Annals of Physics 390 (2018) 192–213

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

On the reduced dynamics of a subset of interacting bosonic particles

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HIGHLIGHTS

- Discusses open quantum systems where system and environment are indistinguishable.
- Perturbative, microscopic treatment of interacting bosonic many-body systems.
- First-order approximation: BBGKY-hierarchy and, as a special case, Gross–Pitaevskii equation.
- Second-order approximation: Nonlinear master equation with interaction-induced decoherence.

ARTICLE INFO

Article history:
Received 3 November 2016
Accepted 27 January 2018
Available online 1 February 2018

Keywords:
Identical particles
Reduced density matrix
Bosons
Open quantum systems
BBGKY hierarchy
Gross–Pitaevskii equation

ABSTRACT

The quantum dynamics of a subset of interacting bosons in a subspace of fixed particle number is described in terms of symmetrized many-particle states. A suitable partial trace operation over the von Neumann equation of an N-particle system produces a hierarchical expansion for the subdynamics of $M \leq N$ particles. Truncating this hierarchy with a pure product state ansatz yields the general, nonlinear coherent mean-field equation of motion. In the special case of a contact interaction potential, this reproduces the Gross–Pitaevskii equation. To account for incoherent effects on top of the mean-field evolution, we discuss possible extensions towards a second-order perturbation theory that accounts for interaction-induced decoherence in form of a nonlinear Lindblad-type master equation.

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https://doi.org/10.1016/j.aop.2018.01.013
0003-4916/

1. Introduction

The effective quantum evolution of some pre-defined subsystem coupled to environmental degrees of freedom, realized by, e.g., a large number of particles, is often conveniently described by the theory of open quantum systems as formulated for clearly distinct system and environment [1–4]. This is no longer true when the effective dynamics of a subset of identical particles is of interest. The natural decomposition into system and environment degrees of freedom which the standard open-system treatment relies upon is then unavailable and the (anti-)symmetrization postulate suggests that the effective dynamics of a subset of particles cannot be inferred without knowledge of the dynamics of the entire interacting system.

In stark contrast to the difficulty of theoretically predicting the subdynamics of identical particles stands the established and rather straight-forward experimental access to, e.g., single-particle observables of a many-body quantum system. In experiments with cold atoms, for instance, the dynamics of the average momentum distribution,

$$p_{\mathbf{k}}(t) = \mathrm{Tr}^{(N)}\{a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}}\rho^{(N)}(t)\}, \tag{1}$$

of an N-body system is easily measured [5,6]. In (1), $a^{\dagger}_{\mathbf{k}}$ creates a particle with momentum $\mathbf{k}$, $\rho^{(N)}(t)$ denotes the quantum state of the full N-particle system at time t, and the trace $\mathrm{Tr}^{(N)}$ is performed over a complete basis of N-particle states. The probabilities $p_{\mathbf{k}}(t)$, in fact, define the diagonal elements of a single-particle density matrix, expressed in a basis of single-particle momentum eigenstates. Knowledge of the evolution of the single-particle density matrix would suffice to predict the expectation values of arbitrary single-particle operators, without necessarily knowing the evolution of the full N-particle density matrix. The same is true, e.g., for correlation functions of $M < N$ particles, given in terms of an M-particle density matrix. A description of the subdynamics of general M-particle density operators ($M \leq N$) in closed form therefore represents a fundamental problem and a long-standing challenge of mathematical and theoretical physics, with immediate relevance for the fields of atomic and solid-state physics, as well as quantum chemistry [7–14].

Existing microscopic descriptions of the subdynamics of *bosonic* particles are based on mean-field expansions, which are well-justified for modeling Bose–Einstein condensates [15], i.e., when the total many-body system is well described by a macroscopically occupied pure quantum state. If, additionally, the particles' interaction is limited to a contact potential, the dynamics of the single-particle state becomes nonlinear and is described by the Gross–Pitaevskii equation [16,17]. While the Gross–Pitaevskii equation has been extremely successful in predicting the dynamics of ultracold quantum gases, it is unable to describe the effects of decoherence, due to the implicit assumption of a pure state for the subsystem at all times.

A more general picture is given by the Bogoliubov–Born–Green–Kirkwood–Young (BBGKY) hierarchy [18–21], which describes the dynamics of the M-particle reduced density operator in the presence of arbitrary pairwise interactions in terms of the $(M + 1)$-particle density operator [8,12]. For a closed description of the M-particle subdynamics, efficient and appropriate approximations for the truncation of the resulting hierarchical expansion must be found, and a general recipe to achieve this is not available.

Presently there is no microscopic open-system theory for the incoherent subdynamics of identical particles. Interaction-induced decoherence of single-particle observables, such as the average momentum (1), however, was predicted by numerical studies [22–24] to manifest in decaying Bloch oscillations, and traced back to chaotic spectral statistics [25]. This prediction was recently confirmed [6] in cold-atom experiments. In this article, we consider a closed system of a fixed number N of bosonic particles, subject to pairwise interactions. We formally derive the equation of motion for the reduced density operator which predicts the quantum mechanical expectation values of any M-particle observable, with $M \leq N$. To do so we employ a description in terms of symmetrized states constructed on a subspace of fixed particle number. Our approach is based on extensions of concepts from open-system theory, such as the partial trace operation, to the considered scenario of indistinguishable particles.

We first show that by performing an appropriately defined partial trace operation on the von Neumann equation of the full many-body system, we recover a BBGKY-type hierarchy of equations