# Quantum-atom optics and dynamical simulations of fermionic many-body systems

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## I. INTRODUCTION AND OVERVIEW

The continuing progress in exploring new states of quantum matter formed by ultracold atomic gases is attracting the attention of even broader scientific communities. At extremely low temperatures, atoms with integer spin (called bosons) enter into a quantum degenerate regime and can form a single, macroscopically occupied quantum state known as a Bose-Einstein condensate (BEC). The BEC, in which the atoms occupy the same quantum state and act like a single entity – a giant matter wave which can be used to make an atom "laser" – was first demonstrated in 1995 [1]. Atoms with half-integer spin (called fermions) form a fermionic counterpart of the BEC – a degenerate Fermi gas [2]. Fermionic atoms can not occupy the same quantum state due to the Pauli exclusion principle. But if two fermions pair up, they can act like a boson and form a Cooper pair, as electrons do in Bardeen-Cooper-Schreiffer (BCS) superconductors. In addition, strongly bound fermionic atoms can form bosonic molecules and molecular BECs, thus resulting in novel Fermi superfluids and unusual systems with a continuous transition from bosonic to fermionic behavior.

An important feature of Bose-Einstein condensates is the presence of atom-atom interactions, which were not considered in the original work of Bose and Einstein. These effects are often taken into account by the "mean-field" approximation, which averages over the condensate, thus ignoring quantum fluctuations and correlations. However, quantum correlations are becoming increasingly important in the understanding of BECs and related strongly correlated systems, especially in newer devices that involve smaller traps, BECs on integrated atom chips, and low dimensional environments.

In general, correlation functions can be thought of as the fingerprints of the underlying order and reciprocal relationships between the particles in complex many-body systems. They facilitate the most in-depth understanding of many-body phenomena due to inter-particle interactions, quantum statistical effects, and external potentials. However, calculating the correlation functions in interacting many-body systems is not an easy task and continues to remain one of the grand-challenges of theoretical physics. In this respect, ultracold quantum gases offer exciting opportunities for new insights in the understanding of quantum many-body correlations because, on the one hand, they can be accurately described by relatively simple and well-defined theoretical models and, on the

other hand, they are amenable to a rather precise experimental control and manipulation.

One of the exciting new research directions in the field of ultracold atoms is quantum-atom optics and *fermionic* quantum-atom optics [3], in particular. This explores analogies with the very successful field of quantum optics with photons, except that (i) we are now dealing with massive particles and (ii) the quantum statistics of underlying particles (e.g., fermionic atoms) is fundamentally different to that of photons.

## II. PROJECT OUTLINE AND AIMS

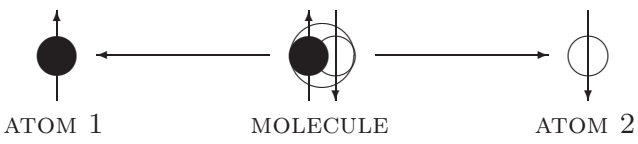
The project consists of two parts, which are complimentary to each other and are developed in parallel.

(A) The first part is concerned with the development of the paradigm of fermionic quantum-atom optics through the theory of correlations between fermionic atoms produced in the dissociation of a Bose-Einstein condensate of molecular dimers.

(B) The second part of the project will be devoted to the development of phase space techniques for dynamical simulations of fermionic many-body systems using the recently proposed Gaussian operator method [4]. This will include the application of the method to specific physical systems, such as the dissociation of realistic, trapped molecular condensates.

### A. Fermionic quantum-atom optics and molecular dissociation

Dissociation of a Bose-Einstein condensate (BEC) of molecular dimers [5, 6] into pair-correlated atoms (see the schematic diagram below) represents the matter-wave analog of two-photon parametric down-conversion. The latter process has been of crucial importance to the development of quantum optics. Owing to this analogy, the molecular dissociation currently represents one of the "workhorses" of the new field of quantum-atom optics [7–17] and offers promising opportunities for the generation of strongly correlated atomic ensembles and fundamental tests of quantum mechanics with macroscopic numbers of massive particles. Examples include the demonstration of the Einstein-Podolsky-Rosen paradox and generation of "squeezed" states with relative number fluctuations below the shot-noise level [8, 9, 14, 18].



The project is concerned with the following questions:

- Can the molecular dissociation be used as a robust source of strongly correlated fermionic atoms that violate a Bell inequality or demonstrate the Bohm's version of the Einstein-Podolsky-Rosen (EPR) paradox?
- What are the best operational measures of correlations between fermionic atoms in molecular dissociation?
- What are the consequences of the fact that the shot-noise for fermions is fundamentally different to that of bosons?
- What are the best strategies to demonstrate relative number squeezing and to achieve shot-noise limited measurements?

The aim of this project is to answer these questions through developing the theory of dissociation of realistic, trapped molecular condensates, and performing quantitative modeling of proposed correlation experiments.

