Coherent Structures in PDEs and Their Applications

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1 Introduction

The goal of this workshop was to bring together researchers that work on various aspects of coherent structures in PDE's. By this, we mean solution features that retain their shape and persist over time. Some of examples that were discussed in this workshop include: vortex and vortex ring structures in Bose-Einstein condensates (BEC); spikes and waves in reaction-diffusion models, and propagation of touch-down singularities in MEMS devices. A common theme was the use of mathematical tools to reduce the complexity of coherent structures by focusing on their most defining characteristics – such as for example, the dynamics of vortex or spike centers. Such reduction allows for a deeper understanding of the essential dynamics of the systems under study.

The workshop was naturally divided into several themes. In the first part of the workshop, practitioners working on BEC presented their recent findings. This included a number of theoretical talks as well as experimental results. In the second part, several participants explored properties of ODE particle models. These models often arise as reduced dynamical systems from PDE's, or as cellular automata models of the underlying processes. There was also a number of talks at the intersection of these two viewpoints.

2 Coherent structures in BECs

The first part of the workshop aimed at exploring the current state of the art and future theoretical and experimental perspectives within the context of coherent structures in Bose-Einstein condensates (BEC) [1]. BECs are typically modelled, at the mean-field level, by a nonlinear Schrödinger (NLS)-type partial differential equation (PDE). A fundamental technique in analysis of many physically relevant PDEs is to approximate their solution using appropriate basic basic building blocks from which more complex solutions can be constructed. These building blocks, which we refer to as "coherent structures", can be analyzed at a level of a reduced system and give valuable insight into the original problem. Within the realm of BECs, these coherent structures (or matter waves) take the shape of solitary waves in one dimension (1D), vortices in two dimensions (2D) or vortex rings in three dimensions (3D) [2] These structures are routinely produced experimentally and a considerable amount of theoretical studies has focused on their mathematical and computational understanding. The interactions of such localized states can be reduced to effective particle systems on the coherent structures main constitutive parameters (positions, velocities, amplitudes, widths, etc.) These effective particle systems, reducing the original PDE dynamics, often take the shape of ordinary differential equations (ODEs) on these constitutive parameters. In particular, these ODEs assume the form of modified Toda lattices in 1D, or of modified classical point-vortex dynamical equations in 2D. Such nonlinear systems of ODEs provide a valuable effective description of the behavior of the condensates. Recent mathematical studies of these ODEs have identified vibrational modes of multiple dark solitary waves in 1D and explored the bifurcations and formation of crystalline lattice structures (and its own vibrational —so-called Tkachenko— modes) for vortices in 2D in close coordination with state-of-the-art experimental results. It is important to highlight here that recent imaging techniques and the ability to externally drive/manipulate such BECs have shown a variety of interesting and novel phenomena including manifestations of symmetry breaking and nucleation events of vortex dipoles and more generally of vortex clusters. These, in turn, raise intriguing mathematical questions and offer non-trivial twists (such as the role of external traps or of anisotropy) to this classical problem of coherent structures and their interactions.

In addition to the 2D setting of vortices, the full geometry of atomic systems (such as BECs) enables the consideration of extensions to 3D. In this case, the vortices extend as elongated vortex filaments (so-called solitonic vortex), and may also acquire more elaborate S- or U- shaped forms. Perhaps most interestingly for the purposes of the ODE reductions, the vortices can "close upon themselves" assuming a vortex ring (VR) form. Such VRs present remarkable dynamics in their own right, exhibiting features such as leapfrogging between two VRs as well as elaborate oblique interactions between few, as well as many rings. Here, too, a reduction containing the dynamics of the position of the center of the ring and the coupled evolution of its radius over time enables a systematic understanding of some of these motions. Nevertheless, obtaining a deeper understanding of the modes of individual 3D vortices and VRs (the so-called Kelvin waves) and especially of the interactions between them is still very much a vibrant area of research that formed an important component of this workshop.

The workshop brought a multidisciplinary group of applied mathematicians together with experimentally oriented condensed matter/atomic physicists as well as with theoretical physicists to identify focus questions that can be jointly addressed and that are emerging as the key questions for the near future in this subject. Specifically, as it will be detailed below, some of the topics within the context of BECs that were covered in the workshop included: techniques to derive the reduced dynamical systems; the analysis of the resulting effective dynamics; numerical computations; comparison with experiments, and identification of important challenges stemming from the general theory and the concrete applications.

