Warszawa, 22 March 2014

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Summary of professional achievements

Contents

1 Curriculum Vitae

1.1 Personal Data

Name: Piotr Paweł Deuar

[redacted] [redacted]

Work address: Institute of Physics, Polish Academy of Sciences (IF PAN)
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1.2 Education

27 II 2005 **Doctor of Philosophy**
University of Queensland, Brisbane, Australia
First-principles quantum simulations of many-mode open interacting Bose gases using stochastic gauge methods.
Subitted 29 VI 2004. (arXiv:cond-mat/0507023)
Supervisor: Prof. Peter D. Drummond.
(Validation in Poland by IF PAN, 12 X 2010)

16 XII 1996 **Bachelor of Science (Hons)**
University of Queensland, Brisbane, Australia
Tests of compatibility between quantum mechanics and macroscopic local realism.
(First Class Honours in Physics)
Supervisor: Dr. Margaret D. Reid.
(Similar to an MSc in the Australian system – allows one to take up PhD studies)

15 XII 1995 **Bachelor of Science**
University of Queensland, Brisbane, Australia

1.3 Employment

VIII 2009 – present	Adiunkt, ON-2.6, Instytut Fizyki PAN, Warszawa, Poland.
IV 2009 – VII 2009	Visiting scientist, LPTMS, Université Paris-Sud, Orsay, France.
IV 2007 – III 2009	Marie Curie Research Fellow, LPTMS, Université Paris-Sud, Orsay, France.
III 2006 – III 2007	Postdoc, Van der Waals-Zeeman Insituut Universiteit van Amsterdam, Amsterdam, The Netherlands.
II 2002 – II 2006	Technical advisor, Deuar Pty. Ltd., Brisbane, Australia.
III 1998 – I 2002	PhD student/Teaching Assistant, Department of Physics University of Queensland, Brisbane, Australia.

1.4 Summary information on scientific publications

Number of publications listed in the Web of Science database:

33

including,

11 Physical Review Letters

10 Physical Review A and B

Number of citations according to Web of Science (14 II 2014):

576

(17.45 citations per publication)

Hirsch index according to Web of Science (22 III 2014):

14

Summed impact factor, according to Journal Citation Reports (JCR):

123,764

(For lack of data, the 2013 impact factor was assumed to be the same as in 2012)

2 List of articles comprising the scientific achievement according to art. 16 ust 2 ustawy z dnia 14 marca 2003 r. (Dz. U. nr 65 poz. 595 z późn. zm)

THEME:

Stochastic methods for macroscopic quantum dynamics and their applications

H1 **P. Deuar**, P. D. Drummond,
Correlations in a BEC collision: First-principles quantum dynamics with 150 000 atoms,
Physical Review Letters **98**, 120402 (2007).

I estimate my contribution to this publication to be **80%**. The idea to carry out calculations on such a large system came from me, as well as the decision to use condensate collisions as our example. I carried out all the calculations and prepared the article. We jointly planned and discussed the research and methods, analysed and interpreted the results, and discussed their broad significance.

H2 **P. Deuar**,
Simulation of complete many-body quantum dynamics using controlled quantum–semiclassical hybrids,
Physical Review Letters **103**, 130402 (2009).

My contribution to this publication was **100%**.

H3 V. Krachmalnicoff, J-C. Jaskula, M. Bonneau, G. B. Partridge, D. Boiron, C. I. Westbrook, **P. Deuar**, P. Ziń, M. Trippenbach, K. V. Kheruntsyan,
Spontaneous Four-Wave Mixing of de Broglie Waves: Beyond Optics,
Physical Review Letters **104**, 150402 (2010).

I estimate my contribution to this publication to be **30%**. The paper was largely experimental (about 50%). Among the theoreticians (PD, PZ, MT, KVK) my contribution accounted for about 60%. This was the first paper to apply the STAB method that I developed for accurate calculations of the properties of the scattered halo. I was responsible for all numerical calculations, and for the idea to interpret the results of Fig. 3 by considering addition and removal of terms in the Bogoliubov Hamiltonian. The majority of the authors, including me, made significant contributions to the interpretation of the results and the editing of the article.

H4 J-C. Jaskula, M. Bonneau, G. B. Partridge, V. Krachmalnicoff, **P. Deuar**, K. V. Kheruntsyan, A. Aspect, D. Boiron, C. I. Westbrook,
Sub-Poissonian number differences in four-wave mixing of matter waves,
Physical Review Letters **105**, 190402 (2010).

I estimate my contribution to this publication to be **15%**. The paper was predominantly experimental (about 75%). Among the theoreticians (PD, KVK) my contribution accounted for about 60%: I was responsible for all the numerical calculations. All the authors contributed significantly to the interpretation and analysis of the results and the editing of the article.

H5 **P. Deuar**, J. Chwedeńczuk, M. Trippenbach, P. Ziń,
Bogoliubov dynamics of condensate collisions using the positive-P representation,
Physical Review A **83**, 063625 (2011).

I estimate my contribution to this publication to be **80%**. The STAB method described in the article was conceived and developed by me, as was the scheme by which it was analysed. All the numerical calculations and the majority of the preparation of the article were my work. All the authors made significant contributions to the form of the article, the analysis and comparison to other methods, and to the final editing of the article.

H6 **P. Deuar**, P. Ziń, J. Chwedeńczuk, M. Trippenbach,
Mean field effects on the scattered atoms in condensate collisions,
European Physical Journal D **65**, 19 (2011).

I estimate my contribution to this publication to be **75%**. I suggested this approach to understand the behaviour of condensate collisions, and was subsequently responsible for all the numerical work and some of the analytics, as well as most of the preparation and editing of the article. All the authors contributed significantly to the form, editing of the article, and the analysis involved.

H7 K.V. Kheruntsyan, J-C. Jaskula, **P. Deuar**, M. Bonneau, G.B. Partridge, J. Ruaudel, R. Lopes, D. Boiron, C.I. Westbrook,
Violation of the Cauchy-Schwarz inequality with matter waves,
Physical Review Letters **108**, 260401 (2012).

I estimate my contribution to this publication to be **20%**. The paper was predominantly experimental (about 60%). Among the theoreticians (KVK, PD) my contribution accounted for about 50%: I was responsible for all the numerical calculations, and for the Gaussian approximation that allowed us to understand the behaviour of the results, while KVK was the originator of the main idea and carried out most of the interpretation. All the authors contributed significantly to the analysis and the editing of the article.

H8 **P. Deuar**, T. Wasak, P. Ziń, J. Chwedeńczuk, M. Trippenbach,
Tradeoffs for number squeezing in collisions of Bose-Einstein condensates,
Physical Review A **88**, 013617 (2013).

I estimate my contribution to this publication to be **60%**. The main calculation method and the Gaussian model used to understand the relationship between correlations and squeezing were both developed by me, and I carried out the majority of the numerical calculation and manuscript preparation. The model used to remove Bose enhancement, its application, and the analytic description of pair correlations in Section III were due to my co-authors. All of us participated significantly in the interpretation and establishing the form of the article, as well as its editing.

H9 R. Ng, E. S. Sørensen, **P. Deuar**,
Simulation of the dynamics of many-body quantum spin systems using phase-space techniques,
Physical Review B **88**, 144304 (2013).

I estimate my contribution to this publication to be **50%**. In this work, I was the expert on stochastic simulation methods for quantum mechanics, while the co-authors were experts on the physics of spin systems. The original idea to tackle this topic was theirs, while the great majority of practical solutions for the problem that are presented in the article were developed by me. About half of the numerical work and manuscript preparation was done by me.

3 Other scientific publications

3.1 Publications in journals listed in the Web of Science database

3.1.1 Published before obtaining a PhD degree (1998-2004)

P10 A. Gilchrist, **P. Deuar**, M. D. Reid,
Contradiction of quantum mechanics with local hidden variables for quadrature phase amplitude measurements,
Physical Review Letters **80**, 3169 (1998).

I estimate my contribution to this publication to be **25%**. I carried out the numerical calculations and took part in discussions about their interpretation.

P11 M. D. Reid, **P. Deuar**,
Macroscopic local realism: how do we define it and is it compatible with quantum mechanics?,
Annals of Physics **265**, 52 (1998).

I estimate my contribution to this publication to be **10%**. I took part in discussions on this topic with my supervisor. She was responsible for the idea and was the main author of this work.

P12 A. Gilchrist, **P. Deuar**, M. D. Reid,
Contradiction of quantum mechanics with local hidden variables for quadrature phase measurements on pair-coherent states and squeezed macroscopic superpositions of coherent states,
Physical Review A **60**, 4259 (1999).

I estimate my contribution to this publication to be **15%**. I carried out part of the numerical calculations presented in this article.

P13 **P. Deuar**, W. J. Munro,
Improving detectors using entangling quantum copiers,
Physical Review A **61**, 010306(R) (2000).

I estimate my contribution to this publication to be **80%**. I was responsible for the idea, calculations, and most of the analysis and writing.

P14 **P. Deuar**, W. J. Munro,
Information transfer and fidelity in quantum copiers,
Physical Review A **61**, 062304 (2000).

I estimate my contribution to this publication to be **80%**. I was responsible for the idea, calculations, and most of the analysis and writing.

P15 **P. Deuar**, W. J. Munro,
Quantum copying can increase the practically available information,
Physical Review A **62**, 042304 (2000).

I estimate my contribution to this publication to be **80%**. I was responsible for the idea, calculations, and most of the analysis and writing.

P16 **P. Deuar**, W. J. Munro, K. Nemoto,
Upper bound on the region of separable states near the maximally mixed state,
Journal of Optics B: Quantum and Semiclassical Optics **2**, 225 (2000).

I estimate my contribution to this publication to be **50%**. The calculations, and part of the ideas, analysis, and manuscript preparation were due to me.

P17 P. Rungta, W. J. Munro, K. Nemoto, **P. Deuar**, G. J. Milburn, C. M. Caves,
Qudit Entanglement.
"Directions in Quantum Optics: A Collection of Papers Dedicated to the Memory of Dan Walls" (Eds. H. Carmichael, R. Glauber, and M. O. Scully, Springer, Berlin, 2001, p. 149-164).
Lecture Notes in Physics **561**, 149 (2001). (arXiv:quant-ph/0001075)

I estimate my contribution to this publication to be **5%**. I took part in some of the research that concerned separability criteria.

P18 **P. Deuar**, P. D. Drummond,
Stochastic gauges in quantum dynamics for many-body simulations,
Computer Physics Communications **142**, 442 (2001).

I estimate my contribution to this publication to be **70%**. I carried out (in close collaboration with my supervisor) the analysis of the stochastic gauge method and the numerical calculations, as well as writing the technical part of the article.

P19 **P. Deuar**, P. D. Drummond,
Gauge P-representations for quantum-dynamical problems: Removal of boundary terms,
Physical Review A **66**, 033812 (2002).

I estimate my contribution to this publication to be **75%**. The analytic and numerical calculations were my work, as well as the idea of diffusion gauges. The initial idea, choice of example models, and the idea of drift gauges were my supervisor's. He also had a large input into the editing of the article.

P20 P. Badziąg, **P. Deuar**, M. Horodecki, P. Horodecki, R. Horodecki,
Concurrence in arbitrary dimensions,
Journal of Modern Optics **49**, 1289 (2002).

I estimate my contribution to this publication to be **10%**. I took part in the early calculations and discussions on the topics covered in the article.

P21 P. D. Drummond, **P. Deuar**,
Quantum dynamics with stochastic gauge simulations,
Journal of Optics B-Quantum and Semiclassical Optics **5**, S281 (2003).

I estimate my contribution to this publication to be **30%**. The calculations in the section concerning the anharmonic oscillator were my work. I also took part in the general development of the method presented in the article, the analysis and interpretation of the method and results, as well as in the writing of the article.

P22 P. D. Drummond, **P. Deuar**, J. F. Corney, K. V. Kheruntsyan,
Stochastic gauge: a new technique for quantum simulations,
Proceedings of the 16th International Conference on Laser Spectroscopy, Australia, 13-18 July 2003 (Eds. P. Hannaford, A. Sidorov, H. Bachor, and K. Baldwin, World Scientific, Singapore, 2004, p. 161-170).
(arXiv:cond-mat/0309537)

I estimate my contribution to this publication to be **30%**. The calculations in the part that concerns the Lieb-Liniger model were done by me. I also took part in the general development of the new method that was described, and in the writing of the article.

P23 P. D. Drummond, **P. Deuar**, K. V. Kheruntsyan,
Canonical Bose Gas Simulations with Stochastic Gauges,
Physical Review Letters **92**, 040405 (2004).

I estimate my contribution to this publication to be **50%**. The main results of the article (calculated with stochastic methods) were my work, as was the development of a practical technique to carry out such calculations. I took part in preparing the article and interpretation of the importance of these results.

3.1.2 Published after obtaining a PhD degree (since 2005)

P24 M. R. Dowling, P. D. Drummond, M. J. Davis, **P. Deuar**,
Time-reversal test for stochastic quantum dynamics,
Physical Review Letters **94**, 130401 (2005).

I estimate my contribution to this publication to be **20%**. I carried out the calculations for one of the two examples presented in the article (the anharmonic oscillator), and contributed to the editing of the article.

P25 **P. Deuar**, P. D. Drummond,
First-principles quantum dynamics in interacting Bose gases I: the positive P representation,
Journal of Physics A: Mathematical and General **39**, 1163 (2006).

I estimate my contribution to this publication to be **85%**. The idea to study this matter in detail was mine, and I carried out all the analytic and numerical calculations, as well as writing the article.

P26 **P. Deuar**, P. D. Drummond,
First-principles quantum dynamics in interacting Bose gases II: stochastic gauges,
Journal of Physics A: Mathematical and General **39**, 2723 (2006).

I estimate my contribution to this publication to be **85%**. The diffusion stochastic gauge concept as well as the idea to study its performance in detail were mine. I carried out all the analytic and numerical calculations, and prepared the article.

P27 P. D. Drummond, **P. Deuar**, J. F. Corney,
Quantum Many-Body Simulations Using Gaussian Phase-Space Representations,
Optics and Spectroscopy **103**, 7 (2007).

I estimate my contribution to this publication to be **20%**. One of the three example calculations in the article (four-wave mixing) was carried out by me. I took part in editing the article.

P28 P. D. Drummond, **P. Deuar**, T. Vaughan, J. F. Corney,
Quantum dynamics in phase space: from coherent states to the Gaussian representation,
Journal of Modern Optics **54**, 16 (2007).

I estimate my contribution to this publication to be **20%**. One of the two example calculations in the article (long-distance interactions) was carried out by me. I took part in editing the article.

P29 **P. Deuar**, A. G. Sykes, D. M. Gangardt, M. J. Davis, P. D. Drummond, K. V. Kheruntsyan,
Non-local pair correlations in the 1D Bose gas at finite temperature,
Physical Review A **79**, 043619 (2009).

I estimate my contribution to this publication to be **40%**. I carried out most of the calculations (corresponding to 12 of the 18 figures) and am responsible for developing the advanced stochastic method whose description comprises a large part of the article. I prepared most of the article text. This collaboration was organised jointly by KVK and me.

P30 S. Wüster, J. Stanojevic, C. Ates, T. Pohl, **P. Deuar**, J.F. Corney, J.M. Rost,
Correlations of Rydberg excitations in an ultracold gas after an echo sequence,
Physical Review A **81**, 023406 (2010).

I estimate my contribution to this publication to be **10%**. In this collaboration, I acted as an advisor on stochastic methods which we used to study this problem, though their results did not make it into the final form of the article. In the meantime I actively contributed to the analysis and interpretation of the results and the writing of the article.

P31 J. Dziarmaga, **P. Deuar**, K. Sacha,
Comment on "Quantum entangled dark solitons formed by ultracold atoms in optical lattices",
Physical Review Letters **105**, 018903 (2010).

I estimate my contribution to this publication to be **35%**. The work was conceived and led by me, and I carried out one of the two numerical calculations presented. I carried on the correspondence with the authors of the article that we were commenting on. All the authors contributed significantly to the interpretation and preparation of the article.

P32 E. Witkowska, **P. Deuar**, M. Gajda, K. Rzążewski,
Solitons as the early stage of quasicondensate formation during evaporative cooling,
Physical Review Letters **106**, 135301 (2011).

I estimate my contribution to this publication to be **30%**. I carried out a large part of the dynamical calculations (EW, the rest). I developed the idea and technique required to rotate away the quantum phase that allowed us to image phase domains in the system, including Fig. 2 which brought the article onto the cover of Phys. Rev. Lett. I contributed significantly to the analysis and interpretation of the results as well as to the preparation and editing of the article.

P33 T. Karpiuk, **P. Deuar**, P. Bienias, E. Witkowska, K. Pawłowski, M. Gajda, K. Rzążewski, M. Brewczyk,
Spontaneous solitons in the thermal equilibrium of a quasi-one-dimensional Bose gas,
Physical Review Letters **109**, 205302 (2012).

I estimate my contribution to this publication to be **30%**. Together with TK, I carried out the dynamical simulations, and took part in the analysis of the results. I carried out the analysis of soliton visibility and the comparison with the Yang & Yang model. I took part in the interpretation of the results, and wrote and edited a large part of the article.

3.2 Publications not listed in the Web of Science database

3.2.1 Published after obtaining a PhD degree (since 2005)

P34 **P. Deuar**,
First-principles quantum simulations of many-mode open interacting Bose gases using stochastic gauge methods,
PhD thesis - University of Queensland.
arXiv:cond-mat/0507023

My PhD thesis.

P35 P. D. Drummond, T. Vaughan, J. F. Corney, G. Leuchs, **P. Deuar**, *Coherence and Correlations in Atom Lasers*,
Proceedings of the 9th Rochester Conference on Coherence and Quantum Optics (CQO9), paper IB_2 (2007). (arXiv:0710.2842)

I estimate my contribution to this publication to be **15%**. One of the two example calculations presented in the article (condensate collision) was my work.

P36 **P. Deuar**, M. Stobińska,
Correlation waves after quantum quenches in one- to three-dimensional BECs,
arXiv:1310.1301, submitted to Physical Review Letters.

I estimate my contribution to this publication to be **90%**. The whole idea of the research as well as all the analytic and numerical calculations were done by me, as was the preparation of the article. We jointly interpreted the results and made later editions of the article.

4 A description of the scientific achievement that is the basis of the habilitation:

Stochastic methods for macroscopic quantum dynamics and their applications

The series of articles listed in Section 2 contains the main results to date from the primary long-term research program that I have been pursuing since obtaining a PhD. Its aim is to develop stochastic methods for describing the quantum dynamics of many interacting particles in a form that is appropriate for treating spontaneous processes in ultra-cold gases. These phenomena are entirely omitted by the semi-classical methods that are usually used in the field, such as mean-field or c-field approaches for nonzero temperature. Apart from the development of the methods themselves [H1,H2,H3,H5,H9], the list includes articles that have applied them to describe correlated pairs of atoms produced during a collision of Bose-Einstein condensates. The applications consist of the analysis of general cases [H1,H6,H8] as well as calculations in direct collaboration with experiments [H3,H4,H7]. My newest research within this theme has extended these stochastic methods to the description of many interacting spins [H9].

4.1 Introduction – spontaneous processes and the stochastic description of quantum mechanics

The physics of ultra-cold gases ("quantum" gases) has seen robust development for about the last twenty years. These gases are macroscopic systems of many mutually interacting particles whose quantum mechanical description is remarkably precisely known. This offers many possibilities for comparison of experiment with theory, as well as for creating analogies with more complicated systems such as liquid helium or solid state systems. The possibility to observe the gases with a relatively simple CCD camera makes them uniquely suited to study all kinds of many-body quantum mechanics. Other experimental "knobs" that one can turn externally are changes in the inter-atomic interactions, and placement of the atoms into a periodic potential generated optically. This allows one to realise many hitherto idealised models from solid state physics (Bose-Hubbard, BCS, ...) directly in the lab. Such setups have been called *quantum simulators*. For bosonic atoms, a sufficiently low temperature leads to the formation of a Bose-Einstein condensate, which is a state of many atoms that occupy the exact same quantum state. This amplifies quantum effects and makes their visibility remarkably strong. However, this simple view of a condensate omits many of the phenomena that are of greatest interest, and are now being studied in the latest generation of experiments. One salient example are non-classical correlations between widely separated particles [1–9][H4,H8].

The last couple of years has seen increased interest in the dynamics and the transient states of quantum gases, as well as in their statistics — examples are studies of *quantum quenches* (a non-adiabatic jump in system parameters) [10–14], correlated atom pairs [1–9][H1,H4,H8], and full distributions of quantum measurements [15, 16]. To describe these, it is essential to go beyond the semi-classical descriptions that were usually sufficient to date – mean field for systems near zero temperature [17], or classical fields (c-fields) for higher temperatures [18, 19]. This is because of the importance here of spontaneous processes, in which atoms are scattered from highly occupied modes (one-particle orbitals) into empty ones. This usually results in a loss of coherence with the source modes in the system, allowing for the creation of more exotic quantum states such as spin squeezing [4, 5] or quantum correlated atom pairs. Most of these phenomena have only become accessible experimentally very recently because their characteristic length scale is the healing length ξ, which has been below attainable resolution. However, some recent advances in experimental techniques have finally made these phenomena accessible: the detection of single atoms in free space with the use of metastable

atoms such as He* [1,9,20][H4] or light sheet imaging [2,21], as well as the growing capability to obtain resolution on the healing length scale either by direct improvement of imaging apparatus [2,5,15,16,21], or with special techniques such as anti-trapping [22].

Even though the quantum description of quantum gases is "remarkably well known", going beyond semi-classical approximations in which the dynamics is governed by Gross-Pitaevskii equations (or linearised fluctuations around them) [17], is a serious challenge. The trouble lies in the exponentially growing number of quantum states that must be taken into account as the number of particles or accessible modes grows. This is the so-called curse of dimensionality – the Hilbert space dimension grows as $\sim d^M$ for M modes occupied by up to $d-1$ atoms. For N fermions, $d=2$ and $M \geq N$, while for bosons the dimension d may even be of the order of N and the number of relevant modes depends on the details of the system. In any case, the number of states is unmanageable in macroscopic systems apart from some special cases with symmetries that allow one to limit the dynamics to a small number of well-known states. They is not usually relevant for experimentally realistic descriptions.

"Brute force" calculations (deterministic evolution of the full state in Hilbert space) become intractable beyond about a dozen (or, in favourable circumstances a few tens) of atoms . Typical experiments contain $10^4 - 10^7$. This problem is particularly onerous for dynamical calculations for which standard Monte-Carlo methods do not work because of the rapid accumulation of phase fluctuations among path integrals, similarly to the famous "sign problem" known from equilibrium calculations with fermions [23]. Some newer approaches based on matrix product states and the DMRG method [24–27] allow to treat up to several hundred atoms, but generally only for one-dimensional systems or quasi two-dimensional strips [28].

