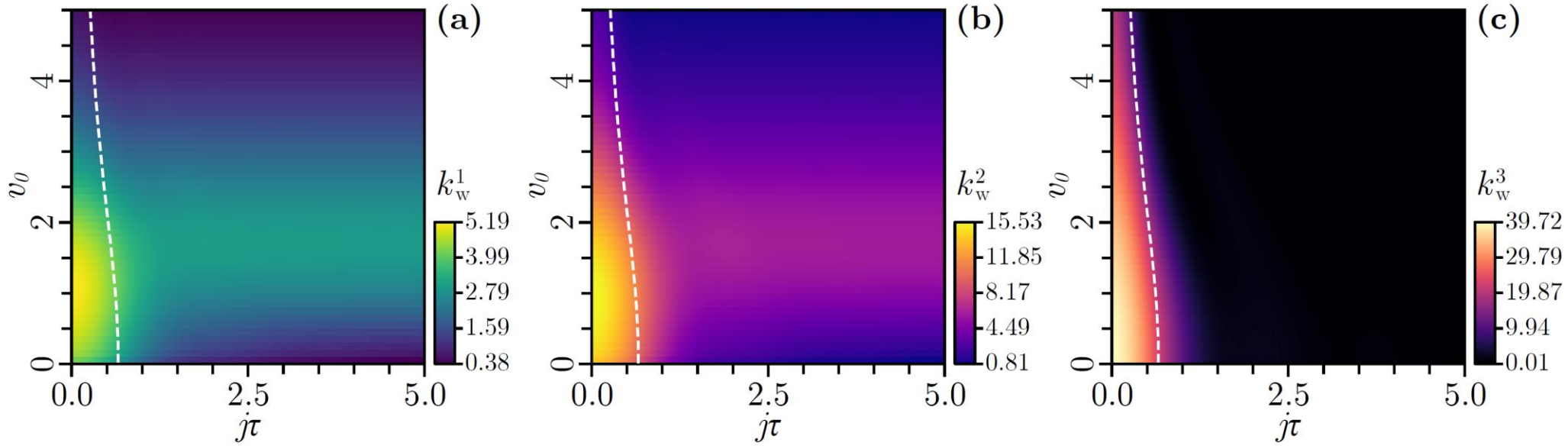


Dissipate work $\langle W_{diss} \rangle / (\delta\lambda)^2$
from sudden quench of the
control parameter
50 sites chain, half-filling
$\beta J = 1, \delta\lambda = 0.01J$.
BI : Band Insulator
BOI : Bond-order insulator [PRL 83, 2014 (1999)]
MI : Mott Insulator

$$\beta k_{\mathrm{w}}^{1} = -\frac{\beta^2}{2} \sum_{ij} \delta\lambda_i \, \delta\lambda_j \, \frac{\partial a_i^{\beta,0}}{\partial \lambda_j^0}$$

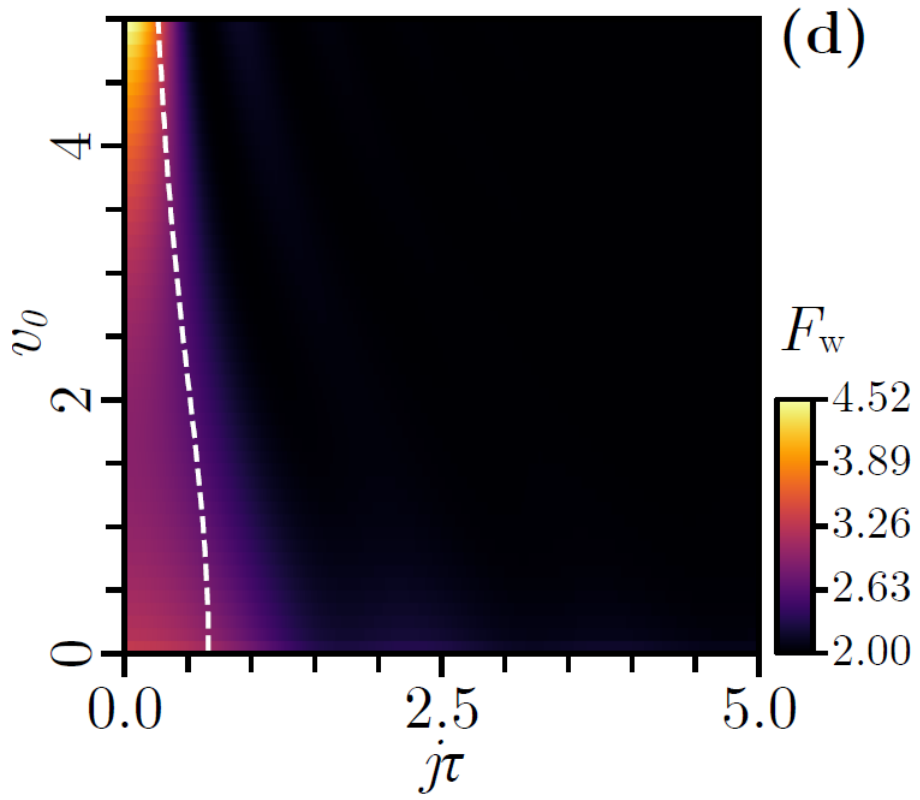
P(W), P(W_{diss}), sudden quench:
A Palamara, F Plastina, A. Sindona
and I. D'Amico PRA 110, 062203 (2024)

Cumulants of the Work Distribution: Adiabatic vs Non-Adiabatic Regime



First 3 cumulants (central moments) of the work distribution vs quench duration τ.
50 sites chain, half-filling, $\beta J = 1$, $\delta\lambda = 0.01J$, $U = 1J$.
Dashed line: crossover from non-adiabatic to adiabatic regimes.

Fano factor



$$F_W = \frac{\mathrm{Var}(W)}{\langle W_{\mathrm{diss}} \rangle} \geq \frac{2}{\beta}$$

TUR is satisfied and saturated
only in the adiabatic regime:
importance of quantum fluctuations
especially in the non-adiabatic region

Conclusions

- Derived a microscopic approach to the relaxation function and hence to the full dissipated work statistics within Linear-Response Thermal Time-dependent Density Functional Theory (LR-thTDDFT) – AD and NA
- Provided a predictive approach applicable to a large class of many-body systems
- Application to the ionic Hubbard model: thermodynamic signatures of Mott, band and bond-order insulating phases
- Improvements: xc potentials / xc kernels beyond LDA /ALDA (dynamic correlations, memory)

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