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Coherence and many-body effects in the transport of Bose–Einstein condensates

by
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Abstract

This thesis presents investigations on the interplay of coherence and many-body effects in the quasi one-dimensional transport of Bose–Einstein condensates (BEC) through scattering potentials. Such configurations can be realized with guided atom lasers that provide a coherent atomic beam. An exact theoretical description of the dynamics is out of reach due to the presence atom-atom interactions. Different levels of approximations are nevertheless possible with their strengths and weaknesses. The mean-field approximation, where the dynamics of the BEC is governed by the Gross–Pitaevskii equation, is most commonly used in the field of ultracold atoms.

In this thesis the *truncated Wigner method* is used to go beyond the standard Gross–Pitaevskii description. This method is adapted in order to study the scattering of Bose–Einstein condensates in one-dimensional waveguides where atom-atom interactions and external potentials are nonvanishing only in a finite region of space. In this case, the truncated Wigner method is combined with the smooth exterior complex scaling method and incorporates *quantum noise* that originate from the vacuum fluctuations in the waveguide. *Inelastic scattering* is shown to play a major role in the resonant transport of BEC through a symmetric double potential barrier effectively forming an atomic quantum dot. Indeed, fully resonant transmission is prohibited and incoherent atoms as well as collective oscillations are detected in the transmitted beam. It is also shown that inelastic scattering destroys Anderson localization in the case of transport through disordered potentials. The classical (incoherent) ohmic transmission is recovered for finite atom-atom interactions.

The validity of the truncated Wigner method is then assessed using the semiclassical van Vleck–Gutzwiller propagator in the Fock space of the many-body system. It is shown that the truncated Wigner method corresponds to the so-called diagonal approximation, and it is possible to identify the leading correction to the truncated Wigner results, which is provided by the so-called *coherent backscattering* (CBS) contribution. Coherent basckattering in Fock space is a genuine quantum many-body effect that lies beyond the reach of any mean-field approach. For the case of closed Bose–Hubbard models, the relevance of CBS is confirmed by numerically comparing the (classical) truncated Wigner evolution probabilities to the exact quantum probabilities in Bose–Hubbard models: While a CBS-induced enhancement of the return probability to the initial state is clearly seen in the exact quantum simulations of the bosonic many-body system, this enhancement is absent in the classical calculations. The magnitude and dependence of the CBS contribution on gauge fields, which break time-reversal invariance, is numerically confirmed. For the case of disordered open systems, it can be shown that this contribution as well as next-to leading order contributions vanish thereby confirming the validity of the truncated Wigner method.

Résumé

Cette thèse présente les investigations réalisées sur la relation entre les effets à plusieurs corps et la coherence lors de phénomènes de transport quasi-unidimensionels de condensats de Bose–Einstein (CBE) à travers divers potentiels de diffusion. De telles configurations peuvent être réalisées avec des lasers à atomes qui créent des faisceaux coherents de matière. Une description exacte de la dynamique à plusieurs corps est hors de portée à cause des interactions entre atomes. Malgré tout, différents niveaux d'approximation sont possibles, chacun possédant leurs forces et faiblesses. L'approximation en champ moyen, où la dynamique du CBE est régie par l'équation de Gross–Pitaevskii, est la plus utilisée dans le domaine des atomes ultrafroids.

Dans cette thèse, la *méthode de Wigner tronquée*, qui est une amélioration de la description fournie par l'équation de Gross–Pitaevskii, est utilisée.

Cette méthode est adaptée pour l'étude de la diffusion de condensats de Bose–Einstein dans des guides d'ondes unidimensionels où les interactions entre atomes et les potentiels extérieurs ont un support fini. Dans ce cas, la méthode de Wigner tronquée est combinée avec la méthode de *dilatation complexe extérieure lissée* (smooth exterior complex scaling) et avec du *bruit quantique*, provenant des fluctuations quantiques dans le guide d'onde. Les effets, non négligeables, des *collisions inélastiques* sont mis en évidence lors du transport résonnant d'un CBE à travers une double barrière de potentiel symétrique formant un point quantique. En effet, une transmission résonnante parfaite est prohibée et des atomes incoherents ainsi que des oscillations collectives sont détectées dans le faisceau atomique transmis. Il est aussi démontré que la diffusion inélastique est responsable de la destruction de la localisation d'Anderson dans le cas du transport à travers des potentiels désordonnés. Une transmission ohmique (incohérente) est retrouvée pour des interactions finies entre atomes.