Instead, for a wide range of problems, these difficulties can be sidestepped with stochastic approaches, often called *phase-space methods*, that are different from traditional Monte-Carlo [29–32][P23,P21,P34]. They rely on the following representation of the state of the system:

$$\hat{\rho} = \int P(\vec{\lambda})\ \hat{\Lambda}(\vec{\lambda})\ d\vec{\lambda}, \tag{1}$$

where $\widehat{\rho} = \sum_a p_a \left|\Psi_a\right\rangle \left\langle\Psi_a\right|$ is the density matrix describing the quantum state or a mixture of them with weights p_a, $\hat{\Lambda}(\vec{\lambda})$ is an operator basis labelled by the parameters $\vec{\lambda}$, while $P(\vec{\lambda})$ is the probability distribution for these parameters. The full quantum state is mapped onto an ensemble of samples $\{\vec{\lambda}^{(j)}\}$ chosen according to the distribution P, and each sample corresponds to a certain set of parameter values. The mapping becomes ever more exact as the number of samples grows. Similarly, the full quantum dynamics is mapped onto a stochastic evolution of the samples. The key element for the stochastic evolution to be practical is to use a basis $\widehat{\Lambda}$ whose parameters are defined locally for each subsystem in the model. That is, $\widehat{\Lambda} = \otimes_{m=1}^{M} \widehat{\Lambda}_m(\boldsymbol{\lambda}_m)$ and $\vec{\lambda} = (\dots, \boldsymbol{\lambda}_m, \dots)$, where the index m counts subsystems, which could be e.g. modes, orbitals, or sites on a computational lattice. The local basis is described by the vector of parameters $\boldsymbol{\lambda}_m$.

This is successful because, firstly: almost all interesting quantities in a large system have contributions from many subsystems; and secondly: just a couple of significant digits of precision are sufficient for almost all purposes. With appropriate choices of the basis operators $\widehat{\Lambda}_m$, the distribution P can be guaranteed real and positive, i.e. a probability distribution. The evolution of the samples is then just diffusion in parameter space and individual samples do not need to accumulate phases, which avoids the sign and phase problems that are chronic in traditional path-integral Monte Carlo dynamics.

The price one pays is limited precision due to statistical fluctuations. Also, the accessible time period can become limited by noise amplification which can occur in the course of the evolution [33][P25,P34,H2,H9]. Nevertheless, in many cases one can obtain useful results that are not attainable with any other contemporary approaches.

Despite this limited precision, one incorporates the *full* quantum dynamics. In contrast to various approximations and simplifications that one can make at the level of the description of the system, here the entire inaccuracy in the results is of a statistical nature, without systematic deviations. It can be reduced by adding more trajectories and, what is more important, can be reliably estimated from a simple statistical analysis of the variation among the generated samples. Another convenient feature is that, as a rule, the dynamical equations have a simple form – typically the mean-field equations plus appropriate noise – and they can be straightforwardly adapted to experimental details. The calculations do not depend on any assumptions of particular symmetries of the system or state, and the calculation is not made appreciably more difficult when arbitrary external potentials, single-particle losses, boundary conditions, or a time-dependent Hamiltonian are added.

The research described in this series of articles developed and adapted phase space methods to the point where they can be used to simulate realistic quantum gases. My point of origin was the positive-P representation [34] that originally proved itself useful in quantum optics, especially in the description of the incoherent dynamics of the optical parametric oscillator and optical solitons [35–41]. Those systems have much in common with spontaneous atom pair production in quantum gases. Later, some initial attempts were made to apply the method to the dynamics of condensates in a number of works, with mixed success [42, 43][P25,P34]. The methods developed by me and described in the series of articles presented here finally made the successful treatment of realistic cases possible [44–47][H1,H3,H4,H6,H7,H8,P27].

An important system that is not well described by any other approach are the halos of scattered atom pairs that form during supersonic collisions of Bose-Einstein condensates [1, 3, 48–53]. The methods developed by me and described in the articles [H1,H2,H5] are the only approaches that have been capable of describing the halo with sufficient accuracy to properly understand the behaviour of the atom pairs produced. The results of my studies of these pairs are presented in more detail in the articles [H1,H3,H4,H6,H7,H8]. They comprise also a good starting point to understand the properties of atoms scattered by the related spontaneous processes such as e.g. pairs created by the decay of excited states in an atomic cloud [2,7,8], during atomic four-wave mixing [54,55], or during superfluid flow of a condensate around obstacles [56–58].

4.2 Development of stochastic methods for Bose-Einstein condensates

The works [H1-H9] took methods that I first came to know during my PhD studies and developed them in a new direction. My doctoral studies under the supervision of Prof. Peter Drummond [P34], were focused on the phase-space methods. We studied their general properties, and devoted the most time to investigation of the so-called (*stochastic gauges*), which specify the additional freedoms available when mapping quantum mechanics to stochastic equations (the mapping is not one-to-one) [P18,P19,P21-P24,P26,P28] (see Section 5.2). The name we used is an analogy to the choice of gauge that is allowed in electrodynamics. We were aiming to apply them to the dynamics of ultra-cold bosonic gases. In the standard case, the relevant Hamiltonian is

$$\widehat{H} = \int d^3\mathbf{x}\, \widehat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) \right) \widehat{\Psi}(\mathbf{x}) + \frac{g}{2} \int d^3\mathbf{x}\, \widehat{\Psi}^\dagger(\mathbf{x}) \widehat{\Psi}^\dagger(\mathbf{x}) \widehat{\Psi}(\mathbf{x}) \widehat{\Psi}(\mathbf{x}), \tag{2}$$

with the Bose field operator $\widehat{\Psi}(\mathbf{x})$, contact interactions of strength g, an external potential $V(\mathbf{x})$, and particle mass m. Apart from the kinetic term, it is very similar to the Hamiltonian of the Kerr nonlinearity ($\chi^{(3)}$) of nonlinear quantum optics, exactly the one for which phase space methods such as the positive-P were very successful [35–41]. We hoped to repeat this success for cold atoms. To this end, we devoted a lot of effort to overcome certain systematic errors that were seen in quantum

optics applications (the so-called boundary term errors) [33] with the help of stochastic gauges. After some initial false leads [P18], we were eventually successful in this endeavour [P19,P23].

Nevertheless, in the later stages of my PhD studies, and later, it began to be clear that applying stochastic gauges to realistic problems would be difficult, and would at the least require the input of further new ideas. Gauges that were very successful at improving simulations for one or two-mode systems lost their effectiveness for many-mode models. There are two reasons: (I) It is difficult to choose a good gauge when the system is complicated, and: (II) the appearance of an additional complex trajectory weight that wrecks the convenient (linear or quadratic) scaling of the size of the calculation with the size of the system [P26]. On the other hand, it also became clear that boundary term errors are not a relevant difficulty when considering the dynamics of (2), because noise amplification always occurs before any systematic deviations can come in to play, and makes further evolution moot [P25,P26].

After I worked out the estimates for the useful simulation time that is possible with both gauged and un-gauged positive-P distributions [P25,P26], It became clear to me that applying just the basic (un-gauged) positive-P method to the dynamics of ultracold atomic clouds can be useful in many experimentally realistic situations. In comparison, access to equilibrium states (which had been the other aim of the doctoral studies of phase space methods) is quite limited because of the growth of fluctuations with simulation time (although not impossible – see Section 5.3). There are also many competing methods for calculating equilibrium states that have been studied in much more detail over the years, such as Monte Carlo and DMRG. The stochastic phase space approach looks, though, to be just made for calculating the dynamics of large two and three-dimensional systems, for which no competing methods to calculate the full quantum dynamics appear to exist.

This was my motivation to attempt to apply the un-gauged positive-P method for the dynamics of macroscopic assemblages of atoms that are not accessible by any other realistic treatment. One such situation occurs when the essence of the physics lies in spontaneous processes that break the coherence of the system.

4.2.1 Full quantum dynamics of a truly macroscopic system [H1]

The positive-P method had previously been applied to ultra-cold atoms [42, 43][P25,P34], but always somewhat shyly, to systems with 10^3 to 10^4 atoms and never for parameters existing in an actual experiment.

For the work in [H1], we took an experimental setup (from the Ketterle group [48]) without making additional simplifications. Our aim was to test whether the positive-P method can be treated as a "black box" that acts on the raw microscopic model (2) for macroscopic numbers of atoms (150 000 in this case). In brief, without going into derivation, the positive-P representation describes the state of the system (1) with an ensemble of samples $\vec{\lambda}$, each of which $\vec{\lambda} = [\psi(\mathbf{x}), \widetilde{\psi}(\mathbf{x})]$ consists of two complex fields ψ and $\widetilde{\psi}$ that correspond to the boson field $\widehat{\Psi}$. Usually, $\psi(\mathbf{x}) \approx \widetilde{\psi}(\mathbf{x})$. The expectation values of operators $\widehat{O}$ correspond to statistical averages $\langle\, f \,\rangle_{\rm stat}$ of appropriate functions of the samples $f(\vec{\lambda}) = \mathrm{Tr}[\widehat{O}\widehat{\Lambda}(\vec{\lambda})]$. The rule for obtaining f is that when $\widehat{O}$ is written in its normally ordered form (i.e. when all $\widehat{\Psi}^\dagger$ are to the left of the $\widehat{\Psi}$) one makes replacements according to the rules $\widehat{\Psi}(\mathbf{x}) \to \psi(\mathbf{x})$ and $\widehat{\Psi}^\dagger(\mathbf{x}) \to \widetilde{\psi}(\mathbf{x})^*$. For example, $\langle \widehat{\Psi}^\dagger(\mathbf{x})\widehat{\Psi}(\mathbf{x}')\rangle \to \langle \widetilde{\psi}(\mathbf{x})^*\psi(\mathbf{x}')\rangle_{\rm stat}$. The samples evolve according to the following stochastic equations in the Ito calculus:

$$i\hbar\frac{d\psi(\mathbf{x})}{dt} = \left\{V(\mathbf{x}) - \frac{\hbar^2}{2m}\nabla^2 + g\,\widetilde{\psi}(\mathbf{x})^*\psi(\mathbf{x}) + \sqrt{i\hbar g}\,\xi(\mathbf{x},t)\right\}\psi(\mathbf{x}) \tag{3a}$$

$$i\hbar\frac{d\widetilde{\psi}(\mathbf{x})}{dt} = \left\{V(\mathbf{x}) - \frac{\hbar^2}{2m}\nabla^2 + g\,\psi(\mathbf{x})^*\widetilde{\psi}(\mathbf{x}) + \sqrt{i\hbar g}\,\widetilde{\xi}(\mathbf{x},t)\right\}\widetilde{\psi}(\mathbf{x}) \tag{3b}$$

Here, ξ and $\widetilde{\xi}$ are white noises, independent at each point of the numerical lattice and each time step Δt. They are specified by the conditions $\langle \xi(\mathbf{x},t)\rangle_{\rm stat} = \langle \widetilde{\xi}(\mathbf{x},t)\rangle_{\rm stat} = \langle \xi(\mathbf{x},t)\widetilde{\xi}(\mathbf{x}',t')\rangle_{\rm stat} = 0$ and the variances

$$\langle \xi(\mathbf{x},t)\xi(\mathbf{x}',t')\rangle_{\rm stat} = \langle \widetilde{\xi}(\mathbf{x},t)\widetilde{\xi}(\mathbf{x}',t')\rangle_{\rm stat} = \delta^3(\mathbf{x}-\mathbf{x}')\delta(t-t'). \quad (4)$$

In practice, they are generated with independent Gaussian random numbers at each point of the numerical lattice and of time with a variance of $1/(\Delta V \Delta t)$ and a mean of zero. ΔV is the volume per spatial point. The evolution (3) differs from the mean field Gross-Pitaevskii equation only by the noise terms and the resultant difference between the ψ and $\widetilde{\psi}$ fields.

The results of the calculations were spectacularly promising. Apart from a successful demonstration, we were able to observe nontrivial dynamics of the scattered atoms in the halo - the first signs that it contains many more phenomena than just the scattering. In fact, even after a series of later studies, some aspects are still not properly understood. Our work also showed the presence of bosonic enhancement of spontaneously scattered atoms. This differs from the traditional kind of four-wave mixing as in [48, 54], where a small coherent seed cloud stimulated the scattering. This observation actually started several years' worth of confusion among the group of theoreticians and experimentalists studying BEC collisions as to the importance of Bose enhancement for the halo's properties. We were only able to untangle the confusion very recently in [H8] – see Section 4.3.3 below.

Our work also showed that the approximate *truncated Wigner* method used previously to describe condensate collisions [59, 60] can produce spectacularly wrong results if the system is insufficiently "classical" (i.e. if the number of atoms is not sufficiently greater than the number of accessible states). An example is shown in Fig. 2. Furthermore, a large proportion of experiments take place in this insufficiently classical regime. An example are the Westbrook group experiments in Palaiseau, with whom we started a fruitful collaboration after this publication. There, $N \sim 10^5$, while the number of relevant modes is $\sim 10^6 - 10^7$. The trouble with the Wigner method is that one has to coax atoms to scatter into empty modes by initially seeding them with random fluctuations at the level of about half a particle per mode. Although after the calculation, these "virtual particles" are removed from the observable measurements, the intervening dynamics does not distinguish true from "virtual" particles and begins to scatter also the virtual ones. This leads to excess occupation in low energy modes, and a vacuum that has been "further depleted" of particles at high momenta. The predicted occupation there is negative.

The work we reported in [H1] were the first simulations of the full quantum dynamics of a macroscopic number of interacting particles (150 000) directly from their microscopic description – not only in the field of cold atoms. The work gained significant visibility in the community and has been cited 50 times so far.

4.2.2 Development of the STAB method to describe scattered atoms [H3,H5]

The capability to accurately calculate the correlations in the halo that was shown in [H1] spawned close collaboration with the experimental group of Chris Westbrook[H3,H4,H7]. It became clear quite quickly that, as could have been suspected, the time that could be simulated with the positive-P method was not very satisfying. A direct calculation with the equations (3) succumbed to an amplification of the noise after about a tenth of the time that it took the condensates to complete the collision.

Since the length of the time interval before noise amplification sets in scales as $\min\{|\psi(\mathbf{x})|^{-4/3}\}$ [P25], a reduction of the density of the quantum field being treated would greatly extend this time. The idea I developed was to approximate the condensates with a coherent wavefunction $\phi(\mathbf{x},t)$ and treat only the fluctuations around this with a fully quantum field $\widehat{\delta}(\mathbf{x},t)$. It contains the entire halo and incoherent scattered atoms that we were interested in. The density of the scattered field is much

smaller because only about 5% of the atoms end up being scattered in this setup. One obtains a description that resembles the Bogoliubov approximation, with a freely evolving condensate in the background. hence the name STAB *(Stochastic Time-Adaptive Bogoliubov)*.

This goes well beyond the standard Bogoliubov approach because firstly, the "condensate" i.e. the coherent source is evolving strongly in time, and secondly because the required number of modes (millions) is too large for the Bogoliubov-de Gennes equations to be solvable in the standard way by diagonalisation. Both hurdles can be avoided by using a stochastic method which treats the scattered field with the positive-P representation.

The general case would require one to preserve orthogonality between the source condensate field ϕ and the scattered fields ψ and $\widetilde{\psi}$. Happily, in the case here, the region of interest (the halo) is clearly separated from the condensates so that they remain effectively orthogonal and it suffices to apply a plane-wave basis for all the fields. This significantly simplifies the whole procedure. The evolution is :

$$i\hbar\frac{d\psi(\mathbf{x})}{dt} = \left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + 2g|\phi(\mathbf{x})|^2\right\}\psi(\mathbf{x}) + g\,\phi(\mathbf{x})^2\widetilde{\psi}(\mathbf{x})^* + \sqrt{i\hbar g}\,\phi(\mathbf{x})\xi(\mathbf{x},t) \quad (5a)$$

$$i\hbar\frac{d\widetilde{\psi}(\mathbf{x})}{dt} = \left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + 2g|\phi(\mathbf{x})|^2\right\}\widetilde{\psi}(\mathbf{x}) + g\,\phi(\mathbf{x})^2\psi(\mathbf{x})^* + \sqrt{i\hbar g}\,\phi(\mathbf{x})\widetilde{\xi}(\mathbf{x},t) \quad (5b)$$

$$i\hbar\frac{d\phi(\mathbf{x})}{dt} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + g|\phi(\mathbf{x})|^2\right]\phi(\mathbf{x}) \quad (5c)$$

The method was applied in [H3] for the first time, and later in our subsequent experimental and theoretical research on condensate collisions [H4,H6,H7,H8]. Its details were presented and analysed in [H5]. That paper paper also performed a detailed check of its correctness in describing the scattered atoms by comparing the STAB result using (5) to that obtained with the full boson field according to the equations (3) that were used in the earlier work [H1]. The agreement was excellent. With regard to computational efficiency, $N \sim 10^6$ atoms on numerical lattices with up to $\sim 10^7$ points are not a problem to calculate on a single modern PC.

We also described the conditions under which the method can be applied – above all, (I) the number of scattered atoms must be small enough that the depletion of the source $\phi(\mathbf{x})$ can be neglected for considerations of the properties of the halo. Also (II), one should restrict analysis to only those atoms that are well separated in momentum space from the source condensates. This second condition allows one to avoid the effect of non-orthogonality between the plane waves used to describe ψ or $\widetilde{\psi}$ and the wavefunction of the condensates ϕ.

A comparison was also made of the statistical uncertainty obtained with STAB and the truncated Wigner representation that was applied in some earlier works [59–61] (Fig. 1). In most cases we found that STAB is a lot more efficient because it does not introduce any initial fluctuations.

The STAB method allowed us to simulate the whole experiment to the end, while keeping a fully quantum description of the scattered atoms in the halo. Significantly, in the majority of similar experiments, only a small percentage of the atoms is scattered, so higher-order effects that are omitted by STAB are in fact completely negligible. This remains so during the later expansion in vacuum in the direction of the detector, because the cloud just becomes even more dilute during this period, and interactions become ever weaker.

4.2.3 Development of the "quantum triangulation" technique to extend accessible times [H2]

Generally the greatest difficulty encountered with these methods is limitation on the time that can be simulated because of noise amplification by nonlinearities in the equations. I have worked out a

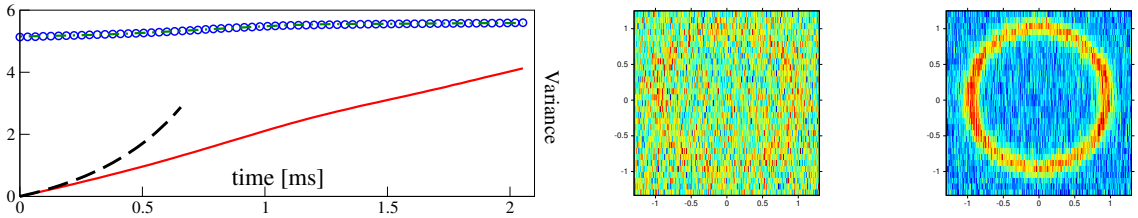

Figure 1: [H5] Left: The level of statistical fluctuations (variance) of local density in the halo of a condensate collision using the methods: truncated Wigner (blue), STAB (red), full positive-P (black). Also, slices through the halo using the truncated Wigner (centre) and STAB (right).

different kind of technique that can be applied in cases when the STAB method can not be used.

As mentioned in the introduction, the power of stochastic approaches (also standard Monte Carlo) stems from the way physically interesting quantities in macroscopic systems have contributions from many particles, and a limited precision is satisfactory. Hence, it is not really necessary to track exactly all the configurations of the system, only a sufficient amount of "typical" ones, provided that we can reliably estimate the statistical uncertainty in our results.

The "quantum triangulation" idea takes this concept a step further: it is also not really necessary to actually carry out the troublesome full quantum evolution *provided that* we can still predict what it would give with a well defined statistical error estimate. Is it possible to obtain such a prediction in a less troublesome roundabout way?

Let us suppose that we have two mutually independent approximate methods that use the sets of equations "$\mathcal{A}$" and "$\mathcal{B}$", and that the time limitation caused by noise amplification does not occur in them (perhaps due to the beneficial effects of the approximation). They are, however, to some degree similar to the full quantum dynamics equations, labelled "$\mathcal{Q}$" such as e.g. (3), which are only useful until the time $t_{\rm sim}$. If the similarities between $\mathcal{A}, \mathcal{B}$ and $\mathcal{Q}$ are sufficiently great, it is possible to construct families of hybrid equations $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\mathcal{B}}$ (possibly in an arbitrary manner) whose members are labelled by a continuous hybridisation parameter λ according to the scheme:

$$\mathcal{H}_{\mathcal{A}} = (1-\lambda)\mathcal{A} + \lambda\mathcal{Q} \quad ; \quad \mathcal{H}_{\mathcal{B}} = (1-\lambda)\mathcal{B} + \lambda\mathcal{Q}. \tag{6}$$

Here, the $\lambda = 1$ hybrids contain the full quantum dynamics, while $\lambda = 0$ gives the initial approximate methods $\mathcal{A}$ and $\mathcal{B}$. The details are not universal and may depend on the system under consideration.

The hybrids $\lambda > 0$ will still contain the noise catastrophe that limits simulation time, *but it will occur at later times* than in the full quantum description $\mathcal{Q}$. The longer times $t > t_{\rm sim}$ that were inaccessible by the full quantum method will be accessible by a part of the hybrid families in the range $\lambda \in [0, \lambda_{\rm max}(t) < 1\,]$.

Now, if the calculated value of the quantity of interest depends smoothly on λ in the family $\mathcal{H}_{\mathcal{A}}(\lambda)$, one can extrapolate to $\lambda = 1$ on the basis of several calculations in the shorter range $[0, \lambda_{\rm max}(t)]$ that is still accessible numerically. As a result, one obtains a prediction for longer times than were accessible with the full quantum description $\mathcal{Q}$. The statistical uncertainty in such an extrapolation can be obtained by various known statistical methods [62]. In my calculations I used the approach to divide all the realisations into a number of sub-ensembles. Then, while the full ensemble gave the best estimate, an extrapolation was also carried out from each sub-ensemble separately. The statistical uncertainty in the best estimate is then calculated from the spread of extrapolated values obtained with the the sub-ensembles.

Naturally, the result of an extrapolation from one family $\mathcal{H}_{\mathcal{A}}$ is not particularly convincing because of the well-known weaknesses of extrapolations. It can, however, be checked with the help of other

independent hybrid families, e.g. $\mathcal{H}_B$. That is what they are needed for. When all the estimates from independent families of hybrids agree, we obtain an "interpolation between extrapolations" that is a much stronger result than any single extrapolation by itself.

Fig. 17 shows an example of how the method is applied. The general concept is similar to that used in e.g. diagrammatic Monte Carlo when one compares the results obtained with different resummation procedures (analogous to different equation families) for a sequence of calculations that retain different orders of diagrams (analogous to different λ) [63].