As part of the research program of the ARC Centre of Excellence for Quantum-Atom Optics (ACQAO), this project is also relevant to the planned experiments at the Swinburne University of Technology (SUT) Node of ACQAO. The team at SUT have produced their first molecular BEC of lithium dimers ($^6Li_2$) in April 2007 [19]. Their future plans include the study of atom-atom correlations in molecular dissociation. We hope that our project will be carried out in collaboration with the experimental effort at SUT and will be able to perform quantitative modeling of their experiments. Currently we have also carried out a theoretical analysis of the BEC collision experiment at CNRS Univ. Paris-Sud (see [20] and references therein).

As already mentioned, the project outcomes may find applications in precision measurements beyond the shot-noise level, as well as in fundamental tests of quantum mechanics with macroscopic number of fermions, such as demonstrations of Bohm's version of the Einstein-Podolsky-Rosen paradox [9] and tests of Bell's inequalities for spin observables. Related proposals have recently been formulated in solid state systems [21], [22] and in subatomic physics [23]. However, the advantage with the ultra-cold fermionic atoms is that they are neutral and therefore the quantum statistical effects are not overwhelmed by long-range Coulomb repulsion, as is the case for charged electrons in condensed matter systems.

### B. Dynamical simulations of fermionic many-body systems

The aim of this part of this research is to develop phase space quantum dynamical simulation techniques for fermions, using the Gaussian operator method proposed by Corney and Drummond [4]. This also means application of the method to specific physical systems, such as the dissociation of trapped molecular condensates.

Simulation of many-body fermionic systems is a topic of widespread interest in many fields of physics, including condensed matter physics, astrophysics, and ultracold atomic and molecular physics. The phase space technique based on the Gaussian operator expansion does not suffer from the well-known sign errors [24], and has been demonstrated to be successful in the treatment of the well-known Hubbard lattice model in 1D and 2D [25–27]. The Gaussian phase-space method for fermions is somewhat similar the stochastic positive-$P$ representation method for bosons which uses a basis of coherent states [28]. However, the fermionic analog of coherent states involves the so-called Grassman algebra [29], which is a mathematical abstraction and can not be implemented on a computer using standard rules of algebra [30].

The Gaussian operator method overcomes this difficulty by using a basis with pairs of fermionic operators, which obeys the usual commutation relations. On the other hand, the phase space methods come with their own disadvantages, which are the large sampling errors that typically develop over long simulation times [31]. This has limitations on the maximum useful time in a quantum dynamical simulation. There are methods to partly overcome this problem, by employing the freedom of choosing an appropriate "stochastic gauge" [32]. The choice of an appropriate gauge, however, is a highly nontrivial problem and is specific to the problem in hand.

As part of this project we plan to develop the Gaussian phase-space method and tailor it to the problem of molecular dissociation. The overall goal is to perform first-principle simulations of molecular dissociation in a multi-mode situation found in typical experiments with trapped condensates. In particular, we would like to find answers to the following questions:

- Is there an optimum "stochastic gauge" for dynamical simulations of dissociation of molecular condensates?
- What is the effect of spatial inhomogeneity of the molecular condensate on the strength of atom-atom correlations created from it?
- What is the role of atom-atom $s$-wave interactions during spatial expansion of the atoms released from the trap?

The simulations will be compared with the results of recent correlation measurements performed at JILA using dissociation of potassium dimers [6], and hopefully with the results of the planned experiments at SUT using lithium dimers.

## III. CURRENT RESEARCH

### A. Previous theoretical work

Early work on molecular condensates (made of bosonic atom pairs) has been carried out by the group at UQ more than ten years ago by Drummond and Kheruntsyan [33]. Related early contributions to the problem of molecular dissociation have been made by Mølmer *et. al.* [7]. More recently first-principle simulations have been carried out by Savage and Kheruntsyan [13, 14]. This work has confirmed the importance of treating the non-uniform shape of the molecular BEC. The role of $s$-wave scattering interactions, which are harder to simulate, seems to be minor for short simulation times. However, the effects of these interactions in the long time limit is still an open question and can be different for bosons and fermions, and will be studied within this project. In all those studies the trap was switched of at $t = 0$. The role of dissociation in a trap was studied in [15] by Tikhonenkov *et. al.*, in addition they have worked on a group theoretical approach to the MBEC dissociation problem [16]. In the case of fermionic atoms the uniform system has been studied analytically within the undepleted pump approximation by Kheruntsyan [3], and with (mean-field) depletion by Jack and Pu [12], and by Davis *et. al.* [17]. While substantially explored for bosonic atoms, the difficulties with fermionic many-body calculations, have so far inhibited investigations of the fermionic atom-atom correlations from first-principle calculations.