La validité de la méthode de Wigner tronquée est évaluée en utilisant le propagateur semiclassique de van Vleck–Gutzwiller dans l'espace de Fock du sytème à plusieurs corps. Il est démontré que la méthode de Wigner tronquée correspond à l'approximation diagonale et qu'il est possible d'identifier la correction dominante appellée *rétrodiffusion cohérente*. La rétrodiffusion cohérente dans l'espace de Fock est un effet à plusieurs corps purement quantique et ne peut être reproduite par aucune théorie en champ moyen. L'analyse numérique des probabilités de transitions quantiques pour des systèmes de Bose–Hubbard confirme la présence de rétrodiffusion cohérente alors qu'elle est absente pour des simulations utilisant la méthode (classique) de Wigner tronquée. L'amplitude ainsi que la dépendance vis-à-vis d'un champ de jauge de la contribution de rétrodiffusion cohérente est confirmée numériquement. Dans le cas de systèmes ouverts désordonnés, il a été montré que la rétrodiffusion cohérente ainsi que les corrections d'ordre supérieur sont inexistantes, confirmant la validité de la méthode de Wigner tronquée.

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Introduction

At the end of the 19th century, nearly all experimentally observed phenomena were explained by two fundamental classical theories of physics. The evolution of a collection of particles could be predicted using Newton's law of motion if the initial positions and momentums were known. The electromagnetic nature of the world surrounding us could be described by waves, or electromagnetic fields, evolving through Maxwell's equations. Fortunately, some troubling experimental observations, and now very well understood effects, such as, *e.g.* the photoelectric effect and black-body radiation, tainted this picture.

The development of quantum mechanics in the early 20th century solved these problems by postulating that particles can be seen as waves and can be described by their associated wavefunction. The evolution of the wavefunction $\psi(\mathbf{r}, t)$ associated with one particular particle is provided by the Schrödinger equation and the wavefunction corresponds to the probability amplitude to find the particle at a particular point $\mathbf{r}$ in space at time t. One can extend this wavefunction picture to a many-body system composed of N particles by introducing a generalized many-body wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ where we dropped the time dependence for compactness. This many-body wavefunction corresponds to the probability amplitude to find particle 1 at position $\mathbf{r}_1$, particle 2 at position $\mathbf{r}_2$, etc... In the case of identical particles, it is not possible to distinguish one particle from another. As a consequence, any observable of the system should remain unchanged under particle (label) exchange. Applying two exchanges to the same pair (i, j) of particles must leave the wavefunction unchanged. We can therefore write that the wavefunction must obey

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j \ldots, \mathbf{r}_N) = \pm\psi(\mathbf{r}_1, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_N) \tag{1}$$

under particles exchange between particle i and j. This fundamental separation of particles into those for which the many-body wavefunction is invariant under particle exchange and those for which the wavefunction changes sign, depends upon a single parameter: their intrinsic spin. This is the result of the spin-statistics theorem [1]. It has to be noted that in the context of quantum field theory, the symmetry property expressed by Eq. (1) follows automatically from the (bosonic or fermionic) quantization of (*e.g.* Klein–Gordon or Dirac) the field.

Particles with half-integer spin are known as fermions. They are anti-symmetric under particles exchange and therefore correspond to the minus sign in Eq. (1). The spin-statistic theorem also states that these particles have to obey the Fermi–Dirac statistics

$$f_{\mathrm{FD}}(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1} \tag{2}$$

which gives, at thermal equilibrium, the probability that particles are occupying a single-particle state of energy ε for a system at temperature T with a chemical potential μ. On the other hand, particles with integer spin are known as bosons. They are symmetric under particle exchange and therefore correspond to the plus sign in Eq. (1). These particles obey the Bose–Einstein distribution

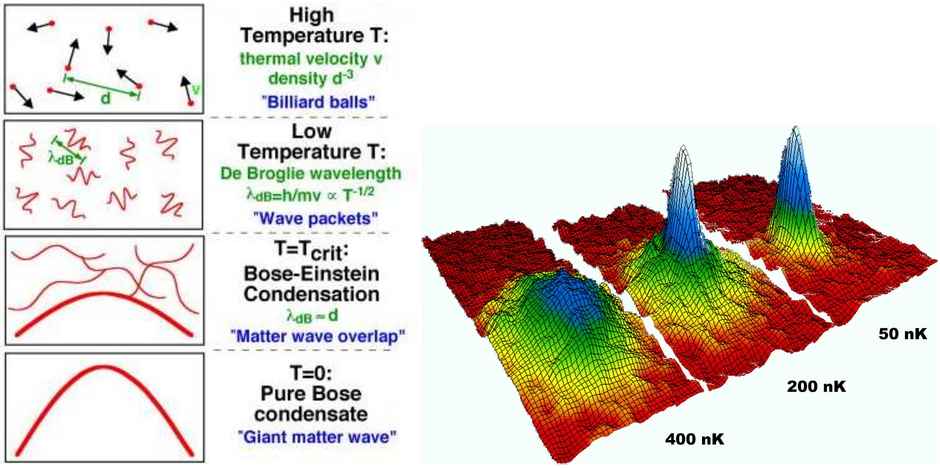
$$f_{\mathrm{BE}}(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} - 1} \tag{3}$$

