Universidade de São Paulo
Instituto de Física de São Carlos

XIV Semana Integrada do Instituto de Física de São Carlos

Livro de Resumos da Pós-Graduação

São Carlos
2024

Ficha catalográfica elaborada pelo Serviço de Informação do IFSC

Semana Integrada do Instituto de Física de São Carlos
(13: 21-25 ago.: 2023: São Carlos, SP.)
Livro de resumos da XIII Semana Integrada do Instituto de Física de São Carlos – Universidade de São Paulo / Organizado por Adonai Hilário da Silva [et al.]. São Carlos: IFSC, 2023.
358p.

Texto em português.
1.Física. I. Silva, Adonai Hilário da, org. II. Título.

ISSN: 2965-7679

122

Approximations for the quantum work extracted from a correlated fermion system

ZAWADZKI, Krissia de[1]; VILLANUEVA FILHO, Orion de Macedo Xavier[1]

orionvillanueva@ifsc.usp.br

[1]Instituto de Física de São Carlos - USP

Understanding how to efficiently extract work from a quantum system out-of-equilibrium is one of the most important questions in Quantum Thermodynamics. In the particular case of a strongly correlated system, this is a very challenging problem, as their dynamics is ultimately determined by many-body interactions which play a crucial role in the possible transitions between excited states during the time evolution. Correlations directly affect the set of degrees of freedom dictating an out-of-equilibrium dynamics and, in that sense, approximations to the many-body problem represent an interesting route to study extraction of work in a strongly correlated quantum system. The present project is inspired by the idea of approximating the work extracted in a quantum interacting system using Density Functional Theory (DFT). One of the key elements in DFT is the Kohn-Sham formulation, which converts the many-body problem in an effective non-interacting one by means of the so-called exchange-correlation functional. It has been shown that dealing with systems at finite temperature by means of DFT approximations built at T=0 (1) could produce accurate results up to a characteristic temperature .While in the previous studies for the quantum thermodynamics of the Hubbard model aforementioned the DFT approximations considered the exchange-correlation potential as that for the ground-state (2), an interesting route to improve their accuracy would be employing approximations constructed in the thermal DFT framework. In this project, we propose to study the extracted quantum work in the driven Hubbard model using density functional approximations based on the Bethe Ansatz LDA approaches (3). Our goal is to identify strategies for designing reliable approximations for quantities of interest of Quantum Thermodynamics in various correlation regimes and thermal ranges.

Palavras-chave: Quantum thermodynamics ; Density functional theory ; Hubbard chains

Agência de fomento: CAPES (88887.992402/2024-00)

Referências:

1 REHR, JOHN J. ; KAS, JOSHUA J. Exchange and correlation in finite-temperature tddft. **European Physical Journal B**, v.91, n.7, p.153, 2018.

2 ZAWADZKI, KRISSIA ; SKELT, A. H. ; D'AMICO, I. Approximating quantum thermodynamic properties using DFT. **Journal of Physics:** Condensed Matter, v.34, n.27, p.274002, 2022.

3 LIMA, N. A. *et al.* Density functionals not based on the electron gas: Local-density approximation for a luttinger liquid. **Physical Review Letters**, v. 90, p.146402, Apr. 2003.