2.1 1D Coherent Structures in BECs

The realm of 1D structures in BECs is undoubtedly the most mathematically studied one. This is a direct consequence of the tractability for some of the existence, emergence, stability, dynamics, and interaction properties of their corresponding coherent structures. However, recent effort has been vested into refining the actual models that are used to describe the evolution in atomic BECs. In particular, it has been argued that mean-field models might not be able to capture the full behavior of BECs, particularly when (i) the system is composed of a limited number of particles (and therefore a mean-field description is not a good approximation) and/or (ii) when the BEC in not close to absolute zero temperature (where additional effects, such as thermal fluctuations, have to be taken into account). For instance, motivated by the talk of Marios Tsatsos, we discussed the possibility of describing BECs beyond the mean-field level. In particular, it is possible to study the fragmentation and quantum correlations in BECs by considering multi-configurational time-dependent Hartree methods to account for the many-body physics of BEC composed of a limited number of particles. This technique might be useful to shed light into experimental investigations in quasi-1D BECs where, e.g., a periodic modulation of the scattering length gives rise to beyond-mean-field phenomena.

Another variant to the standard mean-field model that assumes a *local* interaction is the extension to *nonlocal* interacting terms. These nonlocal terms arise, e.g., when considering BEC consisting boson with dipolar moments. In this case the local nonlinearity in the NLS equation has to be replaced by a nonlocal (nonlinear) interaction term that involves an interaction kernel through a convolution. It is important to characterize the differences in the properties of the coherent structures once the nonlocal terms are considered. Spearheaded by the work of Dimitri Frantzeskakis, we discussed asymptotic approximations for dark solitary waves in nonlocal NLS equations. In particular, it is possible to describe in this setting quasi-1D structures embedded in a 2D geometry. In particular, it is possible to follow the adiabatic dynamics of planar dark soliton and of ring dark solitons that takes into account the nonlocal interaction terms. Important questions then arise for such models relevant in both atomic and optical models, including the role of nonlocality in the stability and dynamics of the excitations. Also within the realm of nonlocal NLS models, when the BEC is subject to a deep external periodic potential, the BEC wavefunction is "partitioned" at the different potential troughs giving rise of a discrete NLS equation. This discrete NLS equation accounts for the BEC population at each lattice trough that is connected to its immediate neighbors (through a term tantamount to quantum tunneling). This discrete model is tightly connected to the work of Panayotis Panayotaros where an extension of this discrete NLS equation was used to model a nematic liquid crystal. This model encompasses the inherent dipolar properties of liquid crystal molecules that naturally induce a nonlocal (nonlinear) interaction term. It is observed in that this system can support intrinsically localized modes (or breathers) corresponding to localized solutions due to the nonlinearity of the substrate rather than to an artificially imposed impurity that could break the spatial symmetry. Again open questions were raised regarding stability properties and systematic nonlinear dynamical features.

Another area of extension that was discussed in the workshop is the possibility of creating BECs in more than one component. These, so-called multi-component BECs, allow for the possibility of condensing two, or more, BEC species. Each of these species can be described by a NLS-type equation that is coupled to the other(s) component(s). The existence of multi species allows for the construction of more exotic solutions. For instance, the work of Pedro Torres showed that it is possible to create and fully describe amplitude waves with nontrivial phases. On the other hand, the work of Panayotis Kevrekidis provided a roadwork to construct in a systematic manner the different combined structures in two and three component BECs. For instance, one could consider some components with an attractive interaction while the other component(s) have repulsive interactions. Through the coupling between the components it is then possible to create mixed conglomerates with, for example, one dark soliton in the repulsive component playing the role of an effective potential to support a bright soliton in the attractive component. Several extensions of this work are possible, including the coupling between only dark solitons, all of which have been achieved in recent experimental realizations of multi-component BECs. Here, numerous exciting developments were presented such as novel states in the form of dark-antidark solitons in two components and dark-dark-bright and dark-bright-bright states in three components that were just reported out of experiments of Peter Engels, but have not been systematically explored theoretically as of yet. The state-of-the-art within such multi-component systems also includes the extension of the above structures to higher dimensional settings. For instance, it is possible to engineer vortex-bright complexes where again a vortex (i.e., a dark structure) provides an effective confining potential to supports a bright 2D soliton in the other component. This type of extensions to higher dimensions gave us a natural springboard to consider the BECs in higher dimensions described in the next two sections.