and will be of interest in this thesis. Both the Fermi–Dirac and Bose–Einstein distributions are well approximated by the Maxwell–Boltzmann distribution at high temperatures, so that no differences between the two type of particles can be spotted. For the case of low temperatures, subtle differences appear.

In 1925, building on the work of Bose concerning the distributional behaviour of photons [2], Einstein formulated the Bose–Einstein distribution [3, 4]. He noted that for massive particles, as the system's chemical potential μ approaches the single-particle ground state energy ε_0 from below, the population of that state would increase to a macroscopic value. This phenomenon is known as Bose–Einstein condensation, while the particles occupying that state are collectively referred to as a Bose–Einstein condensate (BEC).

On the way towards the experimental realization of a Bose–Einstein condensate many experimental difficulties had to be overcome. One important step was the demonstration of laser cooling [5], where the temperature of neutral atoms is lowered by employing the Doppler shifts with laser beams near an atomic resonance. In addition, techniques like evaporative cooling and magneto-optical traps [6] were developed. Nowadays, temperatures in the nano-Kelvin regime can be obtained. It took 70 years to achieve, in 1995, the first Bose–Einstein condensate experimentally in dilute atomic vapor of ^{87}Rb [7], ^{23}Na [8] and ^{7}Li [9] providing a macroscopic quantum entity of the size of $\sim\mu$m. A simplified representation of the process of Bose–Einstein condensation is provided in Fig. 1(a). In Fig. 1(b) is represented the velocity distribution of an atomic Bose gas going through the Bose–Einstein condensation. Since then, a lot of other bosonic species where cooled down to Bose–Einstein condensation such as ^{1}H [10], ^{4}He* [11, 12], ^{6}Li [13], ^{7}Li [9, 13], ^{23}Na [8], ^{39}K [14], ^{41}K [15], ^{52}Cr [16], ^{85}Rb [17], ^{87}Rb [7], ^{88}Sr [18], ^{133}Cs [19, 20], ^{160}Dy [21], ^{162}Dy [21], ^{164}Dy [22], ^{170}Yb [23], ^{168}Er [24], ^{174}Yb [25]. It has to be noted that some condensates were reached using sympathetic cooling [26], thereby forming a mixture with different isotopes or even different species. It has also to be mentioned that an enormous effort has been undertaken in Liège to cool iron atoms [27–29] and a cold atomic cloud of iron has been recently obtained [30].

For the last 20 years, Bose–Einstein condensates and ultracold fermionic (degenerate) gases have been widely studied since they offer a very high accuracy and high flexibility in the control of parameters in the experiments. They allow to study new phenomena, but also to address open questions, which originated in different contexts. For example, it is possible to mimic condensed matter physics and study the BCS-BEC crossover with ultracold spin-1/2 fermions. For attractive atom-atom interaction, the atoms can undergo a BCS transition to a superfluid state of loosely bound Cooper pairs. On the other hand, for weak repulsive atom-atom interactions, they can form bosonic molecules leading to a Bose–Einstein condensate. The beauty is revealed by using Feshbash resonance, allowing to tune the atomic interaction between a repulsion and attraction [see, *e.g.*, Refs. [33, 34] for experimental realizations]. Optical lattices, which are created by a standing wave formed by counter propagating laser beams in all three spatial directions, provide a strong analogy to tight-binding model in solid-state physics. Such an optical lattice has no defects or dislocations, which are encountered in the solid state context. This setup makes it for example possible to study the transition between the Mott insulator state and the superfluid state [35, 36]. Ultracold atoms also provide



(a) **(b)**

Figure 1. (a) Simplified vision of the behaviour of a Bose gas at different temperatures. Due to de Broglie law $\lambda_{\mathrm{dB}} = h/p$, lowering the temperature increases the wavelength of the associated matter wave. Eventually, all the waves will overlap to form a "giant matter wave" at $T = 0$ K. [reproduced from [31]] (b) Images of the velocity distributions of the trapped atoms, on the left frame just before the appearance of the Bose–Einstein condensate; the center frame, just after the appearance of the condensate; the right frame, after further evaporation leaves a sample of nearly pure condensate, reproduced from [32].

a formidable playground for quantum chemistry. Again the high level of control and accuracy permits to achieve a chemical reaction from a desired initial to a desired final quantum state. For example, photoassociation was used in the Mott insulator phase of an optical lattice to form molecules [37], formation of three-body Efimov trimer states was observed [38] and also creation of deeply bound molecules has been reported [39].

