Computer Physics Communications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computer Physics Communications

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

Computer-aided cluster expansion: An efficient algebraic approach for open quantum many-particle systems☆

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ARTICLE INFO

Article history:
Received 27 September 2016
Accepted 11 October 2016
Available online xxxx

Keywords:
Semiconductor quantum optics
Open quantum many-particle systems
Equations of motion
Cluster expansion
Micro laser
Photon correlations

ABSTRACT

We introduce an equation of motion approach that allows for an approximate evaluation of the time evolution of a quantum system, where the algebraic work to derive the equations of motion is done by the computer. The introduced procedures offer a variety of different types of approximations applicable for finite systems with strong coupling as well as for arbitrary large systems where augmented mean-field theories like the cluster expansion can be applied.

Program summary

Program Title: EoM_main.frm
Program Files doi: http://dx.doi.org/10.17632/fjwxr28j3d.1
Licensing provisions: CC By 4.0
Programming language: FORM
Nature of problem: Quantum many-particle systems are an important subject in fundamental and applied research. The calculation of the time evolution of such systems is a key aspect to investigate and understand their properties. In most cases the Hilbert space that represents the quantum mechanical system is too big to be processed by numerically exact methods and approximation methods have to be used.
Solution method: The program automates an equation-of-motion technique that uses the generalized Ehrenfest equation to derive the time evolution for expectation values of physical observables. The cluster expansion is used to close the hierarchy of the equations of motion. The offered method allows for a variety of different types of approximations to solve such problems with small numerical effort [1].

[1] Leymann, H.A.M., Foerster, A., Wiersig, J., 2014. Expectation value based equation-of-motion approach for open quantum systems: A general formalism. Phys. Rev. B 89 (8), 085308.

1. Introduction

Driven open quantum systems represent a broad class of physical systems where an exact solution is not always feasible. However, in many cases numerically exact solutions for the time evolution of the density matrix are not required, and alternative approximation methods can be applied. The focus of this work is on driven open quantum systems, where we are interested in either the dynamics of the system, or in its non-equilibrium steady state. Such systems usually are hard to solve numerically exact (solution of the full von-Neumann–Lindblad equation) due to the large number of interacting particles and the size of the corresponding Hilbert space. The cluster expansion (CE) and related theories are approximation methods that have proven to be useful in various applications in many-body quantum mechanics, e.g. to describe quantum wells [1], BEC in an optical lattice [2], Rabi oscillations in a quantum dot (QD)-cavity system [3], and sub- and superradiance in semiconductor QD-lasers [4,5]. The specification of the method is its comparatively small numerical effort, while the derivation of the equations of motion (EoM) is a tedious algebraic task, especially when higher orders of approximations are required. To overcome this obstacle we introduce a symbolic manipulation program that carries out the algebra, so that the user can focus on the physical modeling and conceptional questions. The aim of this paper is to share our experience in deriving EoM using the presented program and allow the reader to apply the program to related problems. The

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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http://dx.doi.org/10.1016/j.cpc.2016.10.010
0010-4655/

program is written in FORM [6] and we recommend the extensive and profound introduction [7].

The paper is structured as follows: In Section 2 we recapitulate the basic mathematical operations and ideas behind the CE. To this end we define the operators that are generic to the CE: time derivative of an expectation values (EV) with enforced standard order of the quantum mechanical operators, factorization of EVs into correlation functions (CF), re-factorization of CF back to EV, and the actual approximation that neglects certain CFs or EVs. In Section 3 we outline the structure of our program. In Section 4 the generic CE operators that are introduced in Section 2 are implemented into FORM modules. Together with the general procedures to derive EoM, we present an example program that is used to study the threshold behavior of a high β-factor QD microcavity laser. To demonstrate the ability of our approach we present in Section 5 calculations up to the 10th order of the CE (EoM that if derived using pen and paper are usually truncated at the 4th order, for this kind of system [8]). A complete working program that contains all procedures and the QD laser-model is available for download http://dx.doi.org/10.17632/fjwxr28j3d.1.

2. Theory of cluster expansion

In this section we recapitulate the basic ideas of the CE and introduce operators that represent the different calculation steps in the CE. The computer procedures that we present in the following sections are exact implementations of these CE operators. For a more detailed introduction to this operator based formulation of the CE we refer to [9,10].

In most cases, when encountering many-particle systems, one is interested only in specific physical observables (EV/CF) and not in the complete density matrix. The first step of the CE is to calculate the time derivative using the generalized Ehrenfest equation [11,12]

$$\frac{d}{dt}\langle A\rangle = \langle \mathcal{L}(A)\rangle = \frac{i}{\hbar}\langle [H,A]\rangle + \sum_\nu \frac{\lambda_\nu}{2}\langle 2L_\nu^\dagger A L_\nu - L_\nu^\dagger L_\nu A - A L_\nu^\dagger L_\nu\rangle, \tag{1}$$

for the EV of operator A with the system Hamiltonian H, and the collapse operators L_ν with the rates λ_ν representing the influence of the external bath in Lindblad form (cavity losses, spontaneous emission into non lasing modes, scattering, and dephasing) [9,11,13]. For further calculations it is advisable to establish normal order of the operators, after the application of the generalized Ehrenfest equation, which is symbolized by $:A:$. As a combination of both operations we introduce the operator $:\frac{d}{dt}:$ that derives the EoM in normal order:

$$\left\langle :\frac{d}{dt}A: \right\rangle = \langle :\mathcal{L}(A):\rangle\,. \tag{2}$$