2.2 2D Coherent Structures in BECs

When a BEC is contained by a trapping potential with a transverse strength much stronger than two similar longitudinal directions, it is effectively rendered 2D. Given that the transverse direction is tightly trapped and therefore naturally accessible energies are not large enough to even excite the first excited state in the transverse direction, this leads to effectively "freezing" this direction and rendering the system quasi-2D. In 2D, the quintessential coherent structure is a vortex. A vortex is the 2D extension of a 1D dark soliton and possesses a topological charge (or winding number). The work of Carlos Azpeitia, for instance, presented a number of bifurcations of vortices and related solutions (solitonic dipoles etc.) in the 2D BEC realm. Furthermore, as the work of experimental BEC physicist Brian Anderson and theoretical effort by Ashton Bradley showed, the quasi-2D realm of BECs is a fertile ground for the study of novel, and often controversial, topic such as 2D quantum turbulence. In Anderson's lab, collections of vortices are routinely produced —by stirring-type mechanisms— and let to freely evolve, interact and annihilate. This system presents a pristine avenue to study 2D quantum turbulence and its associated entropy/energy cascades. An important open experimental issue is the lack of availability of phase observations within the measurement which renders such cascades experimentally inaccessible and only measurable through theoretical tools. In a related experiment, in this case a BEC in a ring geometry produced at NIST, was driven to create a single unit of circulation carried by the ring (equivalent to a single vortex inside the ring). Then, by using a paddle stirrer in this case to slow down the circulation, the work of Mark Edwards showed that it is crucial to account for finite temperature effects to capture the quantitative aspects of the vortex expulsion responsible for the reduction of the ring's overall circulation. The modeling of thermal condensates via the so-called ZNG formulation that Edwards presented promises to constitute an important avenue for future theoretical work. Hence, while standard zero-temperature BEC models given in terms of the NLS equations might be inadequate to describe the interactions, creation and annihilation of vortices in BECs, a concerted effort needs to be undertaken to quantify such beyond mean-field effects.

2.3 3D Coherent Structures in BECs

Finally, one of the most challenging setups to analytically tackle within the realm of BECs is the case of 3D coherent structures. Some recent efforts have been vested to understand the emergence and stability of vortex lines and vortex rings near the linear limit. For instance, Ricardo Carretero and collaborators have identified the different bifurcations responsible for the emergence of vortex lines and vortex rings from essentially lower-dimensional structures such as dark solitons extended in 2D, namely planar dark solitons. Through degenerate perturbation theory, it is possible to predict, not only the bifurcation structure, but also the bifurcation thresholds (in terms of the total norm of the solution) for the different trap cases comprising isotropic and anisotropic trappings. It is generically found that single and multiple vortex rings are stable as the norm (or density) of the system is increased. This naturally leads to the study of such structures in the large density limit and, in particular, to their dynamics due to the trapping potential and, even more challenging, their mutual interactions. In the large-density limit the NLS equation describing the BEC can be cast, using the so-called Madelung transformation splitting the wavefunction into its density and phase components, into a Eulerian non-viscous fluid. This superfluid, described in terms of its fluid velocity corresponding to the gradient of the phase of the original wavefunction, also contains an extra quantum pressure term that depends on the gradient of the density. Therefore, away from substantial density gradients, namely away from coherent structures, the superfluid behaves like a standard Eulerian fluid for which tools such as the Biot-Savart law can be employed. In fact, using the Biot-Savart law, it is possible to describe the interaction between vortex rings and, in certain cases bearing high symmetry (cf. co-axial vortex rings), reduce the original equations of motion to ODEs on the ring's positions and radii. In cases where the coherent structures' configuration do not bear symmetries, it is still possible to consider approaches based on vortex filament techniques. Within this approach, each vortex filament is treated using a 1D PDE parametrized along the the filament's arclength. In this manner, a collection of N vortex lines, vortex rings, and in general vortex filaments, can be described by a set of N coupled 1D PDEs. The work of Andres Contreras, in particular, posed the problem of examining N such coupled PDEs and revealed such a PDE system whose understanding would enable progress in understanding the collective dynamics of multiple vortex line filaments. Finally, it is worth mentioning that computational methods based on Graphical Processing Units (GPU) architectures, together with high-order compact schemes. are allowing for the numerical integration of the full 3D original NLS-like PDE in almost real time. These new technologies will allow to perform exhaustive parameter and configurational searches for phenomenologies unique to the 3D realm. This is one of the directions that are highly promising for the immediate future, as became transparent from the conference discussions.