As a demonstration, I recalculated the condensate collision described in the pioneering first paper in the series – [H1]. The positive-P equations (3) were, of course, $\mathcal{Q}$, while the approximate method $\mathcal{A}$ was the popular *truncated Wigner* method and the second approximate method $\mathcal{B}$ was the mean field Gross-Pitaevskii description. I showed the accuracy of the predictions using quantum triangulation, and that it was possible now to obtain results for sufficiently long times (∼1.5ms) to reach the end of the collision (Fig. 2). Reaching this time was not possible with the earlier original method. Quantum triangulation turned out later to be essential for the methods developed for the dynamics of spin systems [H9] – see Section 4.5.

4.3 Condensate collisions – properties of the atom pairs in the halo

When two Bose-Einstein condensates collide with sufficient velocity, correlated atom pairs are scattered. This effect becomes appreciable when the relative speed of the condensates exceeds the speed of sound in their densest part. From the point of view of the theory of superfluidity, this corresponds to crossing the critical velocity. For atoms with momentum $\pm\hbar k_0$ relative to the centre of mass, the primary process is $k_0 \;\&\; -k_0 \;\rightarrow\; \mathbf{k} \;\&\; -\mathbf{k}$. Atoms in counter-propagating condensates collide, becoming a pair of toms with opposite momenta $\pm\hbar\mathbf{k}$. In the simplest approximation, energy and momentum conservation requires $|\mathbf{k}| = |k_0|$, leading to the formation of a spherical halo of radius $\hbar|k_0|$ in momentum space. Fig. 3 shows the typical arrangement (on top of a density plot from [H6]).

The halo has been observed in many experiments [1,3,44,48–55,64–68][H3,H4,H7] and analysed in many theoretical works [44,46,59,60,68–79][H1,H3,H6,H7,H8]. The atoms are usually observed after a long free flight through vacuum, during which time their positions come to correspond to the velocity (momentum) distribution that formed at the end of the collision. In addition to the plain absorption image that is taken in ultra-cold atom experiments, two innovative techniques have been developed to register the positions of single atoms and access their correlations. These are: the multi channel plate detector (MCP) [1,20,80], and imaging with the aid of a so-called *light sheet* [2,21,81].

The halo formation is a spontaneous process because the atoms are scattered into a part of momentum space that was initially empty. Due to this, mean field dynamics (5c) can not capture this process – the right hand side of the equation is zero whenever $\phi(\mathbf{x}) = 0$. In consequence, the halo is not coherent with the condensate sources. This is similar to photon pair production by parametric down conversion. Such photon pairs are strongly squeezed, and have been used to study violation of the Bell inequality [82], and even such exotic applications as quantum cryptography [83] or quantum teleportation [84].

Likewise, the pairs of atoms produced in a condensate collision have potential applications for ultra-precise measurements [85], interferometry [5,86–88], or research into the fundamentals of quantum mechanics [89,90]. It is expected generally that situations in which the superfluid critical velocity is exceeded in a condensate will produce a similar halo. BEC collisions constitute, then, an archetypical case of a wider range of related phenomena such as molecular dissociation in a condensate [47,91–105], superradiant atom scattering [106–115], atomic parametric down-conversion [2,7,8,55,116–122], or the interaction of a condensate with barriers and obstacles [56–58,123–126].

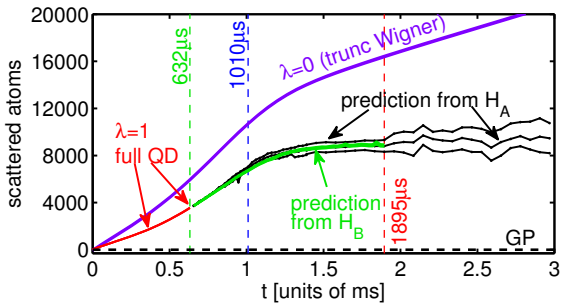

Figure 2: [H2] An application of quantum triangulation to condensate collisions. We compare the raw positive-P (red), extrapolation from hybrid equations (black, green), and the inaccurate: truncated Wigner (purple) and Gross-Pitaevskii (black dashed) methods.

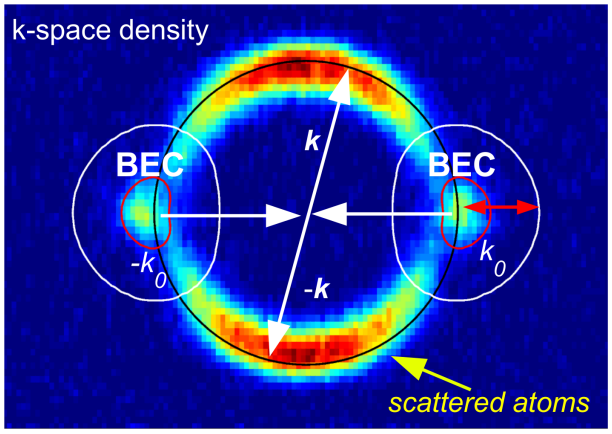

Figure 3: Typical densities of scattered atoms after a collision of BECs with momentum $\pm\hbar k_0$. White arrows show the dominant scattering process.

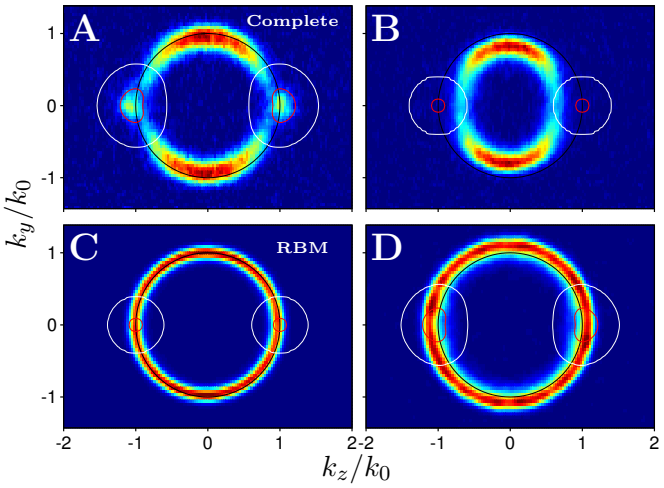

Figure 4: [H6] Density of scattered atoms after the end of the collision for models A, B, C, and D described in the text.

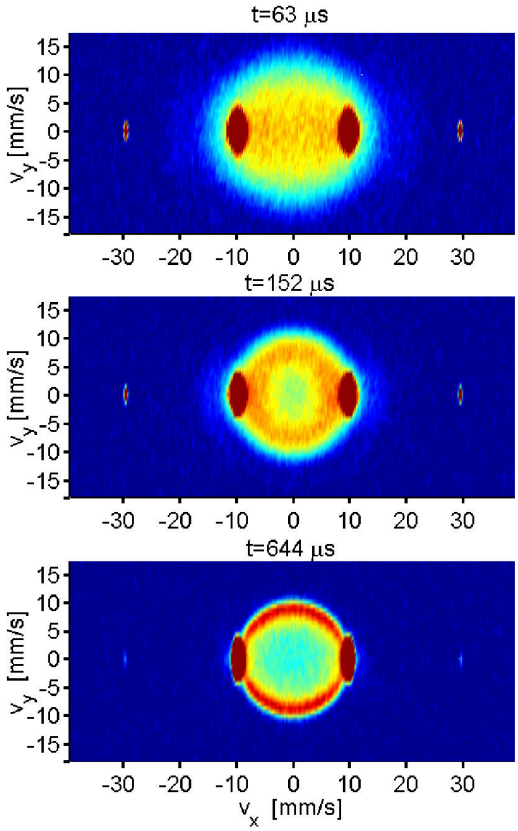

Figure 5: [H1] Time series of scattered atom densities in momentum space.

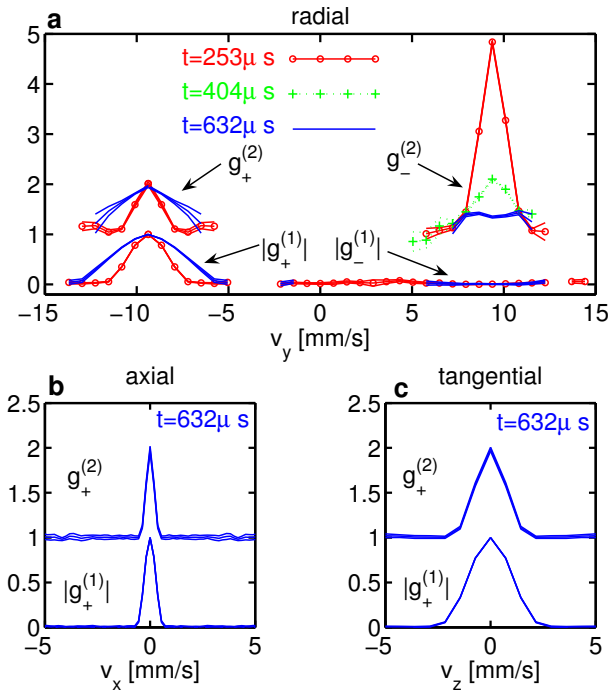

Figure 6: [H1] Two-point correlations between atoms in the halo $g^{(\mu)}(\mathbf{v}_0, \mathbf{v})$, where $\mathbf{v}_0 = (0, -9.37\text{mm/s}, 0)$, and the $\mathbf{v} = (v_x, v_y, v_z)$ differ from $\mathbf{v}_0$ by the values shown on the axes.

It turns out that the simplest description (spherical halo and ideal atom pairs) as mentioned above, is highly insufficient to describe the true physics because many additional processes are occurring at the same time. It cannot be relied on for practical applications. They require one to go beyond analytical calculations that consider coupling between only a few modes, and instead perform numerical simulations.

In [H1], [H6] and [H8] I applied the positive-P and STAB methods to theoretically study the properties of atoms in the halo. The calculations reported in [H3],[H4] and [H7], were on the other hand, made in close collaboration with experimentalists, describing particular experiments. They will be discussed in the later Section 4.4.

4.3.1 The evolution of correlations among the scattered atoms [H1]

In [H1], the dynamics of one- and two-particle correlations were calculated in the halo (Fig. 6) along with the process of its formation (Fig. 5). Only the final momentum distribution is measured in experiments, so the process of the halo's formation can only be studied in detail by performing simulations. We took the parameters from the Ketterle group experiment that first saw a strong halo [48], and studied the collision of clouds that contained a somewhat smaller number of atoms because this is the more physically interesting case. Then, like in most newer experiments [1,55], there are too few atoms for a description with classical fields as in Norrie *et al.* [59,60] to be correct.

Looking generally at the halo's formation, at early times its thickness is very large (Fig. 5) and limited by energy-time uncertainty. Later, as it becomes thinner, its width becomes limited by so-called power broadening [72]. Many of the features seen in halos were first spotted in these calculations of ours [H1]. one effect that turned out to be very important for the interpretation of experiments [H3] was the reduction of the halo radius with respect to $|k_0|$. It is a consequence of the effective potential created by the mean field of the condensates that is felt by the scattered atoms. Its further consequences were analysed in [H3] and [H6].

A weak off-resonant scattering process to high momenta was also observed: instead of the standard k_0 & $-k_0 \rightarrow$ **k** & $-$**k**, one also sees atoms produced by the process k_0 & $k_0 \rightarrow -k_0$ & $3k_0$, which is extremely non-energy-conserving (it requires the input of eight times the kinetic energy of one condensed atom). Later analysis showed that this process is coherent and already present in the mean field description [H6]. It is made possible by two circumstances: firstly, it is strongly Bose enhanced by the presence of the second condensate at $-k_0$ which acts like a seed in four-wave mixing. Secondly, the simultaneous time evolution of the condensate allows for the collective transfer of energy so that the atoms with momentum $\pm 3\hbar k_0$ continue to constitute a part of the condensate that has merely changed its wavefunction to include a component with higher spatial frequencies.

Two-point correlations were the main aim of the calculations. They give insight into the behaviour of the system in a single realisation. The first order correlation $g^{(1)}(\mathbf{k}_1,\mathbf{k}_2) = \langle\widehat{\Psi}^\dagger(\mathbf{k}_1)\widehat{\Psi}(\mathbf{k}_2)\rangle/\sqrt{\overline{n}(\mathbf{k}_1)\overline{n}(\mathbf{k}_2)}$ describes single-particle coherence between momenta $\hbar\mathbf{k}_j = m\mathbf{v}_j$. Here, $\overline{n}(\mathbf{k})$ is the mean density at **k**. The second order correlation $g^{(2)}(\mathbf{k}_1,\mathbf{k}_2) = \langle\widehat{\Psi}^\dagger(\mathbf{k}_1)\widehat{\Psi}^\dagger(\mathbf{k}_2)\widehat{\Psi}(\mathbf{k}_2)\widehat{\Psi}(\mathbf{k}_1)\rangle/(\overline{n}(\mathbf{k}_1)\overline{n}(\mathbf{k}_2))$ gives the typical shape, size, and strength of density fluctuations. The shape, intensity and length of correlations in the halo were calculated, both for local and counter-propagating momenta (Fig. 6). We were able to clear up a whole set of issues which had previously been muddled either due to a lack of calculations, or only ones performed with truncated Wigner classical fields [59,60].

Local density correlations were seen at the level of $g^{(2)} = 2$, like photons in the famous Hanbury Brown-Twiss effect [127], and in agreement with the measurements of C. Westbrook's group [1] and predictions from simplified theories [74,78]. The width of the so-called "phase grains" [59,60], i.e. the width of the phase correlations $g^{(1)}$ is narrower by a factor of $\sqrt{2}$, and corresponds to the width of the initial condensate wavepackets.

The most important quantity from the point of view of further applications are the correlations between counter-propagating momenta, because they speak of the properties of the atom pairs. Their width is similar to that of the local correlations, but they are initially extremely strong because almost all the scattered atoms are in the form of as-yet unperturbed and sparsely distributed atom pairs. This was not seen in older truncated Wigner calculations because of the much greater noise in that method. Interestingly, these correlations remained much stronger than the thermal value of $g^{(2)} \approx 2$ at times $t = 200\mu s$ when the mean occupation of phase grains was well above one. At even longer times, though, $g^{(2)}$ falls below the thermal value of 2 that would be the expected asymptote in simpler models [74].

We also confirmed a lack of phase correlations between counter-propagating atoms, which agrees with the simple, but previously uncertain, model of [74]. Phase correlations can not be measured in present experiments on this system.

Two further unexpected yet prominent effects were seen: a broadening of local correlations in the radial direction as the collision progresses, and the decay of counter-propagating correlations below the value of 2 expected from a simple several-mode description. These were important first clues that the behaviour of the atoms in the halo is much more complex than had been revealed in theory works at the time, and that this may have an influence on the possibilities to observe quantum effects among these atoms. Knowledge of the correlation strength *in situ* is particularly important because it is difficult to estimate from experimental measurements. The width and shape of correlations is relatively easy to measure, but its strength is influenced by a number of technical factors such as the detector's inefficiency, its resolution, and reaction time. Taken together these factors are fairly inaccurately known by the experimental group even today.

It was noticed the the broadening of the phase grains coincides in time with the moment when appreciable bosonic enhancement appears. The latter is evidenced by a growth in scattering rate despite a monotonically decreasing overlap between the source condensates. In discussions with the Palaiseau experimental group we hypothesised that deviations from the simple description in terms of several modes may be due to this Bose enhancement. In the end, this turned out to be a false lead, something that we only realised after about 5 years [H8]. In the meantime it deceived us and hindered our understanding of the relevant dependences in the system. More on this in Sec. 4.3.3.

With regard to the simulation itself, this work demonstrated that it is possible to obtain useful and accurate results in such huge systems, and at the same time showed that the noise amplification was the main limiting factor. In this case, only about half the collision could be simulated. The calculation was later extended to include the whole collision with the help of quantum triangulation [H2] (Fig. 2).

4.3.2 Understanding the effect of the mean field due to the condensates [H6]

Motivated by the theoretical [H1] and experimental [H3] results that showed a nontrivial and unexpectedly large effect from the mean field produced by the condensates, as well as by the inconsistencies between older calculations in Prof. Marek Trippenbach's group [72] and my simulations [H1], we wanted to clear these issues up in a collaboration that led to the article [H6].

Our reference description here is the approximate "reduced Bogoliubov model" (RBM) that has been used in a large proportion of theoretical works on the properties of the atoms in the halo [46, 64, 69–77]. It is the simplest multi-mode model that allows for the creation of atom pairs in the halo and calculation of their density or correlations. It assumes that (I) the condensates pass each other with a constant velocity and do not deform, and that (II) the dynamics of the scattered atoms consists only of free ballistic flight and pair production via collisions only between atoms in counter-propagating condensates. The condensates appear in the equations as a coherent, stable source. The

predictions of this model sometimes agree well with experiment [77], but there are also cases where large discrepancies are seen [46][H1,H3].

On top of explaining the physics that takes place, it has also become important to determine the conditions under which the RBM is still reliable. We concentrated our attention on the width, angular structure, and above all the radius of the halo. The main result was that deviations from the RBM become negligible when the collision is sufficiently strongly supersonic. However, in the majority of experiments this condition is not met. We also determined the importance of various processes in the Bogoliubov description for effects such as a reduced halo radius and a weakening of scattering along the collision axis. The analysis was carried out by considering the numerical results when various terms in the calculation were added or removed. This approach that was developed here was important for later research [H7,H8].

We considered the simplest case that incorporates the phenomena of interest – a collision of initially spherically symmetric condensates that begin as the condensate ground state in a trap that is turned off at the beginning of the collision. The Bogoliubov / STAB description where $\widehat{\Psi}(\mathbf{x}) = \phi(\mathbf{x}) + \widehat{\delta}(\mathbf{x})$, and the number of atoms in the condensate is N, contains the following universal scaling: The scattered field $\widehat{\delta}$ is identical in all systems which share the same geometry and have the same value of gN (or aN, where a is the s-wave scattering length). Its dynamics is then specified by the length scale aN rather than by a or N separately. The remaining important length scales are the initial width of the condensate σ, and the de Broglie wavelength of atoms in the condensates' centre of mass frame $\lambda_0 = 2\pi/k_0$. Since there are three relevant length scales, there are two dimensionless parameters. using the more convenient terminology used in [H8], they are: (I) the Mach number $\mathrm{Ma} = 2v_0/\overline{c}$, i.e. the ratio between the relative speed of the condensates $2v_0$ and the typical speed of sound $\overline{c} \sim \sqrt{\mu/m}$; and (II) the degree of bosonic enhancement $\gamma \sim \sigma m\overline{c}^2/\hbar v_0$. One expects to see appreciable Bose enhanced scattering into the halo when $\gamma \gtrsim 1$ [74].

The general Bogoliubov Hamiltonian for the scattered atoms is:

$$\widehat{H}_{\rm eff} = \int d^3\mathbf{x}\, \widehat{\delta}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \widehat{\delta}(\mathbf{x}) \tag{7a}$$

$$+2g \int d^3\mathbf{x}\, |\phi_L(\mathbf{x}) + \phi_R(\mathbf{x})|^2\, \widehat{\delta}^\dagger(\mathbf{x})\widehat{\delta}(\mathbf{x}) \tag{7b}$$

$$+g \int d^3\mathbf{x}\, \phi_L(\mathbf{x})\phi_R(\mathbf{x})\widehat{\delta}^\dagger(\mathbf{x})\widehat{\delta}^\dagger(\mathbf{x}) + \text{ h.c.} \tag{7c}$$

$$+\frac{g}{2} \int d^3\mathbf{x}\, \left(\phi_L(\mathbf{x})^2 + \phi_R(\mathbf{x})^2\right) \widehat{\delta}^\dagger(\mathbf{x})\widehat{\delta}^\dagger(\mathbf{x}) + \text{ h.c.} \tag{7d}$$

The first line contains ballistic flight, the second the potential caused by the presence of the condensate, the third contains the main resonant process of pair creation that scatters one atom from each cloud, while the last line describes the off-resonant scattering of two atoms from the same cloud. The initial coherent wavefunction is constructed per $\phi = \phi_L + \phi_R$ from the two components $\phi_{L/R}$ that move left (L) and right (R). The maximal cutting down that leaves something nontrivial consists of omitting the second and fourth lines, which we will call the PP (pair production) simplification. The evolution of the condensates (5c) can also be simplified to

$$i\hbar\partial_t\phi_L(\mathbf{x},t) = -\frac{\hbar^2 k_0}{2m}\left(k_0 - 2i\frac{\partial}{\partial z}\right)\phi_L(\mathbf{x},t) \quad ; \quad i\hbar\partial_t\phi_R(\mathbf{x},t) = -\frac{\hbar^2 k_0}{2m}\left(k_0 + 2i\frac{\partial}{\partial z}\right)\phi_R(\mathbf{x},t). \tag{8}$$

where there is only stiff movement of the clouds with a speed $v_0 = \hbar k_0/m$, without any change of shape due to the inter atomic repulsion, interactions between the clouds, and also without the (slower) free kinetic dispersion. We call this the SM (stiff movement) simplification. The simplest description,

the RBM, consists of using both simplifications (RBM ≡ PP+SM). We analysed four variants of the evolution:

(A) full Bogoliubov and full condensate evolution
(B) full Bogoliubov, but only SM for the condensates.
(C) maximal simplification: RBM
(D) simplified Bogoliubov (PP), but full condensate evolution.

The scattered halo after the end of the collision is shown in Fig. 4. Our conclusions were as follows:

The distribution of scattered atoms is spherically symmetric in variants C and D, from which we conclude that the weakened scattering along the collision axis is caused only by the potential (7b) and off-resonant pair creation (7d). The small local clouds of scattered atoms that are seen to form near the condensates appear only when terms in the fourth line (7d) are included.

The dependence of the halo radius is somewhat involved (Fig. 7), but an analysis of the numerical results showed that deviations from the RBM depend primarily on the Mach number Ma. This is explained by the contributions to the conservation of energy in the idealised case of a collision of plane waves. The initial energy of an atom in the condensate is $E_0 + 3\mu/2$, where $\mu = g\overline{n}$ is the chemical potential, $\overline{n}$ the condensate density, and $E_0 = \hbar^2 k_0^2/2m$ the kinetic energy of single atoms in the condensate. The energy of a scattered atom is, however, $E_0 + 2\mu$, according to the Bogoliubov equations. Noting that typically $\mu \ll E_0$, then $k \approx k_0(1+\varepsilon)$ with a relative shift of $\varepsilon = -(1/2)(\mu/E_0) = -10/(\mathrm{Ma})^2$. This shift is several times smaller than that reported in [72] – which turned out to include an error.

Importantly, deviations of ε from the RBM become visible only for sufficiently small Mach numbers. For the parameter in the article this was $\mathrm{Ma} \lesssim 8$ and for faster collisions the RBM gave very good results. The suppression of the linear growth of deviations for large Mach numbers is related to the so-called "skier effect" [H3] caused by the mean field term (7b). During their flight, scattered atoms ride down the potential hill created by the condensates, and can this way recover the energy that they lost in the initial scattering. This evens out the difference between the radii seen in the RBM and the full evolution. however, this can take place only if the collision is sufficiently fast that the atoms can get off the hill before the condensates dilute due to their own internal expansion.