Studying transport phenomena using Bose–Einstein condensates is also an active research field. This is stimulated by its analogy with electronic mesocopic transport at very low temperature where, for instance, quantization of conductance according to the Landauer–Büttiker theory [40, 41] occurs. These conductance steps have recently been experimentally observed [42] with the fermionic ^{6}Li atoms. Moreover, mesoscopic transport processes of electrons lie at the heart of the working principle of logical electronic devices such as transistors, and their understanding is therefore crucially relevant for the development of future microprocessors. While these experiments are in the weakly interacting regime, the next step in this context would consist in the exploration of interaction-related phenomena that are not present in such weakly interacting transport processes. The high degree of flexibility and control that is available in the context of ultracold atoms allows one to study such many-body phenomena with a fully tunable atom-atom interactions strength and without unwanted side effects, which in the solid-state context would be induced by phonons or magnetic impurities, for example.

From a theoretical point of view, the accurate description of interaction phenomena in the transport context represents a formidable task as it most often amounts to accounting for coherence and many-body correlation within a finite scattering geometry that is connected to noninteracting but potentially macroscopic source and drain reservoirs, see *e.g.* Ref. [43] for the most recent achievement in this direction. Up to now, studies on transport were undertaken for the quasi-stationary propagation process of a weakly interacting Bose–Einstein condensate across one- [44–47] or two-dimensional [48, 49] scattering configurations in the framework of a guided atom laser, which create a continuous beam of Bose–Einstein condensed atoms. These studies were, to a large extent, based on the mean-field approximation in terms of the nonlinear Gross–Pitaevskii equation and therefore revealed typical nonlinear transmission features that are also known from nonlinear optics. Recently, transport in the context of atom lasers was also described in the framework of the Hartree–Fock–Bogoliubov approximation [50].

Another path is taken in this thesis in order to go beyond the mean-field description of transport and thereby allowing for stronger atom-atom interaction. We use the truncated Wigner method which, in the case of transport in an atom laser configuration, amounts to a Monte-Carlo sampling of the initial quantum state by classical fields and a propagation according to a slightly modified Gross–Pitaevskii equation. The truncated Wigner method, which was, by now, only used in closed systems, is generalized in this thesis to open systems. This was done with the help of Prof. A. Saenz at the Humboldt University in Berlin. It allowed to uncover the effect of interaction on the coherence of the incoming atomic beam formed by a Bose–Einstein condensate. In particular, for the case of an atomic quantum dot, collective oscillations and inelastic scattering were detected which hinders full coherent transport.

In the same way as the mean-field approximation, the truncated Wigner method is also an approximation. The question of validity therefore rapidly arose during this work. In particular, we want to consistently identify the leading corrections to the truncated Wigner method. Together with the research team of Prof. K. Richter at the University of Regensburg in Germany, in particular with Thomas Engl and Juan-Diego Urbina, we were able to study a generic contribution beyond the truncated Wigner method in closed systems. We used a path integral formulation in the semiclassical limit to derive the van Vleck–Gutzwiller propagator in Fock space. This contribution arises due to coherent superposition (and interferences) in the underlying Fock space and bears the name of coherent backscattering. Our findings provide a better understanding of many-body thermalization and also a better understanding of subtle differences between quantum and classical ergodicity.

Fragmentation of Bose–Einstein condensates were observed during transport through quasi one-dimensional waveguide potentials engineered by atom chips [51]. This observation was explained by inhomogeneities in the atom chip resulting in a disorder potential [52–54] and stimulated the investigation of Anderson localization [55] with Bose–Einstein condensates [56–59]. In 2008, Anderson localization with Bose–Einstein condensates was demonstrated [60, 61]. This observation opened the possibility to study the effect of interaction on Anderson localization, which is, by now, a very active field. In particular, the suppression of expansion of an initially trapped interacting Bose gas was studied [62], as well as localization of Bogoliubov quasiparticles [63, 64] and also the realization of Bose glass phases [65, 66]. Investigation on the effects of interactions on Anderson localization in the context of transport have also been undertaken in the mean-field limit [44, 47] as well as with the Hartree–Fock–Bogoliubov approximation [50]. We describe the transport process across disorder potentials with the van Vleck–Gutzwiller propagator for which the truncated Wigner method is the leading order contribution. There, we find that observables that are averaged over disorder are identical to the ones obtained by the Gross–Piteavskii equation, even if inelastic scattering is not taken into account in the latter equation. We confirmed that the breakdown of Anderson localization is due to incoherent atoms and that even a very weak interaction can lead to drastic departure from the noninteracting case. Finally we showed that the next leading corrections, such as, *e.g.*, coherent backscattering, are vanishing. This essentially means that the truncated Wigner method is accurate for disorder-averaged single-particle observables.