3 Particle Dynamics

3.1 Interacting Particle Models

Many talks involved interacting particle models. Several novel extensions were introduced. For example D'Orsogna discussed what happens for particles moving inside a fluid, which is a reasonable approximation for fish movement. Topaz and Bernoff introduced new continuum limits of interacting particle models, leading to a Cahn-Hilliard-type PDE. They also discussed how external food sources affect population density, and its implications for controlling locust outbreaks. Evers presented extensions of a one-dimensional model to two dimensions. He observed many novel patterns and explained their existence. Iron introduced a new local model of cell adhesion and aggregation.

Many talks studied the effect of the anisotropy on the system. Holm described an intriguing experiment with non-round particles floating in water. Depending on the anisotropy, the particle would align along curves rather than forming clumps. Kolokolnikov discussed how the anisotropy of the feed-rate in a reaction-diffusion system affects overall pattern formation, and can often lead to novel dynamical phenomena such as "creation-destruction loops". Uminsky also discussed how anisotropy affects the formation and stability of three-dimensional hollow-spheres, revealing that it has a strong stabilizing effect, greatly increasing the parameter regime for which hollow spheres appear.

Numerical aspects of particle methods featured prominently. Holm discussed a new technique using geometric gradient flow to do continuum-limit simulations of some particle systems. ODE methods were also used extensively in the work of Whitaker on a near-neighbor coupling model of phosphenes. While most of the talks on particle models concerned "all-to-all" interaction models, Whitaker results showcased a wide range of dynamical situations possible even with near-neighbor coupling.

Most of the talks on interacting particles assumed that the particles are a first-order system, such as for example following a gradient flow. This assumption is realistic in many situations, and is often sufficient to allow for very complex dynamics. However because of Newton's law of motion F=ma, many particle systems are second-order in nature, although they are approximated by first-order when there is sufficient damping present. Fetecau discussed the intricacies involved when trying to approximate a zero-inertia limit in this way. This is especially true when the system has an anisotropy, such as field-of-vision in animal formations.

3.2 PDE viewpoint

Many of the talks combined particle models with PDE's, revealing a rich interplay between these two worlds.

Ward introduced a quorum-sensing model that directly combines ODE's and PDE's by coupling bulk diffusion [PDE] to the surface membrane kinetics [ODEs]. This leads to very rich dynamics and novel spectral problems with eigenvalues at the boundary.

Lindsay presented models of touch-down behavior in MEMS. The touch-down occurs along curves or points corresponding to the singularity of a two-dimensional PDE model. A variety of asymptotic techniques were used to describe the evolution of the singularity set.

Several talks involved reaction-diffusion type models. Short discussed recent developments of crime model, including extensions of the UCLA PDE model of crime. He considered an inverse-type problem, how the model parameters can be fine-tuned based on the existing crime data. The ultimate goal here is to help in devising smarter policing strategies for urban crime. Iron introduced a new reaction-diffusion model of formation of cell aggregates. Rodrigues discussed a class of PDE models that has cross-diffusion as well as nonlocal terms, with an eye on proving rigorous analytical results about existence of solutions. Taking a different approach, Xie and Kolokolnikov used asymptotic methods to study spike dynamics in the Schnakenberg model. Xie's talk was about a single spike in two dimensions. Even a single spike can undergo complex bifurcations which can result for example in a rotating spike. Kolokolnikov discussed how the reduced spike patterns in a reaction-diffusion PDE system lead to a novel particle system with an unusual properties. Conversely, the analysis of a resulting particle model sheds new light on the original PDE system.

4 Conclusion

The workshop presented a timely opportunity for interaction and cross-pollination between applied mathematicians, experimental and theoretical physicists on the topic of coherent structures. By its nature, this topic overlaps many areas in physics and mathematics, and a variety of viewpoints presented during the workshop attest to its continuing vibrancy, and a need for cooperation between different scientists. Bringing various points of view to bear will give a boost to further developing this important field.

References

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