To summarise, it was earlier shown that significant Bose enhancement will take place by the end of the collision when $\gamma \gtrsim 1$ [74]. In [H8], below, it is shown that this value also separates the relevant physical regimes for correlations. On the other hand, here we showed that the governing parameter for halo densities is the Mach number Ma.

4.3.3 Mechanisms that degrade quantum effects and squeezing [H8]

The article [H8] contains a detailed analysis of the relationship between correlations and reduced (squeezed) fluctuations of density between counter-propagating atoms in the halo. It tasked itself with two matters: (I) Reconciling and explaining the discrepancies between predictions of simple few-mode models and the experiment plus its multi-mode description that both measure the properties that have been averaged over spatial regions ("counting bins"), and (II) Understanding the mechanisms that degrade the squeezing and quantum properties of the atom pairs.

Number squeezing Consider measurements of the number of atoms in two subsystems a and b. Let us keep in mind the case of a condensate collision, where they will correspond to two regions in space on opposite sides of the halo. Another common case is when they are the numbers of atoms measured to have two different internal states, as e.g. in [4]. Strong correlations between the atoms can reduce the fluctuations in the difference of numbers measured in the two modes $(\Delta n)^2 = \langle \widehat{n}_a \widehat{n}_b \rangle - \langle \widehat{n}_a \rangle \langle \widehat{n}_b \rangle$. For example, a twin-Fock state $|n, n\rangle$ demonstrated recently in [4] has zero fluctuations, while a coherent state of uncorrelated atoms has Poissonian fluctuations $(\Delta n)^2 = \langle \widehat{n}_a + \widehat{n}_b \rangle$, also called shot noise.

A reduction of these fluctuations below the Poissonian level, often abbreviated somewhat incorrectly in the literature as *number difference squeezing* or just *number squeezing* is a serious indication that the state of the atoms has inherently quantum properties. The normalised difference fluctuations

$$\eta^2 = \frac{(\Delta n)^2}{\langle \hat{n}_a \rangle + \langle \hat{n}_b \rangle} \tag{9}$$

is restricted to values $\eta^2 \geq 1$ for classical states. Furthermore, $\eta^2 < 1$ is synonymous with a violation of the Cauchy-Schwarz inequality when the mean number of particles in a and b is equal. That, in turn, proves that the state cannot be described by any classical boson field [128], and under the right conditions is proof for the further presence of entanglement [129]. In the presence of sufficient single-particle coherence between modes a and b, *spin squeezing* is also present [130, 131], something that is potentially of great use in quantum metrology – measurements with resolution better than that allowed in a non-quantum world [131–133]. Such states have been created in several recent experiments [5, 134–138].

Spatially separated pairs of entangled atoms tempt one with possibilities to study the EPR paradox [89, 139], local realism [82] and test the Bell inequalities [140] for states in which different distributions of rest mass are apparently entangled. This is of great importance to the fundamentals of quantum mechanics because entanglement between states with different masses breaks the superselection rules that are often raised to the status of a fundamental physical principle.

For condensate collisions, large reductions of fluctuations in the occupation difference have been measured in several experiments: in Palaiseau with $\eta^2 = 0.89(2)$ [H4] and $\eta^2 = 0.92(5)$ [7], and in Vienna with $\eta^2 = 0.37(3)$ [2]. After extrapolation to what would presumably be seen with ideal detectors, it is reasoned that in both cases ([H4] and [2]), the squeezing inside the actual atom cloud was $\eta^2 \approx 0.1$.

Few-mode and many-mode descriptions The simplest model that produces atom pairs in two modes from an undepleted source is $\widehat{H}_2 = \widehat{a}^\dagger \widehat{b}^\dagger + \widehat{a}\widehat{b}$. If we start with empty modes a and b, their occupation later is $\overline{n}(t) = \sinh^2 t$. The correlations are $g^{(2)}_{ab} = \langle \widehat{a}^\dagger \widehat{b}^\dagger \widehat{a}\widehat{b} \rangle / \overline{n}^2 = 2 + 1/\overline{n}(t)$ between modes and $g^{(2)}_{aa} = 2$ locally. Interestingly, these values agree with the peak correlation strengths in the many-mode RBM model [74] for local and counter-propagating atoms. Regardless of the Hamiltonian, the relationship between correlations and squeezing in a two-mode system with $\overline{n}$ particles per mode is $\eta^2 = 1 + \overline{n}\left(g^2_{aa} - g^{(2)}_{ab}\right)$. This means that number squeezing requires that the correlation between modes is stronger than the local one. For the above two-mode model, $\eta^2 = 0$ at all times.

Notably, both the above two-mode and RBM results disagree with experiment [H4,H7] and the full calculations [H1]. Firstly, local and counter-propagating correlations in the halo were measured in the experiment [H7]. The height of the maximum of local correlations ($h_{CL} = g^{(2)}(\mathbf{k}, \mathbf{k}) - 1$) was two times greater than that for the counter-propagating correlations ($h_{BB} = g^{(2)}(\mathbf{k}, -\mathbf{k}) - 1$). A similar situation is seen at long times in the simulations (Fig. 6). On the other hand, η^2 calculated from the same data was far below one [H4]. This is in complete disagreement with the relationship gleaned from the two-mode and RBM models. Secondly, the two-mode model has been interpreted as the limit of experimental measurements when the volume of the counting bins becomes very small. Squeezing between very small regions in the simulation give values very close to $\eta^2 \approx 1$, with only minor deviations in the negative or positive directions. This does not resemble the two-mode result $\eta^2 = 0$ in any way (nor the same result obtained in the RBM).

Multimode measurements consist of counting up atoms in momentum regions V_j. The atom number in each is $\widehat{N}_j$. So, the squeezing is $\eta^2 = \langle (\widehat{N}_1 - \widehat{N}_2 - (\overline{N}_1 - \overline{N}_2))^2 \rangle / (\overline{N}_1 + \overline{N}_2)$, where $\overline{N}_j = \langle \widehat{N}_j \rangle$. To re-derive the dependence between two-body correlations and squeezing, we defined averaged correlations according to the same scheme as is used in the experiments [H7]: $\overline{g}^{(2)}_{ij} =$

$(1/\overline{N}_i\overline{N}_j)\int_{V_i} d^3\mathbf{k}\int_{V_j} d^3\mathbf{k}'\langle\widehat{\Psi}^\dagger(\mathbf{k})\widehat{\Psi}^\dagger(\mathbf{k}')\widehat{\Psi}(\mathbf{k})\widehat{\Psi}(\mathbf{k}')\rangle$. In the symmetric situation $\overline{N}_j = \overline{N}$, the relationship between squeezing and correlations takes on a similar form to the two-mode case: $\eta^2 = 1 + \overline{N}\left(\overline{g}^{(2)}_{11} + \overline{g}^{(2)}_{22} - 2\overline{g}^{(2)}_{12}\right)/2$. The primary correlation measurements, however, deal with the local not the bin-averaged correlations. We applied a simplified model that I worked out initially to help with the calculations in [H7]. We assume that the normalised local density correlation function $g^{(2)}$ gas a Gaussian form, which agrees well with both the experimental measurements [H7] and the simulations [H1,H8]:

$$g^{(2)}_{CL/BB}(\mathbf{k},\mathbf{k}') = 1 + h_{CL/BB}\prod_{i=1}^{3}\exp\left[-\frac{(k_i - k_i')^2}{2(\sigma_i^{CL/BB})^2}\right], \tag{10}$$

Here CL/BB indicates correlations between local, co-propagating (CL - collinear) and counter-propagating (BB - back-to-back) atoms, while $i = 1, 2, 3$ denotes the three orthogonal directions in k-space. The parameters are the peak heights h, and correlation widths σ_i.

We compared this model with full Bogoliubov calculations with the STAB method, where we first measured the local $g^{(2)}(\mathbf{k},\mathbf{k}')$ and squeezing η^2 between the bins V_j directly from the numerical calculation, after which (10) was fitted to the correlations to get h and σ_i and then a squeezing estimate $\eta^2_{\rm est}$ was made with only this information. The agreement between η^2 and $\eta^2_{\rm est}$ turned out to be quite good (Fig. 8), although the cases with only small numbers of atoms were treated somewhat worse because of the poor signal-to-noise ratio that we had in the local correlations. After confirming the accuracy of the simple model in this way, the behaviour of $\eta^2_{\rm est}$ in limiting cases allowed us to explain the discrepancy between the simple and many-mode pictures.

(I) When the dimensions of the bin regions V_j are much *greater* than the correlation widths σ_i, one predicts

$$\eta^2 = 1 + (2\pi)^{\frac{3}{2}}\frac{\bar{n}}{2V}\left[h_{\rm CL}\sigma_1^{\rm CL}\sigma_2^{\rm CL}\sigma_3^{\rm CL} - h_{\rm BB}\sigma_1^{\rm BB}\sigma_2^{\rm BB}\sigma_3^{\rm BB}\right]. \tag{11}$$

This form bears resemblance to the two-mode expression, only it turns out that it is not the correlation peak heights (h) that are relevant, but the "peak volumes" $h\sigma_1\sigma_2\sigma_3$. This explained the apparent contradiction between low back-to-back (BB) correlations and strong squeezing – because the width of the back-to-back correlations measured in the experiment was much greater than that of the collinear ones.

(II) When the bin dimensions are are much *smaller* than the correlation widths σ_i, one predicts $\eta^2 = 1 + \frac{\bar{n}}{2}(h_{\rm CL} - h_{\rm BB})$. Here, we recover the $h_{BB} > h_{CL}$ condition for squeezing, but overall η^2 is very close to the shot noise value (one) due to $\overline{n}$ being very small because it is proportional to the counting volume V. This explains why squeezing was so close to 1 in the full calculations. The two-mode estimate of $\eta^2 = 0$ is completely erroneous in this limit because shot noise becomes the dominant effect for atom counting. The shot noise comes about because the chance that an atom whose probability density is spread over the relatively large σ^3 volume happens to get registered in the small box V is itself small. This is an internal feature of the physical state of the system and as such is a cause of squeezing degradation that cannot be alleviated with the help of better detection schemes or detectors.

Degradation of squeezing It is evident that correlations are not ideal in the full STAB calculations from the asymmetry that is seen in single realisations (Fig. 9). Past experience with the related optical systems indicates that both making use of quantum measurements and deeper tests of non-classicality such as the Bell inequalities are even more sensitive to a degradation of entanglement than squeezing is. To progress further in those directions than the present experiments, it will probably be necessary to understand the mechanisms by which the atom pairs are degraded.

Among the different degradation mechanisms that were suggested in the literature or in informal discussions were the following:

- The Skier effect — the pairs are not necessarily created centrally, in which case the rolling down off the mean field potential (7b) will be asymmetric, and the atoms in the pair can end up in non-opposite bins.
- The time-varying source $\phi(\mathbf{x}, t)$ — causes the overlap of pairs with different starting properties in the same $\mathbf{k}$ region.
- Bosonic enhancement — it was noticed in simulations that it occurs at the same time as deviations from the two-mode model and the RBM.
- Non-monochromatic source — (*inhomogeneous broadening*). The wavefunction of the condensates has a certain width in k-space which gives the centres of mass of atom pairs a fluctuation. As a result, two pairs can overlap in k-space in only one of the bins, not both.
- Sharp bin boundaries – the atom counting in experiments is made over bins with sharp well-defined boundaries that cut through the wavepackets of single atoms. Since atom counting is a one-body process, both atoms in a pair, on opposite sides of the halo have independent probabilities to get counted in the relevant bins. This causes shot noise.

The Gaussian model for small bins shows that to avoid the deleterious influence of the last effect one requires bins that are greater than, or comparable to, the coherence volume. We also studied the effect of bin size for large bins – the influence of shot noise becomes weak in this limit in comparison to the other factors discussed below.

For correlations, the γ parameter has much more influence than Ma. We studied two cases in detail: $\gamma = 0.24$ (dilute halo in which phase grain occupation always remains $\ll 1$), and $\gamma = 1.02$ (dense halo in which phase grains are loaded by stimulated scattering in the later part of the collision). They show significantly different squeezing behaviour. For the dense halo (Fig. 8), squeezing is soon lost as the collision progresses, despite it being present initially to some degree. One cannot observe this initial squeezing in the experiment. In the dilute case, though, the initial squeezing remains mostly unchanged until the end of the collision and beyond. This is another coincidence between the presence Bose enhancement and the loss of quantum properties.

We set out to eliminate the above causes by eliminating successive terms in the Bogoliubov description, in a manner similar to what we did in [H6] for halo density.

To study the relevance of the skier effect and the time-varying source, we compared the full Bogoliubov calculation (Fig. 8) with the RBM (Fig. 10). The latter took on the role of an experimental control in which these effects do not occur. The behaviour of η^2 d did not change qualitatively for either of the cases of γ, although the squeezing does last a little longer in the dense case than with STAB. We conclude, then, that neither the skier effect nor the time-variation of the source are the fundamental cause of the degradation that one sees.

Bose enhancement (present also in the RBM) was considered a strong candidate because of the match between the times when degradation and Bose enhancement appear. To study its influence, my co-authors Paweł Ziń, Marek Trippenbach and Tomasz Wasak developed a special stochastic model that excludes the possibility of bosonic enhancement (it is described in [H8]). We compared the behaviour of the full description with the non-enhanced model (Fig. 11). To our major surprise, it turned out that although the degradation of squeezing was reduced after excluding Bose enhancement, it was still very strong. This proves that Bose enhancement is *not* the fundamental cause of the degradation, and its appearance around the same time is not causally related.

Of our initial hypotheses, the non-monochromatic source is what remains. To confirm or deny this hypothesis we compared the collision of spherical condensates with a collision of plane waves of matching density (Fig. 12) – both of them with the full STAB Bogoliubov method. The squeezing from plane waves is very strong ($\eta^2 \approx 0.03$), though still not ideal. This remnant degradation is also

interesting. It turns out that it is caused by the presence of the virtual scattering seen in [H1], as evidenced by its time behaviour (primarily at very early times) and its disappearance in the RBM, which does not include off-resonant scattering. Its remnant long-time presence is due to the time-evolution of the condensate which allows some virtual pairs to stabilise by collecting some energy from the condensate.

We conclude, them, that the non-monochromatic nature of the source (inhomogeneous broadening) is the underlying cause of most of the degradation of squeezing. The shot noise that comes about due to counting bin boundaries also has a role to play, as well as virtual scattering (which was not previously suspected).

One also arrives at another conclusion. Since inhomogeneous broadening causes stray atoms from the k-space neighbourhood to appear in a bin without their pair appearing in the matching bin, this process becomes more onerous the denser the halo. This explains why the squeezing can survive until the end only in the dilute case of $\gamma \ll 1$. The occupation of each phase grain is well below one in this regime, so the k-space neighbourhood is mainly vacuum and there are too few stray atoms around to completely degrade the squeezing between bins.

Summarising, this work brought a number of practical results for use in future experiments: the relationship between multi-mode correlations and squeezing, the simple Gaussian model to describe it, a simulation method that allows one to remove the influence of bosonic enhancement to understand the dynamics, and refutation of the idea that the enhancement is responsible for loss of squeezing and pairing. Above all, the influence of the different processes on the loss of quantum properties were understood, and we were able to determine that the main underlying cause is the non-monochromatic nature of the cloud. On top of this, an important and somewhat unexpected conclusion of our analysis is that in the presence of non-monochromatic sources a dense halo is not, in fact, advantageous. On the contrary, the degradation present can be alleviated by a dilution of the colliding source condensates.

4.4 Condensate collisions – experiments

The series contains three articles [H3, H4, H7] in collaboration with the experimental group of Chris Westbrook (as well as Karen Kheruntsyan from the University of Queensland, and for [H3] with the group of Marek Trippenbach from the University of Warsaw). In these works, comparison to the results of numerical simulations with the STAB method [H5] was important to interpret or understand the experimental results.

The experimental setup is shown in Figs. 13–14 and described in detail in [141][H4]. The initial condensate (or quasicondensate) with $N \approx 10^5$ metastable helium atoms (He^*) is created in a very elongated harmonic trap (the aspect ratio was 25 in [H3] or 200 in [H4,H7]). At $t = 0$ a short laser pulse generates a sinusoidal potential for the atoms which leads to Bragg diffraction that causes the cloud to coherently split into two parts that separate at relative velocities of $v_0 = \hbar k_0/m$. The wavefunction splits according to $\phi(\mathbf{x}, 0) \to \phi(\mathbf{x}, 0)(e^{ik_0 x} + e^{-ik_0 x})/\sqrt{2}$. Simultaneously, the external trapping potential is turned off. What ensues is called a half-collision (Fig. 13a) that lasts typically a few hundred μs during which the halo of scattered atoms forms. At later times, the interaction between atoms becomes negligible because density is reduced by both free ballistic expansion and expansion caused by the repulsive interactions, since the atoms are no longer trapped.

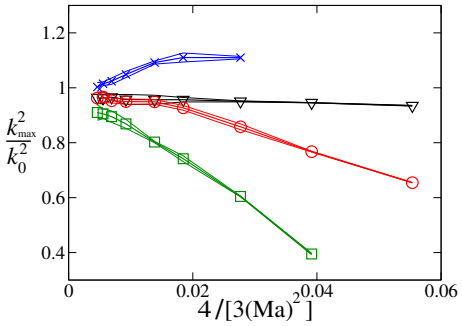

Figure 7: [H6] Deviation of the halo radius from $|\mathbf{k}| = k_0$. Full calculation (red), RBM (black), and variants B (green), D (blue).

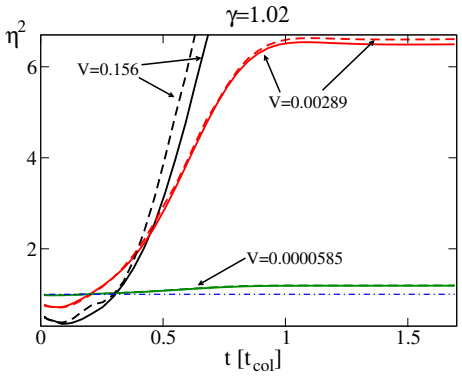

Figure 8: [H8] Evolution of the squeezing η^2 during a BEC collision (continuous) and its estimate on the basis of correlations $\eta^2_{\rm est}$ (dashed). Dense halo case $\gamma = 1.02$.

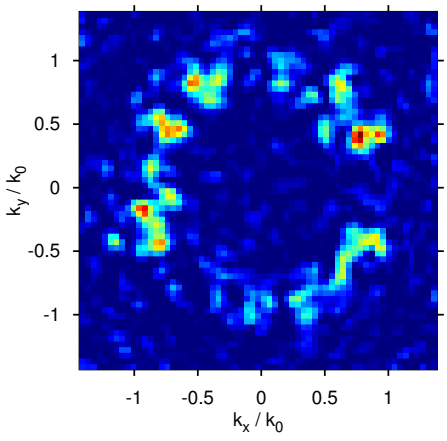

Figure 9: [H8] A slice through the halo for one realisation (colour indicates density).

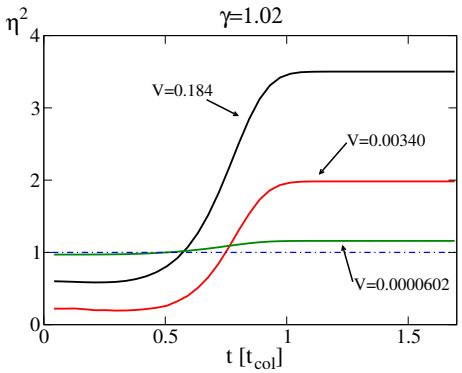

Figure 10: [H8] Evolution of the squeezing η^2 in the RBM.

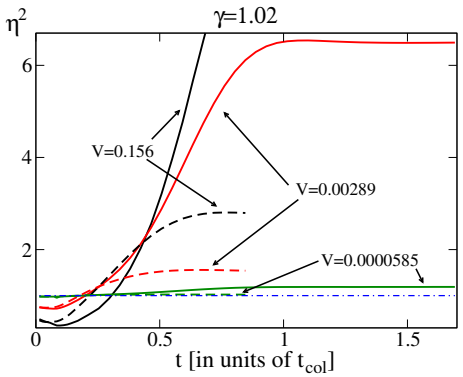

Figure 11: [H8] Evolution of the squeezing η^2 in the full model (continuous) and without Bose enhancement (dashed).

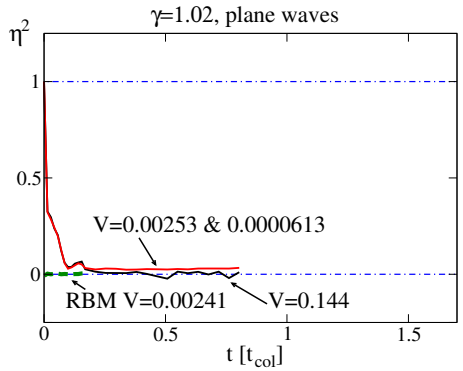

Figure 12: [H8] Evolution of the squeezing η^2 from a plane wave collision. Dense halo case.

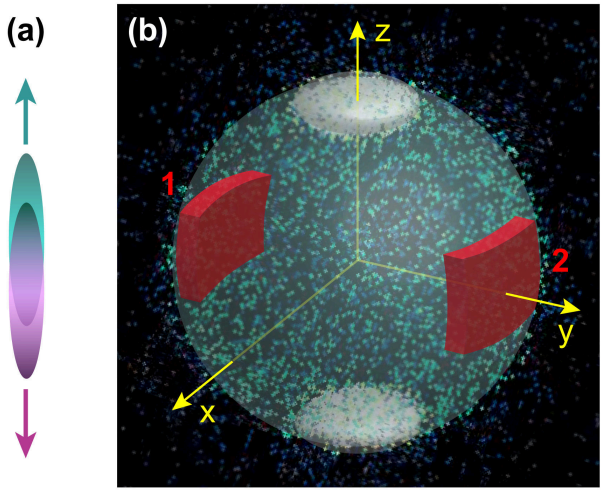

Figure 13: [H7] Placement of bins in the experiment, and an example of measured atom positions.

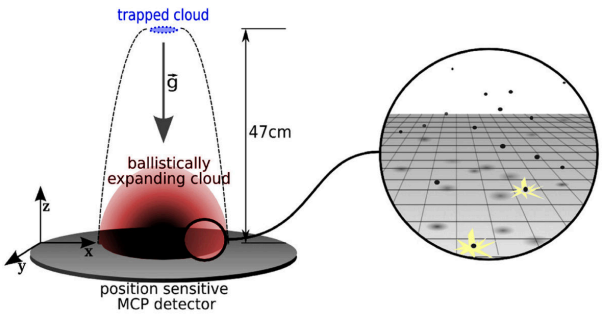

Figure 14: The experimental setup in Palaiseau. (Diagram as in [1]).