### B. Progress to date within this research project

The effective quantum-field theory Hamiltonian describing dissociation of a BEC of molecular dimers can be written in the following form, neglecting atom-atom $s$-wave scattering interaction:

$$\hat{H} = \hat{H}_0 - i\hbar\chi \int d\mathbf{x} \left( \hat{\Psi}_0^\dagger \hat{\Psi}_2 \hat{\Psi}_1 - \hat{\Psi}_1^\dagger \hat{\Psi}_2^\dagger \hat{\Psi}_0 \right). \tag{1}$$

Here $\hat{H}_0$ is the kinetic energy term, $\widehat{\Psi}_0(x,t)$ stands for the molecular bosonic field operator, whereas $\widehat{\Psi}_i(x,t)$ $(i = 1, 2)$ describe the two atomic fields in two different spin states. $\chi$ is the atom-molecule coupling term which is responsible for coherent conversion of molecules into atom pairs, e.g. via Raman transitions or a Feshbach resonance, and hence can be tuned experimentally. The last term

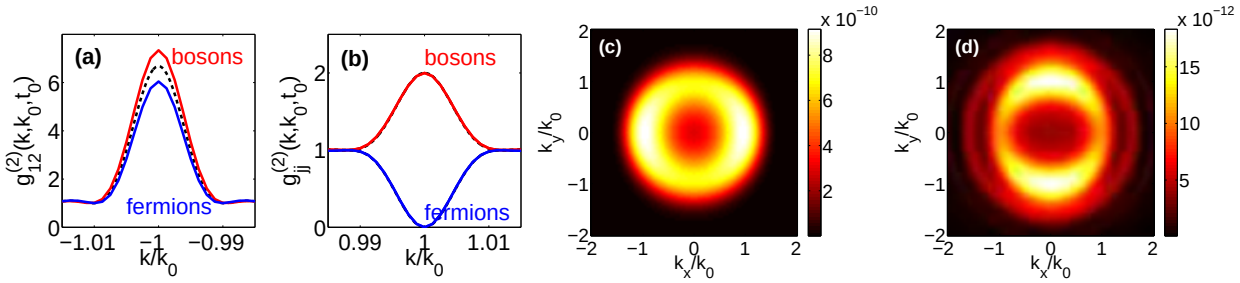



FIG. 1: Back-to-back (BB) (a) and collinear (CL) (b), Glauber's (second-order, equal time) correlation function $g^{(2)}(k, k_0, t)$ as a function of momentum $k$ at a time $t/t_0 = 0.5$. The dashed (black) lines are from our analytic $t \ll t_0$ asymptotes, solid lines are calculated numerically [34, 35]. The two figures on the right are atomic density distribution in momentum space at time $t/t_0 = 3.3$, for bosons (c), and fermions (d) [36]. The MBEC (not shown) is elongated along the x-direction.

in the parentheses, $\hat{\Psi}_1^\dagger \hat{\Psi}_2^\dagger \hat{\Psi}_0$, can annihilate one molecule and create two atoms (one in spin state 1 and one in 2). It's Hermitian conjugate term models the opposite process, recreation of a molecule.

As a starting step, we have employed the undepleted molecular field approximation in which the molecular field is treated classically via the coherent mean-field amplitude $\Psi_0(x) = \sqrt{\rho_0(x)}$, where $\rho_0(x)$ is the molecular BEC density. The undepleted molecular approximation is valid only for short dissociation times, during which the converted fraction of molecules does not exceed $\sim 10\%$ [13, 17]. In this regime, the dissociation typically creates low density atomic clouds for which the $s$-wave scattering interactions are a negligible effect too [13]. In the future we plan to relax the undepleted molecular approximation and perform first-principle simulations of the equations of motion governed by the Hamiltonian (1) without any additional approximations.

To this end we have performed simulations of inhomogeneous molecular condensates within the undepleted field approximation, in one- and two-dimensional geometries [34–36], see Fig. 1 (a), (b) and (c), (d), respectively. Within this approximation, the Heisenberg's equations are linear in operators and can be solved numerically by standard methods of linear operator algebra. Our goal have been to understand the effect of the shape of the molecular BEC (MBEC) on the atom-atom correlations on a simple analytically transparent level, see the dashed curves in Fig, 1 (a) and (b). Those are the analytical short time asymptotes we have derived, as seen in the figures they capture the essential shape of the correlation functions even at a relatively large time. The physical origin of the back-to-back (BB) correlation [Fig. 1 (a)] is the momentum conservation (illustrated on page 2) and is analogous to photon pair correlations in parametric down-conversion. The collinear (CL) correlation [Fig. 1 (b)] is the analog of the famous Hanbury Brown and Twiss effect in optics with photons, except that in the case of fermionic atoms the bunching is reversed into anti-bunching.

In the two-dimensional study we have used an elongated MBEC to quantify the effects of bosonic stimulation [fig 1 (c)] and fermionic Pauli blocking [fig 1 (d)] [36]. As is clearly seen the bosonic and fermionic results are qualitatively very different, due to bosonic stimulation and Pauli blocking.

We have also developed the exact phase space method such that we presently can model more than 300 atomic modes. This would be impossible with the traditional first principles method (numerical diagonalization), since our model system corresponds to a Hilbert space of dimension $2^{300} \simeq 10^{90}$, which is larger than the number of particles in the universe. Atom-atom interactions have been neglected in the work so far.

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