Thesis overview — Among all the exciting topics in the framework of transport Bose–Einstein condensates systems, this thesis focuses on studying the effect of many-body interactions in beams of coherent matter waves.

In Chapter 1, we recall the basics of Bose–Einstein condensation in a trap and also recall the basics of atom-atom interactions using the Lippman-Schwinger equation. We then move to the physics behind the creation of optical lattices for Bose–Einstein condensates. Finally we set the general Hamiltonian describing the ultracold bosonic gas and introduce the well-known mean-field limit described by the nonlinear Gross–Pitaevskii equation.

In Chapter 2, we introduce the theory behind the guided atom laser and briefly describe their experimental realizations. We then directly introduce a novel scattering approach which amounts to transparent boundary conditions rendering the inherently infinite one-dimensional scattering system to a finite but open one-dimensional system. Since the use of numerical computations is required for such systems, we then introduce the smooth exterior complex scaling which is a numerical method that is more efficient than the scattering approach introduced before. Finally, we study transmission across a symmetric double barrier modelling an atomic quantum dot and show the main nonlinear features that we recognize in the transmission spectrum.

In Chapter 3, we formulate quantum mechanics in phase space, which is well known from quantum optics, and concentrate to a particular phase-space distribution, namely the Wigner distribution. We then particularize this method to guided atom laser and show the important role of quantum fluctuations in the process. This allows us to demonstrate the essential role of inelastic scattering and collective oscillations in the transport of Bose–Einstein condensate through an atomic quantum dot.

In Chapter 4, we study many-body interferences in Fock space. To do so, we first introduce the concepts of path integral formalism and propagators. In particular, we show in details the main approximations made to arrive to a semiclassical description, given by the van Vleck–Gutzwiller propagator to uncover the presence of a generic contribution going beyond the (classical) diagonal approximation, namely coherent backscattering, in a (closed) disordered Bose–Hubbard system.

In Chapter 5, we study transport of Bose–Einstein condensate through disorder potentials and in particular the Anderson localization phenomenon, which critically relies on interferences and therefore coherence. We identify, thanks to the truncated Wigner method, that atomic interactions can break Anderson localization due to the generation of incoherent atoms. In a last step, we use the van Vleck–Gutzwiller propagator to show that the diagonal approximation corresponds to the truncated Wigner method and that no other corrections to the diagonal approximation survive the disorder average for one-body observables.

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1. T. Engl, J. Dujardin, A. Arguëlles, P. Schlagheck, K. Richter, and J.-D. Urbina, "Coherent Backscattering in Fock Space: A Signature of Quantum Many-Body Interference in Interacting Bosonic Systems" Phys. Rev. Lett. **112**, 140403 (2014).
2. J. Dujardin, A. Saenz, and P. Schlagheck, "A study of one-dimensional transport of Bose–Einstein condensates using exterior complex scaling" Appl. Phys. B **117**, 765 (2014).
3. J. Dujardin, A. Arguëlles, and P. Schlagheck, "Elastic and inelastic transmission in guided atom lasers: A truncated Wigner approach" Phys. Rev. A **91**, 033614 (2015).
4. J. Dujardin, T. Engl, J.-D. Urbina, and P. Schlagheck, "Describing many-body bosonic waveguide scattering with the truncated Wigner method" arXiv:1502.02890 (2015) [submitted to Ann. Phys.].
5. J. Dujardin, T. Engl, K. Richter, and P. Schlagheck, "Breakdown of Anderson localization in the transport of BEC through 1D disordered potentials" in preparation.

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6. S. Dorbolo, D. Terwagne, R. Delhalle, J. Dujardin, N. Huet, N. Vandewalle, and N. Denkov, "Antibubble lifetime: Influence of the bulk viscosity and of the surface modulus of the mixture" Colloids Surf. A **365**, 43 (2010).

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