The atoms fall under gravity for about 0.5 m in vacuum (Fig. 14). In this time their free ballistic flight converts the initial momentum distribution into a corresponding spatial distribution at the detector that is placed at the bottom of the vacuum chamber. It is a special *multi-channel plate* detector (MCP), that registers the impact of single atoms with a high resolution both in space and arrival time. The detection of single atoms is made possible thanks to the 20 eV of energy possessed by the metastable excitation of the outer electron. This energy is released if the atom nears a conductor in the detector, which then registers the arrival times of the resulting electrical impulses. The detection efficiency for a single atom is about 12%, with the limitation that when the densest part of the cloud (the condensates) impact the detector, it becomes temporarily saturated. In a single run of the experiment, the positions (i.e., indirectly, the momenta of the initial cloud just after the collision) of about every eighth atom in the halo is registered, as shown in Fig. 13b. This allows one to precisely measure not only the density, but also two-particle correlations in the halo or η^2 with the help of appropriate bins.

4.4.1 Atomic four wave mixing beyond the optical regime [H3]

Unlike the later experiments [H4,H7], the collision here was not oriented along the long axis of the clouds like in Fig. 13, but was made "sideways" along one of the short dimensions of the cloud. This led to anisotropy in the plane perpendicular to the collision axis.

It also appeared in the halo cross-section (Fig. 15), a trait that is not predicted in simple models of the RBM type because they are not sensitive to the potential created by the condensates (7b) which is the source of the anisotropy. Anisotropy is also not observed in analogous systems from nonlinear optics that display four wave mixing because the nonlinearities are usually small there, possibly with the exotic exception of the ponderomotive force occurring during high harmonic generation in intense laser fields [142]. Past research in atom optics concentrated on phenomena for which the analogy between the bosonic fields in quantum optics and ultracold atoms held very well. This experiment showed the limits for this analogy – whence the "Beyond Optics" part of its title.

The difference was brought out by observation of the anisotropy, as well as by drawing attention to the completely different phase matching conditions as compared to optical four wave mixing. One of the reasons the anisotropic geometry was studied to begin with was to look at the possibility of atomic superradiance. This would have been analogous to the superradiance that occurs when an elongated condensate is illuminated from the side by laser light [106–115]. There, because the photon has no rest mass the energy-momentum conservation conditions on a scattering between a photon and an atom allow the photon to be scattered along the long axis of the condensate. The atom is scattered at a 135^o angle from the photon. The photons accumulate along the long axis, which bosonically stimulates further photon scattering preferentially in this direction. This greatly amplifies the photon wavepacket along the long axis of the condensate, i.e. the so-called end-fire mode. However, for a collision of two condensates, scattering along the long axis is not possible. The equal rest masses of the particles restrict the energy-momentum conservation conditions, and the minimum deviation from the long condensate axis is 45^o. This allows only for the relatively weak anisotropy shown in Fig. 15(a).

In the experiment, we precisely measured the position and anisotropy of the halo on the plane perpendicular to the collision axis. Measurements and corresponding simulations are shown in Fig. 15(c). An explanation of the anisotropy requires carrying out a more subtle accounting of the energy contributions than was made in Section 4.3.2.

- To take an atom out of the mean field of the condensate to an orthogonal mode costs about $\mu/2$ energy per atom as before. This is an isotropic feature.

- Scattered atoms have, however, the opportunity to recover a large part of this energy if they

roll down the potential hill (7b) created by the condensates — this is the "skier effect" again. This is only possible, however, in directions that deviate sufficiently from X, the long axis of the condensate. Along *this* axis, the atoms do not have time to "roll down" the potential hill because it disappears in the meantime because of the rapidly diluting condensate. The dilution comes about because of the rapid expansion of the condensate in the short directions under its own repulsive interactions as soon as the external trap is released at $t = 0$. Scattered atoms propagating along the log axis have too far to go before they regain any appreciable energy from rolling down. The lack of the skier effect in the long directions is what is ultimately responsible for the anisotropy.

Prior to comparing with the STAB simulations, we couldn't reach a consensus as to what was the principal reason, because of several competing explanations that we had come up with. The numerical simulations ultimately allowed us to identify and unambiguously confirm that the two processes detailed above are what is responsible. The article [H3] was also the first chronologically to describe (albeit briefly) the STAB method. It turned out that it was the only available approach that could give us sufficiently accurate predictions to match these effects in the experiment, at the required level of 2% precision.

4.4.2 Sub-Poissonian density fluctuations in the halo [H4]

This was the first experiment to show number difference fluctuations η^2 below the Poissonian level in atom optics. While pair correlations were seen previously [1, 94], they do not guarantee fluctuations below the shot noise level, nor spin squeezing (an example is given e.g. in [115]), nor entanglement. Our experiment gave the first clear evidence of non-classical behaviour in widely separated atoms in this regard and was an important demonstration that they are a promising field for applications to quantum metrology or quantum information [131–133]. The squeezed atoms are separated here by several cm, which give them much potential for studies of the fundamentals of quantum mechanics such as e.g. nonlocality [82, 89, 139, 140]. Other later experiments in several similar systems also showed squeezing of a similar strength between well separated identical atoms [2, 7].

This experiment was done in a refurbished apparatus with a much more elongated cloud than in [H3], and the collision was now along the long condensate axis. This led to a denser halo, although it remained deep in the "dilute halo" regime ($\gamma \ll 1$) from the point of view of the squeezing degradation analysis of Section 4.3.3. To measure the number difference fluctuations η^2, the halo was divided into a certain number of bins – originally 16. This is shown in Fig. 16(a-b). The neighbourhood of the condensates was excluded from the analysis due to being complicated and/or influenced by detector saturation. The number of atoms per bin was measured in each realisation, and they were used to calculate the squeezing parameter η^2 for each pair of bins.

Significantly, fluctuations below the shot noise level ($\eta^2 \sim 0.9$) were seen only between opposite bins (8 pairs), while those between all the other pairs of bins were on the shot noise level $\eta^2 = 1$. This is shown at the bottom of Fig. 16. After factoring in the inefficiency of the detector, we estimated that the actual degree of squeezing in the scattered atoms is about -10dB ($\eta^2 \approx 0.1$).

To confirm that we had the correct understanding of the situation, we compared the dependence of η^2 on the division into bins with the theoretical description. To this end we simulated the system while varying the number of bins N_z into which the halo was divided. The agreement between experiment and STAB was satisfactory. As a side benefit, this study allowed for a more accurate determination of the efficiency of the detector (12%) by comparing the simulated and the detected squeezing.

4.4.3 Violation of the Cauchy-Schwarz inequality by atomic fields [H7]

This experiment demonstrated that distant atoms in the halo do not satisfy the classical Cauchy-Schwarz (CS) inequality. This proves that they cannot be described by any classical boson field [128]. This is a very substantial step on the way to demonstrating violations of the Bell inequality by superpositions of states that differ in their mass distribution. The experimental demonstration of such a violation, which is the long-term goal of our common research, would constitute a proof of the breakdown of local realism for systems composed of massive particles. This would be an important result for the fundamentals of quantum mechanics.

The halo was divided into spatial bins (as shown in the small diagrams above Fig. 18). This time we measured the two-bin correlations $\overline{G}^{(2)}_{ij} = \overline{g}^{(2)}_{ij}\overline{N}_i\overline{N}_j$ between them, similarly to the description from [H8]. We showed analytically that when the ratio of counter-propagating to collinear correlations, $\mathcal{C} = \overline{G}^{(2)}_{12}/\sqrt{\overline{G}^{(2)}_{11}\overline{G}^{(2)}_{22}}$, is above 1, the CS inequality is violated. This was then also demonstrated in the experimental data. It is shown in Fig. 18, along with the lack of violation for neighbouring rather than opposite bins. The classical limit was exceeded for many different partitions into bins (M, number of zones, in Fig. 18).

An additional substantial result of this research was that the inequality violation, and consequently unequivocally quantum effects, only become visible when the measurements are made in a sufficiently multi-mode manner. A two-mode simplification was not capable of reproducing either $\mathcal{C}$, nor its relationship to the correlations measured. The ideas touched on here were later developed more fully in the theoretical/numerical work [H8]. The comparison to simulations with the STAB method were the element that confirmed our understanding of the behaviour of the scattered atoms, and the relationship between the few- and multi-mode description and observables.

The numerical simulations were also essential to weed out the importance of fluctuations of the total number of atoms N on the results. The actual number of atoms in the experiment fluctuates quite significantly from run to run, by several tens of percent. What is more, the number in a particular run can not be determined precisely mostly because of the nonlinear saturation of detectors by the condensate. The dependence of the number of scattered atoms in the halo depends non-linearly and rather strongly on N because the scattering rate is proportional to the local density squared, and that density depends in turn non-linearly on N. As a result, it is difficult to quantify the influence of these fluctuations on the halo, though the variation between runs is generally seen to be large. I carried out simulations for different values of N to estimate whether its fluctuations influence the interpretation of our results. In the supplement of [H7] this was explained in detail. – generally the fluctuations of N do not have an important influence on $\mathcal{C}$, but can have on the anisotropy studied in [H4].

This was also the first publication where I introduced the next innovation for incoherent atom wave dynamics, one that opens the road to simulating a much greater variety of systems — extension of the STAB method to nonzero temperature. It turns out that the scattering from pairs of colliding *quasi*-condensates can be simulated in quite a simple way by replacing the source condensate wavefunction by a statistical ensemble that realises the classical fields description of the quasicondensate. Here, each stochastic realisation of the Bogoliubov evolution is paired with a different, independent, source wavefunction taken from this classical fields statistical ensemble. In our case we used the approximate form found by Petrov *et al.* [143] to prepare the condensate [144].

This was important for our research into the CS violation because the source cloud in the experiment [H7] is sufficiently elongated to be almost one-dimensional, and in fact has quasicondensate phase fluctuations. We estimate that there are about 10 phase domains per cloud. This has particular importance for correlations because the thermal broadening of the momentum distribution in the quasicondensate causes a corresponding broadening of the back-to-back (BB) correlations for counter-propagating atoms. Taking that broadening into account was necessary to reconcile the low

correlation peak in the halo with the strong number difference squeezing $\eta^2 < 1$, as was explained in [H8]. The question for us here was whether this thermal broadening has an effect on the CS violation ($\mathcal{C}$) in the experiment. The new thermal STAB method was used, and it turned out that the thermal influence on $\mathcal{C}$ is small in comparison with the dependence on total number of atoms N.

The results published as [H7] constitute the latest stage of the long-term program of the Palaiseau group to test the Bell inequalities with separated massive particles. The sequence to date includes the first measurements of non-classical correlations in the atom clouds [20, 80], across the halo [1], sub-Poissonian fluctuations of the number difference [H4], and the violation of the Cauchy-Schwarz inequality [H7]. A recent theoretical work [129] shows that our exceeding of the CS inequality indicates also that the atoms in the halo are in fact usefully entangled. This last conclusion is particularly interesting given that most experiments that have hitherto showed the entanglement of atom clouds [5, 134–138] proved this by showing spin squeezing. There is no spin squeezing in our experiment because of the negligible phase coherence (shown in [H1]), so the entanglement that appears here is of some different kind.

4.5 Dynamics of large systems with spins [H9]

A somewhat separate branch of my research on simulations of full quantum dynamics concerned spins. In collaboration with Prof. Erik Sørensen and his student Ray Ng, we developed a stochastic method for the dynamics of spins systems (with spin 1/2 per site). In this, I was the expert on quantum simulation methods, and the co-authors experts on the physics of spin systems.

We benchmarked the usefulness of the new method on the example of the Ising model that undergoes a quantum quench (a non-adiabatic jump in system parameters) in the transversely applied magnetic field [164, 166, 168]. This scenario has been intensively studied recently [145]. Achievements in the last few years with cold atom systems confined in optical lattices indicate the possibility to realise so-called quantum simulators [146–152] in which the internal atomic degrees of freedom duplicate those present in spin systems. This has extra importance for states with frustration because knowledge about their dynamics has to date been quite poor . Recent experiments [153–162] have made major advances towards the creation of such simulators. For example, a simulator was implemented for 9 spins [157, 159], while systems with about 300 spins were created with trapped ions [161] as well as neutral atoms in optical lattices [158, 163]. Some of these experiments model exactly quantum quenches in the Ising model [153, 155, 157, 161].

We derived stochastic equations that correspond to the full quantum dynamics of the Heisenberg model on a lattice of arbitrary geometry with a transverse magnetic field:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \left[\hat{S}_i^z \hat{S}_j^z + \Delta \left(\hat{S}_i^y \hat{S}_j^y + \hat{S}_i^x \hat{S}_j^x \right) \right] - h(t) \sum_i \hat{S}_i^x, \tag{12}$$

Here J is the interaction strength for pairs of spins denoted $\langle i, j \rangle$ (the interaction is via the spin projections onto the axis z), $h(t)$ is the strength of the transverse magnetic field in the x direction x, and Δ the interaction strength of spin projections onto the x, y plane. The Ising model is the special case of $\Delta = 0$, while the isotropic Heisenberg model has $\Delta = 1$. In comparison with a boson field of cold atoms or photons in quantum optics, spin dynamics is generally intrinsically "hard" numerically. This is because the noise in the stochastic equations comes from the interaction J which is large or greater than the magnetic field strength h for physically interesting cases. In comparison, in condensate dynamics the noise is relatively small in comparison with the mean field evolution.

In our calculations we looked at the fairly standard case when the initial state at $t = 0$ is the Ising ground state of the $h = 0$ model. At $t = 0$, the transverse field is suddenly switched to its final value that we usually chose as $h/J = 0.5$. This is the critical point of the one-dimensional system, and here

the correlation length in equilibrium diverges. In our case, of course, the correlation length grows with time and tends to infinity only as times get very long. The purpose of the simulation is to track its evolution. Example results are shown in Fig. 19.

The representation that turned out to be successful uses the local basis $|z\rangle = e^{z/2}|\uparrow\rangle + e^{-z/2}|\downarrow\rangle$ parameterised by the complex number z. This basis differs significantly from coherent states $|\alpha\rangle = e^{\alpha\widehat{a}^\dagger}|0\rangle$ that are used for boson fields in the positive-P representation, but does retain some features of coherent states that are essential for the simulation of large systems: a linear scaling with the number of spins, N, of the size of the configuration $\vec{\lambda}$, the number of equations and the numerical effort required. I also keeps the independence of the realisations, Gaussian local noise during evolution, and a lack of global phase factors. This differs from from all incarnations of path integral Monte Carlo. On the other hand, like positive-P for bosons, noise amplification occurs also here after a certain time, and this finally establishes the limits of the method. As there, the time limitation does not depend on the number of spins, and only weakly on the dimensionality of the lattice (i.e. the number of neighbours). We analysed this scaling similarly to the way it was done previously for boson fields [P26,P27] and, in particular, we estimated its dependence on the main dimensionless parameter of the system, h/J. As in other numerical phase-space methods, breaking of the translational symmetry, time-dependence of the coefficients, and the form of the boundary conditions do not affect the numerical difficulty. The correctness of the results was demonstrated on the case of a relatively small system of 10 spins that could be solved exactly by diagonalising the Hamiltonian (Fig. 17, right).

To determine its usefulness for large systems, we calculated the dynamics of systems of 10000 spins in one and two dimensions (Fig. 19). These calculations each took about a day on a standard PC. Using the quantum triangulation technique developed by me [H2], we were able to extend the simulation time to $2.8\hbar/J$.

This is a time that is sufficiently long to observe nontrivial dynamics, including propagation of correlations and the bulk of the decoherence [169]. Generally, the rather trivial early-time perturbative physics occurs in a time $\hbar/J$ that is accessible without the triangulation, whereas the majority of the decoherence lasts several units of $\hbar/J$. An earlier attempt to develop a related stochastic method by the Sørensen group using Schwinger bosons [165] was only able to obtain times around $0.6\hbar/J$ and had unfavourable scaling with N — essentially, the simulation of 100 or more spins was not possible.

It is also worth mentioning that while the simplest case – the one-dimensional Ising model with a transverse magnetic field — can be solved exactly with the help of the Jordan-Wigner transformation [166] for the uniform case, or calculated with DMRG methods for up to several hundred spins up to times of $t/J \sim 100$ [167], that is no longer possible for 2D or 3D systems. For our method, an increase of the dimensionality does not constitute a problem.

There is a whole spectrum of problems for which times of several $\hbar/J$ are sufficient to obtain important information. Apart from quantum quenches themselves, e.g. the Löschmidt echo method allows to localise phase transitions [170], while coherence properties can be investigated by looking at the dynamics under an appropriate sequence of changes of external parameters [171, 172][P24,P30]. This last technique is particularly useful for lossy systems because it avoids the need to track the system over very long times.

4.6 Summary

In brief, the main results of the series of articles [H1-H9] presented above, are:

- Development and demonstration of a method for the calculation of the full quantum dynamics of systems composed of huge numbers of ultracold atoms [H1]. Full quantum calculations on systems as large ($10^5 - 10^6$ atoms) were previously considered impossible. The ease with which these results were obtained encouraged many uses of this stochastic approach since both with my collaboration [H1,H3,H4,H6,H7,H8,P27] and without [44–47].
- Development of the STAB method that treats the scattered atoms in a fully quantum manner [H3,H5]. This allows precise simulations of many cold atom experiments when atoms are scattered into empty modes, something that is not possible with more approximate methods such as the RBM or mean field, or of dubious accuracy when using the truncated Wigner method.
- Understanding and explanation of the relationship between correlations and squeezing among the scattered atoms, and of the relationship between the halo's two-mode and many-mode descriptions [H1,H6,H7,H8].
- Revealing the causes of the degradation of squeezing in the halo and, by implication, of the entanglement of the halo atoms [H8].
- Development of a method for the simulation of the full quantum dynamics of large systems of interacting spins [H9], and of the quantum triangulation method [H2] that was subsequently found essential for the spin simulations. This opens new perspectives for future calculations on systems of spins in two- and three-dimensions, and even ones that lack translational symmetry.
- A series of experimental studies with the Westbrook group from Palaiseau, for which my numerical simulations played an important role in coming to an understanding of the results. Sequentially, the experiments revealed the significant differences between atom and photon optics [H4], non-classical sub-Poissonian fluctuations of density between widely separated atoms [H5], and a violation of the Cauchy-Schwarz inequality that proves the impossibility of describing the halo atoms with classical fields [H7] and their entanglement [129]. These are successive steps in the long-term campaign to observe a violation of the Bell inequality, and incompatibility with local realism, for massive particles in states with different distributions of mass.

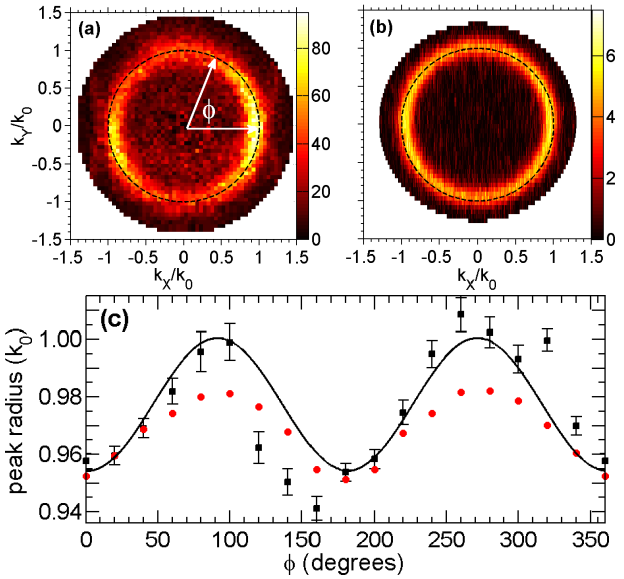

Figure 15: [H3] A slice through the halo in the experiment (a) and STAB simulation (b). The condensates are elongated along X. The halo radius as a function of the angle ϕ is shown in (c) for the experiment (black), and simulation (red).

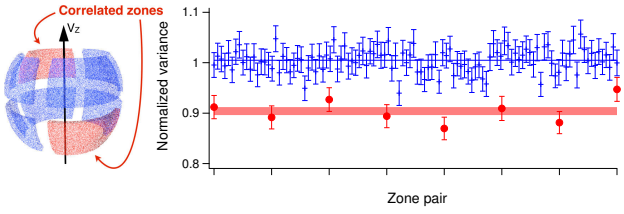

Figure 16: [H4] Measurement of sub-Poissonian fluctuations. Division into bins (left); η^2 between all bin pairs (right), with opposite bins in red, all others in blue.

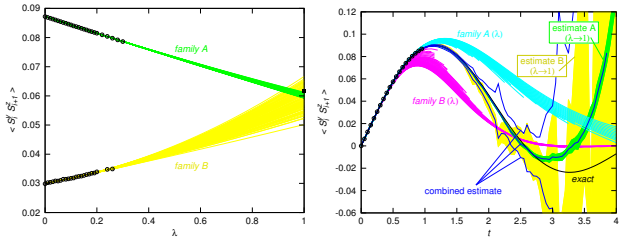

Figure 17: [H9] Quantum triangulation. Left: extrapolation of two equation families to the full quantum value. Right: estimates from each family, and the final combined estimate (dark blue). Outer lines estimate the statistical uncertainty.

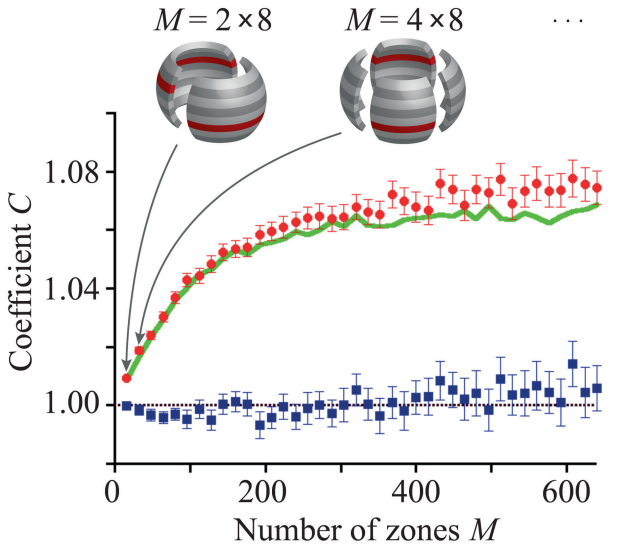

Figure 18: [H7] Violation of the Cauchy-Schwarz inequality $\mathcal{C} \leq 1$ by measurements on opposite bins (red). Results for neighbouring bins in blue. STAB calculation in green. The top diagrams show the geometry of division into bins.

