VISTA Seminar

Seminar 66

April 3, 2024

10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm CST Beijing

TOC:

1. Presenter 1: Prof. Frank Grossman, Technische Universität Dresden, Germany………………………………………………………………….…. page 2

2. Presenter 2: Mr. Yulong Qiao, Technische Universität Dresden, Germany page 3

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**Different trajectory-based approaches to Bose-Hubbard dynamics**

Frank Grossman

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Description automatically generatedA person in a blue shirt and hat standing in front of a rocky cliff

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We give a brief review of trajectory-based methods to solve the time-dependent Schrödinger equation for Bose-Hubbard (BH) models and related model systems of chemical physics. In order of increasing accuracy these are the truncated Wigner approximation [1], the Herman-Kluk propagator [2], the coupled coherent states approach [3] and a fully variational multi-configuration Gaussian method [4]. We then discuss the results of calculations for BH model systems with small well numbers and highlight the fact that some of the more advanced methods are very well suited to uncover genuine quantum effects beyond initial state preparation [5].

**References:**

[1] M. Hillary et al, Phys. Rep. 106, 121 (1984)

[2] D. V. Shalashilin and M. Child, JCP 113 10028 (2000)

[3] M. Herman and E. Kluk, Chem. Phys. 91, 27 (1984)

[4] M. Werther, S. Loho Choudhury and F. Grossmann, IRPC 40, 81 (2021)

[5] Y. Qiao and F. Grossmann, Front. Phys. 11, 1221614 (2023)

**Applications of generalized coherent states in the dynamics of Bose-Hubbard model**

Yulong Qiao

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The Bose-Hubbard (BH) model is an ideal platform for distinguishing quantum effects from classical behaviour, due to its clear classical counterpart. This work aims to develop a new variational approach to capture quantum effects, such as quantum revivals that classical dynamics is not able to describe [1]. To this end, we begin with a half-filling Glauber coherent state (CS), which is far from equilibrium, and calculate the time-evolved autocorrelation function.

To solve this dynamical problem, we introduce a variational ansatz using generalized coherent states (GCS) [2] which can be used to expand Glauber CS [3,4]. By increasing the multiplicity of our ansatz, we prove that the numerical error in comparison to the exact dynamics decreases with a favourable scaling in the 4-site BH model.

**References**

[1]. S. Tomsovic, P. Schlagheck, et al., Phys. Rev. A 97, 061606 (2018).

[2]. A. Perelomov, Generalized Coherent States and Their Applications (Springer-Verlag, Berlin, 1986).

[3]. P. Buonsante and V. Penna, J. Phys. A: Math. Theor. 41, 175301 (2008).

[4]. Y. Qiao, F. Grossmann, Phys. Rev. A 103, 042209 (2021).

**How to connect**

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 66

Time: Apr 3, 2024 10:00 PM Eastern Time (US and Canada)

Join Zoom Meeting

<https://buffalo.zoom.us/j/92663090079?pwd=VlhPcnRBVTJvT2RLLzNRaWQyWGxQUT09>

Meeting ID: 926 6309 0079

Passcode: 536690