To obtain the dynamics of a many-particle problem one encounters a hierarchy of EoM that couples equations of $\mathcal{O}(N)$ to equations of $\mathcal{O}(N+1)$. By order $\mathcal{O}(N)$ we mean the number of particles that are addressed by an EV or CF. In all practical cases the hierarchy has to be truncated, which can be accomplished in two ways by the truncation operator $\Delta_{\delta/\langle\rangle}$, either by neglecting CFs of order larger than N

$$\Delta_{\delta(N)}\delta(N+1) = \delta(N), \tag{3}$$

or by neglecting EVs of an order larger than N

$$\Delta_{\langle N\rangle}\langle N+1\rangle = \langle N\rangle\,. \tag{4}$$

Which one of these two truncation schemes is more appropriate depends on the physical system. We introduce two particular examples where the truncation leads to the exact solutions: For the ideal gas consisting of non-interacting particles one can set all N-particle CFs larger than $N=1$ to zero, i.e. apply $\Delta_{\delta(1)}$. Whereas an interacting two-particle-system is highly correlated, but $\Delta_{\langle 2\rangle}$ truncates the hierarchy of EoM since all three particle EVs vanish exactly in this system.

To neglect CFs one needs to factorize EVs into CFs, i.e. one needs to express an EV by CFs and vice versa. In the following we recapitulate the factorization according to [10] which is strongly orientated on [14]. We define a set of indices $I=\{1,2,\ldots,k\}$ and a product of Bosonic operators $b^I = b_1 b_2 \cdots b_k$. P is a partition of the set I meaning a set family of disjoint nonempty subsets J of I with $\cup_{J\in P} J = I$, and P_I is defined as the set of all partitions of I. The EV $\langle b^I\rangle$ is factorized into CFs $\delta(b^I)$ by applying the operator $\mathbf{F}$

$$\mathbf{F}\langle b^I\rangle = \sum_{P\in P_I}\prod_{J\in P}\delta(b^I). \tag{5}$$

One can define the inverse operation to re-factorize CFs into EVs as well by

$$\mathbf{F}^{-1}\delta(b^I) = \sum_{P\in P_I} c_P \prod_{J\in P}\langle b^I\rangle, \tag{6}$$

with $c_P = (-1)^{\#(P)-1}(\#(P)-1)!$. To close the infinite hierarchy of EoM of EVs induced by Eq. (1) for a system with a very large number of photons (type I) interacting with a small finite number of atoms (type II) we would have to apply $\mathbf{F}^{-1}\Delta^{I+II}_{\delta(N)}\mathbf{F}\Delta^{II}_{\langle M\rangle}$. Where M is chosen according to the amount of atoms and N according to the interaction strengths. The algebraically most costly part is the factorization $\mathbf{F}$ and the inverse operation $\mathbf{F}^{-1}$. These operations are the reason why higher orders in general cannot be derived using pen and paper. To give an impression of the complexity of the factorization problem we display the factorization of the non-normalized photon-autocorrelation function $\langle b^\dagger b^\dagger b b\rangle$ with the Bosonic creation and annihilation operator $b^\dagger$ and b

$$\begin{aligned}\mathbf{F}\langle b^\dagger b^\dagger b b\rangle &= \delta(b^\dagger b^\dagger b b) + 2\delta(b^\dagger b^\dagger b)\delta(b)\\ &+ 2\delta(b^\dagger b b)\delta(b^\dagger) + \delta(b^\dagger b^\dagger)\delta(b b)\\ &+ \delta(b^\dagger b^\dagger)\delta(b)^2 + 2\delta(b^\dagger b)^2 + \delta(b^\dagger)^2\delta(b b)\\ &+ 4\delta(b^\dagger)\delta(b^\dagger b)\delta(b) + \delta(b^\dagger)^2\delta(b)^2.\end{aligned} \tag{7}$$

This example elucidates the high combinatorial complexity originating from the fact that every partition of the operators has to be regarded. Additional work steps are required for the factorization of EV of Fermionic operators, when the shift in sign has to be taken into count for every commutation of the Fermionic operators.

3. FORM and general concepts

We use the symbolic manipulation system FORM version 4.1 (Jan 13 2014 64-bits) [6]. We assume that the reader is familiar with the basic syntax and concepts of FORM. An introduction to FORM can be found at https://www.nikhef.nl/%7eform/. The advantage of FORM is that the user has full control over the working procedures, in contrast to commonly used computer algebra systems. The calculations performed in our program can actually be regarded as a combination of search and replace commands. Our implementation of the CE consists of procedures that are the implementation the CE operators introduced in the previous section, i.e. the Ehrenfest EoM of EVs with established standard order of the operators ($\langle :\frac{d}{dt}A:\rangle$), and the application of the factorization and truncation operators ($\mathbf{F}$, $\mathbf{F}^{-1}$, $\Delta_{\langle N\rangle,\delta(N)}$), see Eqs. (2)–(6). The basic working principle of the program is illustrated in the flowchart depicted in Fig. 1. At first we have to set up the problem by defining a Hamilton operator H and the collapse operators L_i in the dissipator in Lindblad form. The set