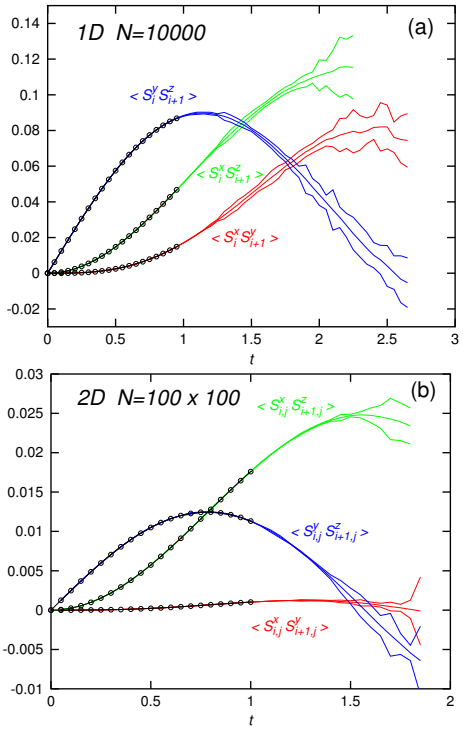

Figure 19: [H9] Spin correlations in macroscopic systems: one-dimensional (a), two-dimensional (b). External lines indicate uncertainty, circles – results obtained without quantum triangulation.

5 Results in other areas and research history

5.1 Local realism in quantum mechanics

In Australia, where I spent most of my youth and childhood, the standard study path after a BSc for those interested in research goes through a fourth year of study dubbed the *honours* year. It takes the place of the two-year Masters' program in European universities and involves both coursework and a research project in approximately equal proportion. If one obtains a good enough grade, PhD studies can then be undertaken directly upon obtaining this BSc (Hons) degree. My research project concerned investigation of the fundamentals of quantum mechanics under the supervision of Dr. Margaret Reid, who is a respected authority on the topic.

We found and demonstrated an example of a quantum state for which a violation of the Bell inequalities occurs with the results of measurements of macroscopic quantities only. In this context, macroscopic is understood to mean such quantities whose measurement uncertainty is itself macroscopic, i.e. much greater than the spacing between the neighbouring discrete measurement values allowed by quantum mechanics. This was the first demonstration of the incompatibility of quantum mechanics with *macroscopic* local realism. This result deviates much more from the classical way of perceiving the world than earlier studies of Bell inequality violations with measurements of particle spins or with single photons. It shows that also the results of some continuous or macroscopic measurements can not be described by any local hidden variable theory.

The idea was in its entirety my supervisor's, while the calculations were my work. I calculated correlations between homodyne measurements of phase quadratures [173, 174] made on a macroscopic boson field that was composed of an appropriately chosen superposition of coherent states. We showed that the boundary given by the Bell inequality was violated by 1.5% using measurements of continuous quantities with only a macroscopic resolution. We estimated the influence of imperfect detection efficiency. the results were published as [P10,P12]. I also took part in preparing the article [P11] which formally defined and made precise the difference between macroscopic and microscopic local realism.

5.2 Stochastic gauges and research into the general properties of phase-space representations

The leading topic of my PhD research with my supervisor Prof. Peter Drummond at the University of Queensland was developing the stochastic gauges idea for phase-space representations, and its application to ultracold atoms. In the years 1998-2002 I worked at the University of Queensland as a full-time PhD researcher, and later as an external student in the years 2002-2004 (I submitted my thesis in June 2004) being simultaneously a research employee of the engineering firm Deuar Pty. Ltd. The engineering research is described below in Section 5.6.

The general course of my research into stochastic gauges has already been briefly laid out in the introduction to Section 4.2. The initial topic was a search for local basis states $\widehat{\Lambda}_m$ that would improve on the the behaviour of the positive-P representation for dynamics and thermodynamics simulations (see Section 5.3). We considered several kinds of bases, including squeezed states more general than those studied earlier in [175], atypically normalised variants of the positive-P basis, and Hermitian basis operators [P18]. These investigations led us to formulate a general theory of phase-space representations and to recognise which features of a basis are important from the point of view of applications to many-body systems. This was described most fully in my PhD thesis [P34]. Some of the ideas developed then by us turned out to be useful later for the development of the so-called Gaussian bases by J. Corney and P. Drummond [176–178], and appear in a couple of articles we wrote together on this topic [P22,P27,P28]. Gaussian bases are one of the best candidates for the calculation of the

full quantum dynamics of many-*fermion* systems in 2D and 3D (for example, see [179–181]), which is important for the theory of condensed matter systems and the dynamics of heavy ion collisions.

To describe the stochastic gauge idea, which in the end we used to overcome the problems with boundary term errors [P19]and to improve simulation times [P23,P26], it is necessary to explicitly show some details of how quantum mechanics is described with stochastic equations. According to (1), there are three equivalent ways to describe the quantum state: the density matrix $\widehat{\rho}$ itself, the distribution $P(\vec{\lambda})$, or the set of realisations $\{\dots \vec{\lambda}^{(j)}, \dots\}$. The master equation $i\hbar\frac{\partial\widehat{\rho}}{\partial t} = [\,\widehat{H}, \widehat{\rho}\,]$, gives the dynamics, possibly with additional contact with an environment such as a thermal reservoir [182]. It can also be written as an evolution equation for $P(\vec{\lambda})$ or for the realisation $\vec{\lambda}^{(j)}$. In many cases, the equation for P takes the form of a Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = \sum_n \left\{ \frac{\partial}{\partial \lambda_n}(-A_n(\vec{\lambda})) + \sum_m \frac{\partial^2}{\partial\lambda_n \partial\lambda_m}\frac{D_{nm}(\vec{\lambda})}{2} \right\} P \tag{13}$$

where the indices n, m count the variables that enter into the full configuration $\vec{\lambda}$. Usually, this is equivalent to stochastic equations for single realisations:

$$\frac{\partial \lambda_n}{\partial t} = A_n(\vec{\lambda}) + \sum_k B_{nk}(\vec{\lambda})\xi_k(t). \tag{14}$$

The relationship between the noise matrix B and diffusion matrix D is $D = BB^T$, and $\xi_k(t)$ are independent real noises like in (4).

Phase space representations have the general property that many different distributions $P(\vec{\lambda})$ can describe the same quantum state, although not necessarily with the same statistical efficiency. The degrees of freedom associated with this are described by a number of functions that can be chosen arbitrarily (the stochastic gauges). The initial idea, *drift gauges*) invented by Prof. Drummond is built on the observation that if we define a new operator basis $\widehat{\Lambda}_G = \Omega\widehat{\Lambda}$ that includes an additional weight Ω, then $\widehat{\mathcal{Z}} = \widehat{\Lambda}_G - \Omega\frac{\partial}{\partial\Omega}\widehat{\Lambda}_G = 0$. In that case it is possible to add the term $\int d\vec{\lambda} P\mathcal{G}\widehat{\mathcal{Z}} = 0$, multiplied by any *arbitrary function* $\mathcal{G}$ to the master equation. That, in turn, allows one to introduce terms containing $\mathcal{G}$ together with $\frac{\partial}{\partial\lambda_n}$ and $\frac{\partial}{\partial\Omega\partial\lambda_n}$ into the Fokker-Planck equation (13). In this way we can introduce any arbitrary change (mediated by the function $\mathcal{G}$) into the deterministic part of the equations of motion (14). The price we pay is an additional evolution of the weight Ω. This weight then enters into all calculations of observables. The changed equations of motion with added gauges $\mathcal{G}_k$ are now

$$\frac{\partial \lambda_n}{\partial t} = A_n(\vec{\lambda}) + \sum_k B_{nk}(\vec{\lambda})[\xi_k(t) - \mathcal{G}_k(\vec{\lambda})] \qquad ; \qquad \frac{\partial\Omega}{\partial t} = \Omega\sum_k \mathcal{G}_k(\vec{\lambda})\xi_k(t). \tag{15}$$

An appropriate modification can, for example, remove *boundary term errors*. The initial, not very successful, attempts to apply this idea were published in [P18]. Further research led us to some important conclusions about the properties required for a successful gauge, and we were able to implement the idea. The successful removal of boundary term errors was demonstrated on a number of notorious examples that had previously been afflicted with systematic errors because of them in [P19].

Unfortunately drift gauges have one serious flaw that appears for large systems – the amount of noise in the *logarithm* of the weight $\log\Omega$ grows linearly with the system size. When the variance of this logarithm becomes greater than about 10, the weight Ω becomes inherently badly sampled, and observable calculations from the ensemble cease to be trustworthy. This again restricts the useful simulation time and system size that can be correctly described with the help of the method.

While studying the general properties of phase-space distributions, a work of Plimak *et al.* [183] caught my attention because it exploited a different freedom in the equations of motion than the drift gauges. I developed the idea further into a general description of the freedoms in the choice of noise terms – what we called *diffusion gauges*. They constructively describe the remaining freedom in choosing B once D has been specified. What is most interesting, this choice can have a very large influence on the size of statistical fluctuations during the evolution – a very relevant issue for practical applications. For example, for the anharmonic oscillator $H = \widehat{a}^{\dagger 2}\widehat{a}^2$, which is the simplest one-mode analogue to an interacting gas of bosons, the evolution of the plain positive-P equations lasts for at most several phase oscillations before it is destroyed by noise amplification. With an appropriate diffusion gauge, however, the simulation stays well behaved right through the end of decoherence (hundreds or thousands of phase oscillations). The scaling of the accessible time interval with the system parameters were analysed in detail for one, to and many-mode systems in [P25,P26]. The result obtained in [P25], that the expected useful simulation time for the Hamiltonian (2) in the raw positive-P representation is $t_{\mathrm{sim}} \approx 2.5\hbar(\Delta V)^{1/3}/[g n_{\mathrm{max}}^{2/3}]$, proved to be extremely useful for later research. It allows one to quickly and accurately estimate how long a simulation time we can expect for the system at hand. Here , n_{max} is the maximum local density in the gas, and the rest of the symbols are the same as in (3).

In the long term, both types of gauges proved useful. The article [P21] describes the working of both kinds of gauges in detail, and together with [P22] gives examples of applications to several relatively simple Hamiltonians such as a one-dimensional Bose gas, molecular dissociation, and the anharmonic oscillator. In [P24] we studied the possibilities of stochastic gauges for models with few modes but so many particles that a brute force calculation on the many-particle basis is ruled out. We simulated the full quantum dynamics of a mole of atoms ($\langle \widehat{N} \rangle = N_A = 6.022 \times 10^{23}$) by using both kinds of gauges together, and were able to observe both the decoherence, and even the quantum revival. The last is quite remarkable considering that the equations of motion are. It is an expressive proof that the same quantum state can be represented by completely different distributions $P(\vec{\lambda})$.

Wrapping up this topic, let me also mention that an extension of the stochastic positive-P equations to the case of non-local interactions between the atoms was presented in [P28]. This has become of greater importance recently due to the great growth in interest in applications of ultracold dipolar atoms. Finally, two collective works published in 2007 contained a number of calculations made by me as examples [P27,P35].

5.3 Thermal calculations with stochastic gauges

A somewhat different topic were applications of stochastic gauges to thermal equilibrium calculations. This has actually been the most useful application of the drift gauges so far. There is a notable similarity between dynamics and the sequence of thermal equilibrium states as temperature changes. The grand canonical ensemble $\widehat{\rho}(\beta, \mu)$ with $\beta = 1/k_B T$ and chemical potential μ, follows the sequence $\frac{\partial \widehat{\rho}}{\partial \beta} = [\widehat{\rho}, \widehat{H} - \mu \widehat{N}]_+$. The stochastic equations that result from this resemble those obtained for dynamics from the master equation under the exchange of $t \to i\beta/2$. For this reason, such an approach has been dubbed the "imaginary time;" method. Importantly, $t = \beta = 0$ corresponds to infinite temperature, and the equilibrium state there is trivial and its P distribution is easily written down and sampled. In this way, integrating over β, one can obtain thermal states for a long range of temperatures from infinity down to some T_{min} that is limited by the statistical properties of the equations.

Two serious inconveniences had to be overcome to obtain useful results in practice. Firstly, in contrast to dynamics, the boundary term errors rear their head here. We were able to find a drift gauge that removes the errors and deal with this problem. Initial calculations on a single-mode system

were published in [P21], while the correctness of the gauged simulation was demonstrated in [P23] on a one-dimensional gas.

The second difficulty comes about because of the deterministic terms in the evolution of the weight Ω. It forces one to take care in the way that the initial state is sampled. In particular, *importance sampling* of the initial states at $\beta = 0$ must be carried out, and a wise choice of the dependence of $\mu(\beta)$ is also helpful [P29].

The article [P29] describes research made long after the end of my PhD. It presents a detailed analysis and exposition of the ranged density and phase correlations in a one-dimensional gas at finite temperature. This physical system has been attracting a great deal of attention in recent years due to its very unusual physical properties (e.g. the lack of thermalisation [184]), the prevalence of one-dimensional traps in ultra cold atom experiments, and due to the usefulness of such gases for the study of phase fluctuations or other phenomena such as solitons or shock waves. Interestingly, even though the $T = 0$ case was solved "exactly" by Lieb and Liniger in 1963 [185], and the thermal gas soon after [186], this "exact" solution does not mean that all observables can be calculated in practice. In particular two-body correlations are a problem, apart from the local ones $g^{(2)}(0) = \widehat{a}^{\dagger 2}\widehat{a}^2/n^2$ described in [187]. We approached the matter on a broad front by several methods in different ranges of temperature and interaction strength γ. While the coldest and hottest regimes were accessible by analytical methods, numerical calculations with stochastic gauges were essential to obtain results in the regime dubbed "decoherent quantum" and in the transition region between the low and high temperature regimes. One of the notable things we found was a prominent maximum in the density correlations at nonzero distance (Fig. 21). It is particularly prominent in gases which have transition values of both the interaction strength and the temperature.

5.4 Dynamics of Rydberg atoms

I also took part in studies of the dynamics of correlations in a system of Rydberg atoms together with Dr. Sebastian Wüster and his collaborators from Dresden [P30] in 2009-2010. I joined the collaboration as their advisor on stochastic methods for quantum dynamics. We studied the influence of Rydberg excitations and the so-called Rydberg blockade on the inter-atomic correlations. The system consisted of an ideal gas of atoms in its ground state that was subjected to an external field that caused the excitation of some atoms to a Rydberg state. In that state they interact via a "long-range" van der Waals potential $\sim 1/r^6$. In the end, the stochastic calculations did not produce satisfactory results in this case, but I participated fairly intensively in the analysis and interpretation of the results obtained with approximate methods. We found that an "echo" type impulse that is used in experiments [171, 172] allows one to generate a state of the gas with highly unusual correlations between the Rydberg atoms – they are preferentially separated by a quite well defined spacing. This pair creation effect is best seen for low densities, which has some parallels to the case of atoms scattered in condensate collisions.

Dynamically, the system we studied has a lot in common with the spin system discussed in Section 4.5: single atoms can be in one of two states, and the Hamiltonian of the system can be conveniently written with the help of pseudo-spin operators. It would be interesting to re-visit this topic with the new, working, method for dynamics that was developed in [H9].

5.5 Quantum information theory

During my PhD studies I also carried on research in the field of quantum information theory, at a time when this field was just starting up. First in collaboration with Dr. William Munro of the Physics Department at the University of Queensland, later also with Prof. Ryszard Horodecki and his group from Gdańsk.

The first set of research concerned quantum copiers. We showed that even having imperfect detectors and copiers, one can still obtain more information about the input state with the help of the detectors and the copier, than one could with just a single detector [P13]. This proved that quantum copiers can be useful despite the *no-cloning* theorem which proved that an ideal copier cannot be constructed [188]. We studied this in more detail in the longer paper [P15], where we also took into account the possibility of dark counts in the detectors. We found the range of parameters for which the quantum copiers are helpful in this setup. The copier is most helpful when the detector's efficiency is very low and the frequency of dark counts is negligible.

In the next paper we described the transfer of information between the input state and the copies in a number of copier variants [P14]. In this context, we calculated the optimal kinds of copiers for several schemes of coding information in a sequence of signal input states. One of the main conclusions was that when information is coded and received via single states at a time, the optimum copier is of the Wooters-Zurek type [188, 189]. We also specified the conditions for optimal cloning under the condition that the copies cannot be entangled.

Next, we studied the criteria for separability for states having subsystems with several ($d > 2$) internal states – i.e. more than qubits which have $d = 2$. Hence, the title of one of the resulting articles was "qu*d*it entanglement" [P17] in contrast to the popular "qu*b*it". In [P16] we found the bounds on the amount of noise (the maximally mixed state) that can be added to the maximally entangled GHZ states to make them separable. Our bounds were stronger than those found in previous works [190, 191]. It was revealing to compare the scaling of the noise percentage with the number of subsystems (exponential) to the scaling with the size of the local Hilbert space d (polynomial). In [P17] we calculated the size of the separable parameter region in the neighbourhood of the maximally mixed state, taking into account both an arbitrary number of subsystems and (most importantly) any number d of local states.

The research that I participated in in the Horodecki group [P20] was aimed at a better characterisation of the entanglement in $d > 2$ systems. Precisely, while the entanglement in a bipartite system of qubits is fully characterised by one number known as the concurrence, we showed that for $d > 2$ a greater number of parameters is required for this. As a consequence, we introduced a multi-element object that is the generalisation of concurrence to higher dimensional bipartite systems, and analysed its meaning for the characterisation of entanglement in such systems. On this basis we indicated an object, the *biconcurrence*, whose trace is then an unambiguous indicator of the presence of entanglement. This was the simplest unequivocal criterion for the presence of entanglement in general bipartite systems.

5.6 Testing the strength of electric power poles while in use

In the years 2002-2005, while continuing the physics research described above, I also worked for my parents' company Deuar Pty. Ltd. in Brisbane. It is a small engineering research enterprise that employs several people in total, started and run by my father, Dr. Krzysztof Deuar. The business revolves around precise testing of the remaining strength of standing (primarily wooden) electricity poles during the course of their normal use. The tests are carried out using a specialised method and equipment, both of which were invented and designed as part of the company's activities, and have been patented in many countries (Australia, USA, Canada, Europe, and others), and are being continuously perfected. The company has been present on the market for these services for over 25 years. A large part of its activities consist of further research and development work with the aim of improving the equipment and the test methodology. It and Dr. Krzysztof Deuar are recognised experts on the subject.

I participated in the research, and to some degree the commercial activities of the company. The research was carried out as under the auspices of an Australian research grant, the AusIndustry R&D

Start Agreement "Integrated System for comprehensive testing of *in-situ* Power Poles for strength and longevity" in the years (2003-2005).

In brief, the *Mechanical Pole Testing* (MPT) method (one variant is presented in Fig. 22) involves attaching specially designed hydraulic equipment to the pole, making contact in two or three places: at ground level, at a height of about 1.2 m above ground, and about 0.5 m below the ground level (in some versions). A force of the order of $10^4 - 10^5$ N is applied in various sequences to impart stress on the pole, and a measurement of the rotation of local segments of the pole with regard to the gravitational field is made at several heights simultaneously. The Young's modulus of the wood is calculated on the basis of the measured rotations, the applied force and its geometry, and the properties of the conductors attached to the upper part of the pole. The force is applied several times in an appropriate sequence whose aim is to eliminate unknown parameters related to the properties of the soil as much as possible. The pole is stressed on almost its whole length because there are also two reaction forces present: the reaction of the ground and of the conductors at the top of the pole. The rotation measurements are made with electronic protractors with a precision of 0.001 degrees. Calculations are made by an original dedicated program that si installed on a hand-held computer, on the basis of data about the pole, the test parameters and the measurements, the last being input either by the operator or automatically by the apparatus during the cycle of force applications. The configuration of the pole, and especially of the conductors is taken into account to assess the actual required strength of the pole. After calculating the Young's modulus, known correlations between it and the ultimate breaking strength of the material (dependent on the species of wood and a few other inputs) is used to estimate the actual breaking strength of the pole.

The tests are carried out on standing poles with the conductors transmitting current during their normal work cycle, but the method has also been adapted to measure the strength of new poles still at the depot before being placed in the ground.

The biggest thing in all of this is to use a very limited number of measurements on the pole, but still obtain an accurate (especially, not an exaggerated) result for the strength. A larger number of measurements means a longer test sequence and larger costs. It is also very important that the equipment is sufficiently light that it can be carried to poles in difficult to access locations, and ones that lie far from the nearest road (these are common troubles). Equally important is that the final procedure is sufficiently simple and transparent that an operator without an engineering education can learn it after several weeks of instruction (The operators are usually employees of the energy / transmission companies).

The method is much more accurate than the ubiquitous "traditional" method, which basically entails judging the amount of rot inside the pole by listening to the sound it makes when hit with a hammer or finding it by drilling holes in the wood. The MPT method is also more accurate than other more refined approaches such as scanning the internal structure of the pole with ultrasound. Its greater reliability has been demonstrated in comparison studies carried out by independent research institutions in several countries around the world. The method is, however, significantly more expensive per each test, which limits its wholesale use for typical situations when safety is not treated as an especially high priority. Economic analyses have shown that economic savings due to extension of the average pole life appear after 5-10 years of applying the method.

My research input concerned several aspects of the development of the method, and customising variants of the method for particular industry clients (energy or transmission companies). The decidedly largest input I had was into numerical and analytic modelling of the strains on the pole and ground during the test. We were especially concerned with optimising the sequence of force applications during the test so as to eliminate as much of the influence of the unknown soil properties as possible. The soil's properties are generally very difficult to quantify or measure, which constitutes one of the two largest sources of uncertainty in the final estimate. (The other is the imperfect correlation between the Young's modulus and the breaking strength).

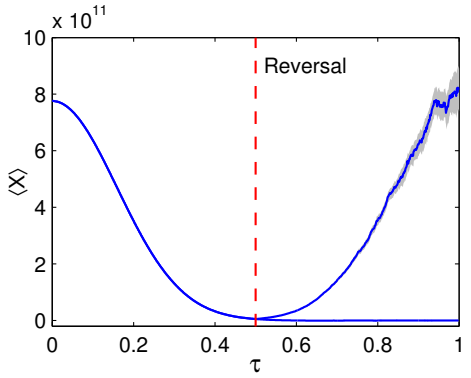

Figure 20: [P24] Coherence $\langle X \rangle \leq \sqrt{N}$ of the anharmonic oscillator with $N = 6.022 \times 10^{23}$ atoms. For the upper curve, the sign of the interaction was flipped after $\tau = 0.5$.

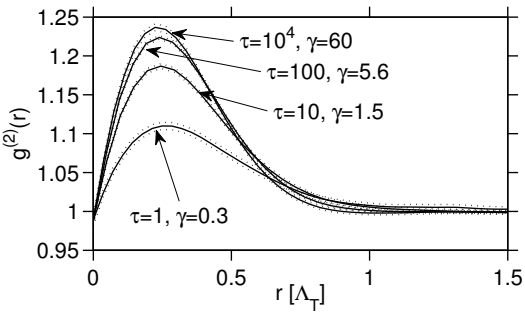

Figure 21: [P29] Spatial density correlations in a uniform Bose gas, showing the correlation maximum at a nonzero inter-atomic distance.

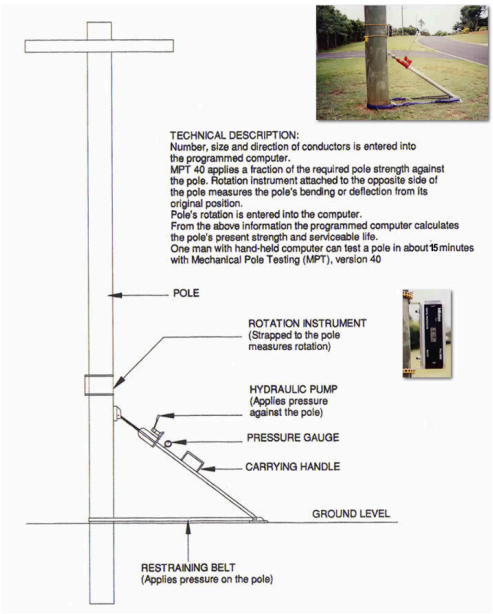

Figure 22: Outline of the Mechanical Pole Testing method (MPT) for electric power poles. [Deuar Pty. Ltd.]

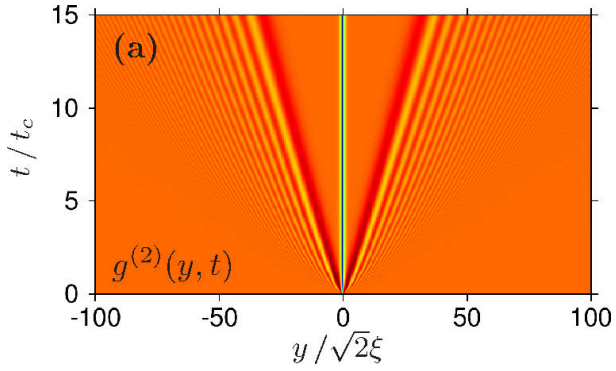

Figure 23: [P36] Density correlations after a quantum quench in the uniform Bose gas.

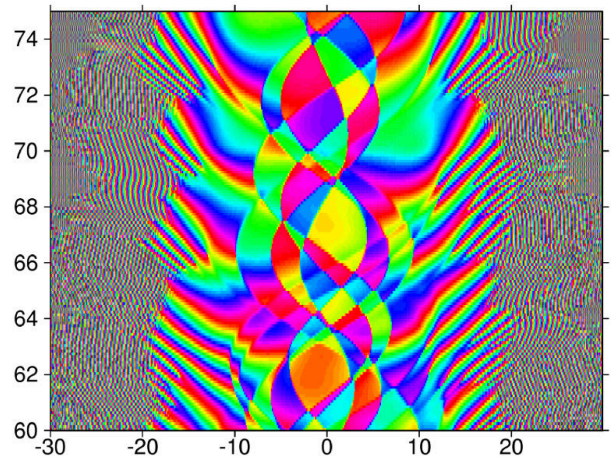

Figure 24: [P32] Phase domains in a one-dimensional gas, some time after rapid evaporative cooling.

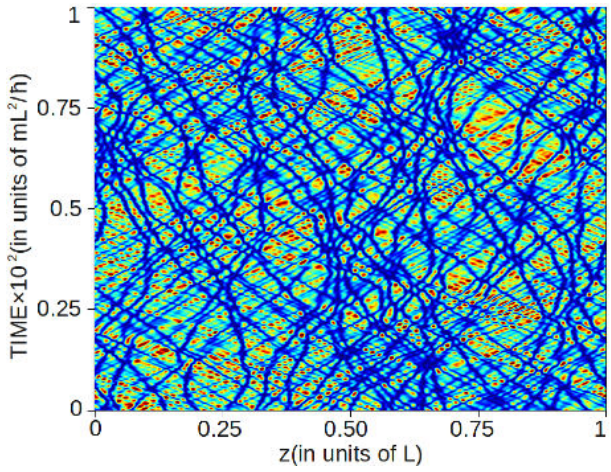

Figure 25: [P33] Spontaneous solitons in the thermal equilibrium state of a uniform one-dimensional Bose gas.

5.7 Quantum quenches in condensates

Preliminary calculations that I made on the one-dimensional Bose gas as a test of the positive-P method [P25] brought my attention to an interesting phenomenon in the observed correlations: While the mean density was unchanged, in the density correlation, a wave could be seen propagating at around twice the speed of sound. Since the initial state was taken to be the coherent wavefunction, the ground state of a non-interacting gas, while at later times the Hamiltonian (2) contains nonzero interactions, this was a realisation of a so-called *quantum quench* (i.e. a non-adiabatic jump in external system parameters).

A quantum quench occurs whenever changes in externally controlled parameters are too rapid for the system to be able to react adiabatically. In the field of ultracold atoms this is a very common phenomenon – it can occur, e.g. when the trap is changed during the preparation phases, and from tuning a Feshbach resonance or changing the transverse trap width for low-dimensional (1D and 2D) gases. The change can be a controlled one, or a side-effect as happens e.g. when initial states are prepared and for instance rapid laser pulses are applied to the gas to shift the atoms into the desired hyperfine state. One expects that such effects are present in many existing experiments with quasicondensates in 1D, but the typical imaging resolution is slightly too coarse to see the produced correlations without special preparation.

Studies of the dynamics of correlations after a quantum quench have come to prominence recently as a consequence of several relevant experiments in strongly interacting systems [10–14], where evolution of the correlations was measured.

In article [P36] (submitted to Physical Review Letters at the moment), we studied phase and density correlations in *dilute* uniform gases of bosons governed by the standard Hamiltonian (2), with the help of Bogoliubov theory. The correlations are caused by production of counter-propagating atom pairs. We obtained a universal expression for the correlations that is applicable for all times after the initial jump in interaction strength. We concentrated on dilute superfluid gases, which correspond to experiments in wide traps in a superfluid state such as [14, 15, 200, 201], rather than on the case of deep optical lattices in which the atoms are closer to the Mott isolator state [10, 11]. The first novelty we encountered was that we could obtain results for one, two, and three-dimensional gases in exactly the same framework, which allowed us to clearly compare these cases. Examples of the correlations that are seen are shown in Fig. 23. In all regimes, there are two basic zones in which the correlations have a different behaviour:

- *Timelike zone*: For points sufficiently close that correlations travelling at twice the speed of sound had time to cross the distance since the time of the quench. here one sees no density correlations apart from local repulsion on distances of ξ, while phase correlations drop off in a way that is characteristic for the gas's dimensionality (linearly in 1D, logarithmically in 2D, locally exponentially falling to a constant nonzero value in 3D).
- *Spacelike zone*: For more distantly separated locations in space. Here there is no density correlation apart from short-wave spatial oscillations, while the phase correlation is constant with distance but globally falling in time at the characteristic rate for the dimensionality, taking on the same value that is reached by the spacelike correlations at the edge of the sound cone.
- Around the boundary between these two regions there are very prominent density-density correlation waves (and also some less prominent oscillations in the phase correlation).

Some of these correlations were known previously for special cases [192, 193], or for strongly interacting one-dimensional gases which correspond to a fermionised system [194–199]. In our work, on the other hand, we describe the general case for gases in the superfluid regime, and obtained succinct

closed expressions for the correlations in most of the regimes that are interesting in practice. They will be a useful reference for any future attempts to measure this phenomenon.

Knowledge of the behaviour of a uniform gas is also very useful for most realistic non-uniform gases provided that the mean density does not change significantly on distances of the order of ξ. Such a *local density approximation* (LDA) is very accurate in many cases, e.g. recently in the one-dimensional gas [201].

The most urgent and arguably the most important element of the research was the demonstration that the density correlations can in fact be observed *in situ* even when the actual imaging resolution is much worse than the healing length ξ. It turns out that of the whole train of correlation waves, in the 1D gas only the man wave that moves at twice the speed of sound survives to be seen in a poor resolution setup. Its width grows in time as $t^{1/3}$. This indicates that if the eaves are able to propagate essentially undisturbed for long enough (e.g. to the edge of the cloud) then they will become visible even with the available resolution.

We analysed the situation for two contemporary experiments: Jörg Schmiedmayer's in Vienna [14, 15] and Isabelle Bouchoule's in Palaiseau [200, 201]. In both cases, we calculated that the imaging resolution and width of the cloud are sufficient for correlation waves to become visible after averaging over 1000-2000 realisations. That would allow one to make direct measurements of atom pairs *in situ* in the trapped gas, instead of observing just their traces and symptoms in the distribution of dilute atoms after expansion that have been able to be observed till now e.g. in condensate collisions.

5.8 Grey and thermal solitons in one-dimensional boson gases

An important branch of my research in the last three years has been the analysis of dark solitons in the one-dimensional gas and their dissipation or formation due to spontaneous and thermal processes. Dark solitons are long-lived dips in the density of the gas that have a well defined relationship between depth, speed, and the phase jump across the dip, and that are robust against mutual collisions and moderate changes in the surrounding gas.

Like two-body density correlations, solitons are at the edge of visibility in these gases because they also have this characteristic width of a healing length. As a result, while externally prepared solitons were already seen 10 years ago [202, 203], naturally occurring solitons that do not form in a pre-determined position are much more elusive. After averaging over realisations no sign of them remains. Spontaneous, naturally forming solitons are, though, an extremely interesting dynamical phenomenon in quantum mechanics. They are a perfect example of a phenomenon that cannot be observed by looking at low-order correlations, becoming visible only in the full distribution of single experimental runs. A full distribution approach to quantum systems has only come to the attention of researchers in our field a couple of years ago [5, 15]. Happily, the newest advances in experimental techniques allow one to achieve a resolution that is close the soliton widths *in situ* [2, 5, 15, 16, 21].

Solitons and two-body correlations: My initial foray into this field began after came across some works from Lincoln Carr's group [204, 205] that studied the filling in – "greying" of black solitons during quantum evolution. While the filling in and broadening of the density and correlation dips shown in these articles was unambiguous, their interpretation that the filling in of the density correlation dip allegedly is evidence that the solitons themselves are filling in seemed inappropriate, knowing the earlier works of Jacek Dziarmaga and Krzysztof Sacha (from the Jagiellonian University in Cracow). They showed that the profile of the mean density of a soliton does not necessarily correspond to the shape of the soliton seen in single realisations [206]. That work showed, rather, that the cause of such a broad lowering of the mean density can be that the solitons' positions fluctuate. After mutual discussions on the topic with JD and KS, we published a comment in Phys. Rev. Lett. on L. Carr's article [204] , in which we gave a counter-example. In that, deep solitons with a normal narrow

width, but placed with a fluctuating position led to the appearance of wide objects in the density correlations [P31]. The shape of this correlation profile was in no way related to the shape of a dip in any single experimental realisation. This clearly showed that profiles of two-body correlations do not indicate the presence of solitons or their lack. The explanation of this somewhat counter-intuitive result is that a soliton dip under normal circumstances displaces many more than two atoms, so only sufficiently high order correlations can distinguish it from other fluctuations and say something about its properties. For example in [P31], solitons even formed a *maximum* in two particle correlations, because of the increase in mean density fluctuations when the possibility to encounter the very low density at the centre of a soliton arises.

A recent article using an analysis of single realisations taken from a DMRG-type calculation was able to show for the first time that spontaneous quantum evolution of a dark soliton leads to random position fluctuations and not to any filling in or greying of the soliton dip [207].

Further extensive soliton studies were carried by me as part of a large collaboration (that also included: Kazimierz Rzążewski, Mariusz Gajda, Mirosław Brewczyk, Tomasz Karpiuk, Emilia Witkowska, Przemysław Bienias, Krzysztof Pawłowski) This cooperation has so far resulted on two articles in Phys. Rev. Lett. to which I made large contributions.

Solitons formed during the evaporative cooling of a gas: In [P32] we described research into the dynamics seen during the evaporative cooling of an ultra-cold gas of bosons. This was the first reasonably realistic numeric model of this process that was capable of capturing the long-time dynamics. Evaporative cooling is the definitive way to achieve quantum degenerate gases since the birth of the field, however quantum simulations of the actual process up to its end have been very hard to achieve.

We calculated the dynamics of evaporative cooling in a 1D Bose gas for a range of situations that led to trapped condensates or quasicondensates of various temperatures and coherence lengths in the final state. We used the classical fields method [18, 19] together with a sampling of the initial high-temperature state generated with the help of a dedicated Monte Carlo algorithm [208].

Our calculations confirmed past suspicions [209] that solitons are formed during the cooling, and that their production initially has features of the Kibble-Żurek mechanism [209–214]. However, the later evolution leads to a dissipation of all or most of the solitons. In the case of slow cooling, the disappearance of the last solitons coincides with the appearance of a true Bose-Einstein condensate.

For faster cooling, one firstly obtains a metastable state in which the cloud has a smooth density profile dissected by sparse deep solitons that separate well defined phase domains. A snapshot of the phase domains from this work (Fig. 24) was chosen as the cover of its edition of Phys. Rev. Lett. These solitons later convert into equilibrium fluctuations via a dissipative thermalisation process, achieving finally a quasicondensate state at various temperatures.

One of the surprising discoveries was the observation that despite this dissipation, a trace of the starting solitons remains in the phase correlations – they essentially remain unchanged during this later evolution just change the manner that they are represented in the single experimental realisations. The coherence length in the final quasicondensate is practically unchanged from that seen in the early soliton-rich state. We also showed that the coherence length in the soliton-rich state corresponds remarkably well to the mean distance between the solitons, and so they are responsible for almost all the phase fluctuations. Thus, the solitons can be considered as the early ("larval") stage of the later equilibrium phase fluctuations in the final quasicondensate.

The soliton phase of thermal equilibrium: Our subsequent discovery, published in [P33], was that solitons are in fact ubiquitous in the thermal equilibrium state of elongated ultracold Bose gases. This can be interpreted as a new phase with previously unsuspected properties: the soliton phase.

Our data from the earlier study of cooling ([P32]) showed that at long times, in cases when the equilibrium quasicondensate has relatively high temperatures, solitons were both forming and disappearing as time went on. This led us to suspect that they may be a natural and prevalent component of the thermal equilibrium state, something that was not previously realised by the community.

We calculated the time evolution of individual realisations of the thermal equilibrium ensemble [208], but this time without any changes in the trapping potential. Solitons were seen everywhere in the quasicondensate (Fig. 25), and appear without any need to seed them by some external perturbation. Deep solitons appear for a wide range of temperatures above the level set by the chemical potential $k_BT \sim \mu$, that corresponds tho the crossover between the thermal- and quantum-dominated quasicondensate. The upper temperature limit for their existence appears to be far in the degenerate quantum gas. The μ temperature scale (typical of many experiments) indicates that solitons may be present en masse in existing experiments but are not seen merely due to the limited resolution and sensitivity of the imaging apparatus. Other numerical studies of dynamical phenomena in these gases also showed that solitons are easily formed as a side effect whenever the gas is violently perturbed [215, 216], which also indicates that solitons are a natural and easily created phenomenon.

Our simulations showed spontaneously forming solitons both in the uniform and the trapped one-dimensional gas, as well as in an elongated but three-dimensional trapped gas. At low temperatures below μ, only shallow grey solitons that are difficult to distinguish from other excitations are seen.

In particular, we investigated the energy-momentum relation for the observed density dips, and by comparison with known dispersion curves [218, 219] confirmed the interpretation of the dips as solitons. Importantly, this also confirmed their interpretation as the type II excitations of Lieb [217], which was previously suspected [218–221], but was never demonstrated in a spontaneous thermal state. hence, the thermal equilibrium state in one-dimensional gases can, then, be interpreted as a remarkable case of the coexistence of two kinds of bosonic excitations – Bogoliubov phonons, and type II Lieb excitations. Indeed, along with the solitons, many other excitations are also seen.

Furthermore, we also demonstrated the presence of large density fluctuations (up to 40%) in the quasicondensate state. Until now it was usually thought that the quasicondensate is sufficiently described by purely phase fluctuations, as was captured in the Petrov-Shlyapnikov model [143, 222]. The reason for the discrepancy and the long time before its discovery is the fact that phase and density fluctuations are only weakly couple here. The density fluctuates on the healing length scale that is hard to observe experimentally, so that experiments to date have been well described by the simple model that includes only phase fluctuations.

Our results are close to and compatible with the level of thermal fluctuations that can be calculated from the exact Yang and Yang model [186] after taking into account a correction that subtracts the zero-temperature shot noise that cannot be described with classical fields. We confirmed thus that the thermal fluctuations calculated with the classical fields method agree with the Yang and yang solution in the local density approximation. This is an important test of the correctness of the classical fields approach because it depends on deviations from ideal gas results to a degree much greater than previous checks.

We described two ways in which one can obtain experimental confirmation of the presence of solitons despite insufficient imaging resolution to resolve a single soliton dip *in situ*. One way is to count density dips only in the very outer edges of the cloud where solitons are relatively deeper and also wider (this approach catches only deep solitons that can make it so close to the edge of the cloud). The second approach relies on the analysis of the statistics of phase jumps in the cloud. A Gaussian distribution indicates a lack of deep solitons (it comes about merely as a consequence of summing many small phase shifts caused by phonons), while a distribution with visibly broader tails indicates already the presence of solitons. This criterion is robust to loss of resolution, including up to many soliton widths.

Generally, our discovery of the soliton phase has met with quite large interest in the community.

6 Other scientific achievements

6.1 Research grants led

VII 2013 – VII 2018 **National Science Centre (NCN) grant 2012/07/E/ST2/01389**
Procesy spontaniczne w ultrazimnych gazach o niezerowej temperaturze.
(Spontaneous processes in ultracold gases at nonzero temperatures).
(1458K PLN ≈ 350K €)

XII 2010 – III 2013 **Polish Government (MNiSW) grant 1697/7PRUE/2010/7**
Charakteryzacja podstawowych elementów dynamiki kondensatów Bosego-Einsteina poza przybliżeniem pola średniego. (Characterisation of the basic elements of BEC dynamics beyond the mean field).
(239K PLN ≈ 60K €)

IX 2010 – VIII 2012 **National Science Centre (NCN) grant N N202 128539**
Dynamiczne zmiany koherencji w gazach kwantowych.
(Dynamic changes of coherence in quantum gases).
(169K PLN ≈ 42K €)

IV 2010 – III 2013 **E.U. 7th Framework program research grant PERG06-GA-2009-256291**
Quantum Dynamics.
(45K €)

IV 2007 – III 2009 **Marie Curie Intra-European Fellowship MEIF-CT-2006-041390**
QuantumGases.
(152K €)

II 2001 – IV 2001 **University of Queensland Graduate School Research Travelling Award.**
For a research visit to Prof. Keith Burnett in Oxford University, and Prof. Ryszard Horodecki, at the University of Gdańsk.
(5K AU$ ≈ 4K €)

Partner in overseas research projects:

I 2013 – XII 2015 **Australian Research Council (ARC) project DP130100949**
Quantum properties of high-spin ultra-cold matter.
2 Chief Investigators (Swinburne University of Technology),
1 Partner Investigator from IF PAN
(20K AU$ ≈ 14K € for collaboration with IF PAN within the project)

6.2 Prizes for scientific research

6 XII 2010 r.
The Stefan Pieńkowski Prize of the Polish Academy of Sciences in the field of physics for the year 2010.
Awarded by the III Division: Mathematical, Physical, and Chemical Sciences, for a series of articles on ultra-cold bosonic gases.
(articles [H1,H2,H3,P29] in the labelling used here).

6.3 Conference presentations

See `http://info.ifpan.edu.pl/~deuar/talks/talks_deuar.html`

6.3.1 Invited talks

1. *Complete quantum dynamics of bosons and spins in phase-space with the help of noise*,
   P. Deuar,
   Advances in time-dependent methods for quantum many-body systems, (ECT*, Trento, Italy, 14-18 October 2013).

2. *Nonclassical atom pairs in collisions of Bose-Einstein condensates*,
   P. Deuar,
   2nd Poznan Workshop on Quantum Engineering, Quantum Information, and Semi-Quantum Biology (QEIB2012) (Poznan, Poland, 16-18 October 2012).

3. *Violation of the Cauchy-Schwarz inequality with matter waves*,
   P. Deuar,
   Quantum Technologies Conference III (Warsaw, Poland, 10-14 September 2012).

4. *Quantum dynamics of correlated atom pairs using the positive-P method*,
   P. Deuar,
   Workshop "Correlated atomic pairs" (Palaiseau, France, 2-3 April 2012).

5. *Bogoliubov quantum dynamics at $T \geq 0$ (even without a condensate)*,
   P. Deuar,
   FINESS 2011 Finite-Temperature Non-Equilibrium Superfluid Systems (Heidelberg, Germany, 18-21 September 2011).

6. *Simulations of incoherent atom dynamics in supersonic BEC collisions*,
   P. Deuar,
   CIGMA Workshop (TU Darmstadt, Darmstadt, Germany, 18-19 February 2010).

7. *The superfluidity of dipolar Fermi gases*,
   P. Deuar,
   Quantum Optics VII conference (Zakopane, Poland, 8-12 June 2009).

8. *Excitations of ultracold Fermi dipolar gases*,
   P. Deuar
   Workshop on Dipolar Quantum Gases (Université Paris-Nord XIII, Villetaneuse, France, 25 June 2008).

6.3.2 Other oral presentations

9. *Solitons as the early stage of quasicondensate formation during evaporative cooling*,
   P. Deuar, E. Witkowska, M. Gajda, K. Rzążewski,
   DAMOP11 Meeting of the American Physical Society (Atlanta, GA, USA, 13-17 June 2011).

10. *Solitons as the early stage of quasicondensate formation during evaporative cooling*,
    P. Deuar, E. Witkowska, M. Gajda, K. Rzążewski,
    LPHYS'11 20th International Laser Physics Workshop (Sarajevo, Bosnia and Herzegovina, 11-15 July 2011).

11. *Superfluid excitations of dipolar Fermi gases*,
P. Deuar, M. A. Baranov, G. V. Shlyapnikov,
March Meeting of the American Physical Society (Pittsburgh, PA, USA, 16-20 March, 2009).

12. *Excitations in dipolar Fermi gases below BCS critical temperature*,
P. Deuar, M.A. Baranov, G.V. Shlyapnikov,
LPHYS'08 17th International Laser Physics Workshop (NTNU, Trondheim, Norway, 30 June – 4 July 2008).

13. *A controlled transition from classical field simulations to full quantum dynamics*,
P. Deuar,
DAMOP08 Meeting of the American Physical Society (Pennsylvania State University, State College, PA, USA, 27-31 May 2008).

14. *Simulating the quantum dynamics and correlations of many interacting bosons beyond the GP equation*,
P. Deuar, P. D. Drummond,
International Workshop "Quantum Gases" 2007 (Institut Henri Poincaré, Paris, France, 23 April - 20 July 2007).

15. *First-principles simulation of interacting Bose gases using stochastic gauges*,
P. Deuar, P. D. Drummond and K. V. Kheruntsyan,
Quantum Limited Atom Optics workshop (Hannover, Germany, 8-12 March 2004).

16. *First-principles simulations of Bose gases using stochastic gauges*,
P. Deuar, P. D. Drummond, and K. V. Kheruntsyan,
Soliton and many-body quantum simulations workshop (Veilbronn, Germany, 11-12 December 2002).

17. *First-principles simulations of 1D Bose gases using stochastic gauges*,
P. Deuar, P. D. Drummond, and K. V. Kheruntsyan,
ACOLS 2001 Australasian Conference on Optics, Lasers and Spectroscopy (Brisbane, Australia, 3-6 December 2001).

6.3.3 Poster presentations

18. *Quantum quenches of dilute Bose gases in 1D, 2D, 3D, at zero and finite temperatures*,
T. Świsłocki, M. Stobińska, **P. Deuar**,
FINESS 2011 Finite-Temperature Non-Equilibrium Superfluid Systems (Queenstown, New Zealand, 16-20 February 2013).

19. *Spontaneous solitons in the thermal equilibrium of a quasi-one-dimensional Bose gas*,
P. Deuar, E. Witkowska, M. Gajda, T. Karpiuk, M. Brewczyk, P. Bienias, K. Pawłowski, K. Rzążewski,
Dynamics and Thermodynamics in Isolated Quantum Systems (KITP, Santa Barbara, USA, 20-24 August 2012).

20. *Spontaneous solitons in the thermal equilibrium of a quasi-one-dimensional Bose gas*,
P. Deuar, E. Witkowska, M. Gajda, T. Karpiuk, M. Brewczyk, P. Bienias, K. Pawłowski, K. Rzążewski,
Lyon BEC 2012 Theory of Quantum Gases and Quantum Coherence (Lyon, France, 5-8 June 2012).

21. *Tractable Bogoliubov dynamics of non-equilibrium systems in a positive-P representation*,
P. Deuar, K. V. Kheruntsyan, M. Trippenbach, P. Ziń,
EuroQUAM 2010 Cold Quantum Matter Achievements and Prospects (Ischgl, Austria, 12-16 September 2010).

22. *Obtaining complete quantum dynamics via a controlled extrapolation from semiclassical methods*,
P. Deuar,
FINESS 2009 Finite-Temperature Non-Equilibrium Superfluid Systems (Durham, UK, 14-17 September 2009).

23. *Superfluidity and excitations in fermionic dipolar gases*,
P. Deuar, M. A. Baranov, G. V. Shlyapnikov,
Conference on Research Frontiers in Ultra-Cold Atoms (ICTP, Trieste, Italy, 4-8 May 2009).

24. *Superfluidity and excitations in fermionic dipolar gases*,
P. Deuar, M.A. Baranov, G.V. Shlyapnikov,
Frontiers of degenerate quantum gases conference (Tsinghua University, Beijing, China, 20-24 October 2008).

25. *A controlled transition from semiclassical to complete quantum dynamics for atomic gases*,
P. Deuar,
Frontiers of degenerate quantum gases conference (Tsinghua University, Beijing, China, 20-24 October 2008).

26. *Correlations in 1D Bose gases at ranges shorter than "long"*,
P. Deuar, K.V. Kheruntsyan, P.D. Drummond,
LT25 25th International Conference on Low Temperature Physics (Amsterdam, Netherlands, 6-13 August 2008).

27. *First-principles quantum dynamics of a colliding BEC with 150 000 atoms*,
P. Deuar, P. D. Drummond,
Quantum Optics VI (Krynica, Poland, 13-18 June 2005).

28. *Stochastic gauges in quantum dynamics for many-body simulations*,
P. Deuar, P. D. Drummond,
CCP 2000 Conference on Computational Physics (Gold Coast, Australia, 3-8 December 2000).

6.3.4 As a co-author *(presenting author in bold)*

29. *Dark solitons in quasi one dimensional Bose gas*,
K. Rzążewski, M. Gajda, M. Brewczyk, P. Deuar, P. Bienias, K. Pawlowski, E. Witkowska, T. Karpiuk,
CQO X Rochester Conference on Coherence and Quantum Optics (Rochester NY, USA, 17-19 June 2013). Talk.

30. *Solitons as the early stage of quasicondensate formation during evaporative cooling*,
E. Witkowska, P. Deuar, M. Gajda, K. Rzążewski,
FINESS 2011 Finite-Temperature Non-Equilibrium Superfluid Systems (Heidelberg, Germany, 18-21 September 2011). Poster.

31. *Quantum atom optics with metastable helium: squeezing and phase matching*,
J-C. Jaskula, M. Bonneau, V. Krachmalnicoff, V. Leung, G. B. Partridge, **D. Boiron**, C. I. Westbrook, P. Deuar, P. Ziń, M. Trippenbach, K. V. Kheruntsyan,
EuroQUAM 2010 Cold Quantum Matter Achievements and Prospects (Ischgl, Austria, 12-16 September 2010). Poster.

32. *Ab initio simulations of collisions of Helium condensates*,
K. Kheruntsyan, P. Deuar, V. Krachmalnicoff, J-C. Jaskula, G. Partridge, M. Bonneau, D. Boiron. C.I. Westbrook,
FINESS 2009 Finite-Temperature Non-Equilibrium Superfluid Systems (Durham, UK, 14-17 September 2009). Poster.

33. *Excitation of Rydberg atoms in an ultracold gas by a rotary echo sequence*,
S. Wüster, C. Ates, T. Pohl, P. Deuar, J.F. Corney, J.M. Rost,
DPG 73rd Annual Meeting of the German Physical Society (Dresden, Germany, 22-27 March 2009). Poster.

34. *Stochastic gauge theory for quantum many-body problems*,
S. Wüster, C. Ates, T. Pohl, P. Deuar, J.F. Corney, J.-M. Rost,
International workshop on "Atomic Physics" (MPIPKS, Dresden, Germany, 24-28 November 2008). Poster.

35. *First-principles quantum dynamics with 150,000 atoms: Correlations in a BEC collision*,
P. Deuar, **P. D. Drummond**,
IQEC International Quantum Electronics Conference (Munich, Germany, 17-22 June 2007). Poster.

36. *First-principles quantum simulations of interacting Bose gases*,
P. D. Drummond, P. Deuar,
CCP 2004 Conference on Computational Physics (Genoa, Italy 1-4 September 2004). Poster.

37. *Stochastic gauge: a new technique for quantum simulations*,
P. D. Drummond, P. Deuar, J. F. Corney, K. V. Kheruntsyan,
ICOLS 2003 16th International Conference on Laser Spectroscopy (Palm Cove, Australia, 13-18 July 2003). Talk.

38. *Stochastic gauge simulations of Bose gases*,
P. D. Drummond, P. Deuar, K. Kheruntsyan,
IQEC 2002 International Quantum Electronics Conference (Moscow, Russia, 22-28 June 2002). Talk.

39. *Canonical ensembles using stochastic gauge equations*,
P. D. Drummond, P. Deuar,
2nd Mathematical Physics Winter Workshop (Coolangatta, Gold Coast, 5-8 July 2001). Talk.

40. *Entangling quantum copiers: An application to improving detection efficiency*,
W. J. Munro, P. Deuar,
QELS 2000 Quantum electronics and Laser Science Conference (San Francisco, California, USA, 7-12 May 2000). Poster.

41. *Contradiction of quantum mechanics with local hidden variables for quadrature phase amplitude measurements*,
M. D. Reid, P. Deuar, A. Gilchrist,
IQEC 1998 International Quantum Electronics Conference (San Francisco, California, USA, 3-8 May 1998). Talk.

6.4 Other invited talks *(outside of the employing institution)*

- *Correlated atom pairs in collisions of BECs: from nonclassical states to Bell test proposals*,
Institut Für Theoretische Physik, Leibniz Universität Hannover, Germany, 14 August 2013.

- *Phase and density correlations in Bose gases after a quantum quench*,
Dept. of Physics and Astronomy, McMaster University, Hamilton OT, Canada, 25 March 2013.

- *Phase and density correlations in Bose gases after a quantum quench*,
BEC Seminar, CFT PAN, Warsaw, Poland, 14 November 2012.

- *Quantum dynamics of correlated atom pairs*,
Faculty of Engineering & Industrial Sciences, Swinburne University of Technology, Melbourne, Australia, 18 April 2012.

- *Soiltons as the early stage of quasicondensate formation during evaporative cooling*,
Department of Physics, University of Queensland, Brisbane, Australia, 17 April 2012.

- *Bogoliubov quantum dynamics for uncondensed atom clouds at* $T \gg 0$,
Optical Seminar, Dept. of Physics, University of Warsaw, Poland, 20 October 2011.

- *Solitons and phase domains during the cooling of a one-dimensional ultra-cold gas*,
Dept. of Physics and Astronomy, McMaster University, Hamilton OT, Canada, 23 June 2011.

- *Szczegółowy wgląd w proces chłodzenia jedno-wymiarowego gazu bozonów*,
(A detailed look at the process of evaporative cooling of a one-dimensional Bose gas)
Institute of Physics, Jagiellonian University, Kraków, Poland, 18 April 2011.

- *Chłodzenie jedno-wymiarowego gazu bozonów*,
(Cooling a one-dimensional Bose gas)
Optical Seminar, Dept. of Physics, University of Warsaw, Poland, 14 April 2011.

- *Dynamika kwantowa ultra-zimnych gazów*,
(The quantum dynamics of ulra-cold gases)
Konwersatorium IF PAN, Warsaw, Poland, 1 March 2011.

- *Bogoliubov dynamics and the dissection of a condensate*,
  BEC Seminar, CFT PAN, Warsaw, Poland, 17 November 2010.

- *Two body correlations vs. Single experiment snapshots*,
  BEC Seminar, CFT PAN, Warsaw, Poland, 12 May 2010.

- *Two body correlations vs. Single experiment snapshots*,
  BEC Seminar, CFT PAN, Warsaw, Poland, 12 May 2010.

- *Simulating quantum dynamics in colliding Bose-Einstein Condensates "directly" from the microscopic Hamiltonian*,
  School of Mathematics and Statistics, Newcastle University, Newcastle, UK, 13 November 2009.

- *Nadciekłość gazów fermionowych dipoli*,
  (The superfluidity of a gas of fermionic dipoles)
  Institute of Physics, Jagiellonian University, Kraków, Poland, 26 October 2009.

- *Naddźwiękowe zderzenia kondensatów i jak oblicza się występującą tam dynamikę*,
  (Supersonic condensate collisions, and how to calculate its dynamics)
  BEC Seminar, CFT PAN, Warsaw, Poland, 21 October 2009.

- *Kolizje Kondensatów BEC i symulacja mikroskopowej dynamiki kwantowej*,
  (BEC collisions and the simulation of microscopic quantum dynamics)
  Optical Seminar, Dept. of Physics, University of Warsaw, Poland, 9 October 2009.

- *BEC collisions – Quantum dynamics simulation in a macroscopic system*,
  ENS-Lyon, Lyon, France, 2 July 2009.

- *The superfluidity of dipolar Fermi gases*,
  Los Alamos National Laboratory, New Mexico, USA, 26 March 2009.

- *The superfluidity of dipolar Fermi gases*,
  University of Virginia, Charlottesville VA, USA, 23 March 2009.

- *Superfluid dipolar Fermi gases and their excitations*,
  Seminarium BEC, CFT PAN, Warsaw, Poland, 9 January 2008.

- *Dynamics of quantum correlations in BECs from first principles*,
  Van der Waals-Zeeman Instituut, Universiteit van Amsterdam, Netherlands, 12 December 2005.

- *First-principles simulations of interacting Bose gases*,
  Dept. of Physics, Nicolaus Copernicus University, Toruń, Poland, 10 May 2004.

- *First principles quantum simulations of interacting Bose gases*,
  BEC Seminar, CFT PAN, Warsaw, Poland, 27 March 2003.

- *Simulating the quantum dynamics of a Bose-Einstein condensate*,
  University of Gdańsk, Poland, 6 April 2001.

- *Simulating the quantum dynamics of a BEC*,
  Clarendon Lab, University of Oxford, United Kingdom, 5 Apr 2001.

7 Teaching, outreach, and international cooperation

7.1 Teaching

7.1.1 Lectures

III	2010 – IV	2009	*Simulating the quantum dynamics of boson gases using the positive-P method*, a series of 3 lectures at the Physics Department, University of Warsaw.
XI	2009 – XII	2009	"Współczesne Problemy Fizyki" *(Contemporary problems in physics)*, lectures to 5th year students, Warsaw University of Technology.
IX	2009		*Ultracold Fermi Gases*: Lectures at the CIKAS summer school on Quantum Engineering, Warsaw University.

7.1.2 Tutorials, Exercises

X	2009 – I	2010	Tutorials "Mechanika Kwantowa" *(Quantum mechanics)*, 4th year , Cardinal Stefan Wyszyński University in Warsaw
	1998 –	2000	Tutorials and lab exercises in physics and engineering, 1st year students, University of Queensland, Australia.

7.1.3 Supervision of student researchers

- I informally take part in supervising Mr Ray Ng, a PhD student of Prof. Erik Sørensen from McMaster University in Canada. Our collaboration in this respect began in the second half of 2009. Mr Ng's MSc and, later, PhD research concerns primarily the application of phase space methods (in which I am an expert) to spin systems (in which Prof. Sørensen is an expert). As part of our cooperation, Mr Ng has twice visited IF PAN (X 2010, XI 2012), and I have also paid two working visits to McMaster University (VI 2011, III 2013). We recently published our first joint paper [H9].

- In several calendar years I took scientific care of winners of the "First Step to Nobel Prize in Physics" competition, who as part of the prize would come to the IF PAN institute for a month of research experience. They were young students who has just finished high school or were just starting their first year at university. We prepared the research from their prize-winning contribution to the competition for publication in scientific journals, and I introduced them to some relatively simple research tasks. They were, in chronological order:

  1. 2009: Ms Hadass Tzaban from the Ulpenat Bnei Akiva school, Netivot, Israel.
     Contribution title: *Turbulent convection in sciences and nature.*
  2. 2010: Mr Eli Gudinetsky from the Religious Comprehensive "Amit" High School / Ben-Gurion University of the Negev, Be'er-Sheva, Israel.
     Contribution title: *Theoretical Study of the Generation of Large - Scale Turbulence with Homogeneous Wind Shear.*
  3. 2011: Mr Ivan Maslov from the Chelyabinsk Physics-Mathematical Lyceum 31.
     The research was published as *Deformation of high-speed meteor bodies by the atmosphere*, I. V. Maslov, A. V. Gorshkov, European Journal of Physics **33**, S17 (2012).

7.2 Conference organisation

- I am a co-organiser of the annual international *Quantum technologies* conference series in the field of ultra-cold gases and quantum information theory, since its inception. To date there have been four meetings in the years 2010, 2011, 2012, 2013. The conferences are organised in various locations in Poland, and attract a large international contingent that constitutes slightly more than half of the participants. In 2013 there were about 60 participants in total.

- In 2000, I helped organise the *CCP 2000 Conference on Computational Physics*, in the Gold Coast, Australia, on 3-8 December 2000.

- I have been chosen as the *Local Organiser and Chair* of the next edition of the cycle of bi-annual international FINESS conferences (Finite-Temperature Non-Equilibrium Superfluid Systems) which I will be organising in Poland in autumn 2015. These are some of the most important world conferences in my subfield of the quantum dynamics of many-body systems. Past participants included Nobel laureates in our field such as - Prof. William Phillips. The conferences have been organised since 2007 (2007 Copenhagen, 2009 Durham, England, 2011 Heidelberg, 2013 Queenstown, New Zealand) and usually attract about 100 participants.

7.3 International cooperation

7.3.1 International research collaborations

Currently active

- Institut d'Optique, Palaiseau, France: Chris Westbrook, Alain Aspect, Denis Boiron and their PhD students: Jean-Christophe Jaskula, Guthrie Partridge, Marie Bonneau, Josselin Ruaudel, Rafael Lopes, Valentina Krachmanicoff, Vanessa Leung

- McMaster University, Hamilton, Canada: Erik Sørensen, Ray Ng, Duncan O'Dell.

- University of Queensland, Brisbane, Australia: Karen Kheruntsyan, Tod Wright.

- Technische Universität Wien, Vienna, Austria: Jorg Schmiedmayer and PhD students: Tim Langen, Max Kuhnert.

- Swinburne University of Technology, Melbourne, Australia: Peter Drummond, Margaret Reid, and PhD students: Laura Rosales-Zarate, Simon Kiesewetter

- Newcastle University, England: Nikolaus Proukakis and PhD students: Stuart Cockburn, Donatello Gallucci.

- University of Amsterdam, Netherlands: Miłosz Panfil.

- Universitat de Barcelona, Spain: Miguel Garcia-March.

- Colorado School of Mines, Golden, USA: Lincoln Carr.

- Leibniz Universität Hannover, Germany: Temo Vekua.

- BEC center, Universita di Trento: Italy: Marek Tylutki.

- Université Paris Diderot VII, France: Giuliano Orso.

Active in the past

- Université Paris-sud XI, Orsay, France: Gora Shlyapnikov.
- University of Innsbruck: Mikhail Baranov.
- Max Planck Institute for Physics of Complex Systems, Dresden, Germany: Sebastian Wuster.
- University of Birmingham, England: Dmitry Gangardt.
- National University of Singapore: Tomasz Karpiuk.
- University of Virginia, Charlottesville, USA: Vanessa Leung.
- University of Queensland, Brisbane, Australia: Joel Corney, Matthew Davis, Bill Munro, Kae Nemoto, Gerard Milburn.

7.3.2 Research experience gained overseas

- PhD studies and earlier undergraduate study at the University of Queensland, Brisbane, Australia: 1993-1996, 1998-2005. In this time, and also since 1983 I lived in Australia. My supervisor during my PhD was Prof. Peter Drummond, and supporting supervisors were Dr. William Munro, later Dr. Karen Kheruntsyan. My *Honours thesis* supervisor was Dr. Margaret Reid.
- Postdoc at the Van der Waals-Zeeman Instituut, Universiteit Van Amsterdam, in The Netherlands in 2006-2007. The head of the group was Prof. Jook Walraven, my direct superior was Dr. Mikhail Baranov.
- Marie Curie Fellow at the Université Paris-sud XI (LPTMS instutite), Orsay, France in 2007-2009. I was employed from my own EU grant money for independent research with Prof. Georgy Shlyapnikov in an oversight role. After finishing the two year Fellowship, I continued research as a scientific visitor at the same institution for several more months.
- Applied engineering research in Deuar Pty. Ltd. in Brisbane, Australia. This is a small engineering R&D business run by my father. The research concerned analysis of the behaviour of in-service wooden electricity power poles when a test force is applied with special hydraulic apparatus. The force is applied to determine the strength of the pole *in situ* based on measurements of its deflection under the strain. The research was funded by the Australian research grant: AusIndustry R&D Start Agreement *Integrated System for comprehensive testing of in-situ Power Poles for strength and longevity* (2003-2005).
- Visiting Academic, University of Queensland, Brisbane, Australia (1 month, V 2012).
- Short-term research visits:
  - Leibniz Universität Hannover, Germany (several days VII 2013).
  - McMaster University, Canada (1 week III 2013).
  - University of Queensland, Brisbane, Australia (2 weeks III 2013).
  - Swinburne University of Technology, Melbourne, Australia (2 days V 2012).
  - McMaster University, Canada (2 weeks VI 2011).
  - Institut d'Optique, Palaiseau, France (1 week V 2011).
  - Institut d'Optique / Université Paris-sud XI, Palaiseau / Orsay, France (2 weeks VI 2010).

– Newcastle University, England (1 week XI 2009).
– ENS-Lyon, France (several days VII 2009).
– Los Alamos National Laboratory, New Mexico, USA, (1 week III 2009).
– University of Virginia, Charlotteville, USA, (several days, III 2009).
– Boston University, USA (several days VI 2008).
– Erlangen University, Germany (several days XII 2002).
– Erlangen University, Germany (1 week VIII 2002).
– Universytet Gdański, Poland (1 month, IV 2001).
– University of Oxford, England (1 week IV 2001).

7.3.3 Membership of scientific societies

- American Physical Society (since 2008)

7.4 Refereeing

7.4.1 Grant proposals

- For the National Science Centre *(Narodowe Centrum Nauki)* (23 projects since 2011).
- For the Research Executive Agency (European Commission) (19 projects since 2013).

7.4.2 Publications

- 20 for Physical Review Letters (2002-2013).
- 17 for Physical Review A (2002-2013).
- 11 for Journal of Physics B (2009-2014).
- 4 for Journal of Physics A (2008-2012).
- 3 for EPL (2010,2011,2012).
- 3 for New Journal of Physics (2009,2011,2013).
- 2 for Physical Review E (2002,2003).
- 1 for Electronic Journal of Theoretical Physics (EJTP) (2006).
- 1 for Physical Review B (2007).
- 1 for Optics Express (2010).
- 1 for Annals of Physics (2012).

In total: 64

7.5 Grant assessment panels

- Panel of experts of the National Science Centre *(Narodowe Centrum Nauki)* – for the assessment of research proposals (panel ST-2 – basic elements of matter) (August 2011)
- Panel of experts of the European Commission (for the Research Executive Agency) – for the assessment of research proposals for FP7 Marie Curie Fellowships (panel PHY – physics) (September 2013)

- Newcastle University, England (1 week XI 2009).
- ENS-Lyon, France (several days VII 2009).
- Los Alamos National Laboratory, New Mexico, USA, (1 week III 2009).
- University of Virginia, Charlotteville, USA, (several days, III 2009).
- Boston University, USA (several days VI 2008).
- Erlangen University, Germany (several days XII 2002).
- Erlangen University, Germany (1 week VIII 2002).
- Universytet Gdański, Poland (1 month, IV 2001).
- University of Oxford, England (1 week IV 2001).

7.3.3 Membership of scientific societies

- American Physical Society (since 2008)

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7.4.1 Grant proposals

- For the National Science Centre *(Narodowe Centrum Nauki)* (23 projects since 2011).
- For the Research Executive Agency (European Commission) (19 projects since 2013).

7.4.2 Publications

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- 17 for Physical Review A (2002-2013).
- 11 for Journal of Physics B (2009-2014).
- 4 for Journal of Physics A (2008-2012).
- 3 for EPL (2010,2011,2012).
- 3 for New Journal of Physics (2009,2011,2013).
- 2 for Physical Review E (2002,2003).
- 1 for Electronic Journal of Theoretical Physics (EJTP) (2006).
- 1 for Physical Review B (2007).
- 1 for Optics Express (2010).
- 1 for Annals of Physics (2012).

In total: 64

7.5 Grant assessment panels

- Panel of experts of the National Science Centre *(Narodowe Centrum Nauki)* – for the assessment of research proposals (panel ST-2 – basic elements of matter) (August 2011)
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P. Deuar
22/3/2014

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