FINAL TECHNICAL REPORT By Dr Chjan Lim RPI december 18 2013

Four related projects were carried out with the overall aim of developing computational models for estimating key thermodynamic properties - specific heat and confinement radii - in electron plasmas, rotating superfluids, trapped Bose-Einstein condensates and geophysical flows. Generalized vortex filaments and fully 3D spin-lattice models are fundamental to all these applications and form the basis of the proposed work on cooperative phenomena in macroscopic fluid systems.

Broader Impact

The proposed projects involved the collaboration and input from Dr. Bryan Taylor FRS, Drs. Hermann Clerxc and Gertjan van Heijst at Eindhoven, the Netherlands and Dr. Marie Farge's group at CNRS France. International collaborations with former M.Sc student Syed M. Assad from Singapore, and collaborations with former PhD students Dr. Joseph Nebus and Dr. Tim Andersen continued. The research involved the training of PhD and MSc students and undergraduates at RPI. Funds for one PhD student in the form of an RA-ship was included in each year of the project. The PI ran a weekly research seminar on the applications of modern statistical mechanics and numerical simulation methods to geophysical and astrophysical problems. Aspects of the results from proposed projects have been included into a new graduate course on Monte - Carlo simulations and statistical mechanics in fluid flow. These results has been widely distributed through publications in high impact scientiifc journals and invited presentations at domestic and international conferences in the field. The PI's research group at RPI consisted of a female PhD candidate and a new graduate student from an under-represented minority.

PROJECT DESCRIPTION

I Introduction

Effective radii of confinement and specific heats of quasi-2D vortex filaments and 3D spin-lattice models of vorticity-dominated flows are key thermodynamic properties critical to plasma containment in fusion technology, heat transfer in oceanic and atmospheric flows and trapped Bose-Einstein condensates (BEC). Researchers have used statistical mechanics - in particular the information-theoretic form of entropy - and modern computational methods to calculate order parameters pertaining to the collective behaviour of many-body problems and predict the formation of self-organized structures in a wide range of macroscopic fluid systems. However, few results are available for performing these calculations for quasi-2D vortex filaments and fully 3D rotating flows that exhibit cooperative phenomena. The overall objective of this proposal is to exploit parallels between vortex filaments, magnetic flux lines and quantum path-integrals and develop effective computational and analytical models of vorticity dominated flows capable of predicting properties such as anomalous expansion and negative specific heat. This DOE-funded study consists of four related projects:

1. *Mathematical characterization of isolated systems of vortex filaments - calculation of negative specific heat.*

The objective accomplished here is to characterize most probable states in isolated systems of generalized vortex filaments. Methods from quantum field theory will be used to estalish relations between microcanonical ensembles and their canonical counterparts that are consistent with their non-equivalence and develop numerical simulation (PIMC) methods for microcanonical ensembles. Analytical microcanonical calculations of specific heats and other cooperative properties of generalized vortex-filament models will be based on these relations and mean-field methods for canonical ensembles. The point is that the mathematical non-equivalence between canonical and microcanonical ensembles of non-extensive vortical systems enables isolated vortex filaments to have negative specific heat when their canonical counterparts – vortex filaments in contact with an energy reservoir - are required to have strictly positive specific heats. Negative specific heat of isolated vortex filaments is a fundamental result with wide-ranging impact on extreme confinement and other run-away phenomena in plasmas.

2. *Development of a path-integral Monte-Carlo (PIMC) method for isolated systems of generalized vortex filaments.*

The objective accomplished here is two-fold - (A) formulate a unified theory for nearly parallel defect lines in electron-magnetohydrodynamics (EMH) and Bose-Einstein condensates at the level of rigor attained in vortex-filament models for nearly inviscid fluids and (B) develop a meshless numerical algorithm that overcomes inherent technical obstacles in Monte-Carlo (MC) simulations of microcanonical Gibbs ensembles. Generalized vorticity models from EMH that represents the vorticity of the electron fluid and the magnetic field as a single entity will be refined with a view towards rigorous size estimates for filament core, radii of curvature and inter-filament separations. To this end, a single energy expression similar to the London energy will be derived to represent the self-induction and inter-filament interactions of these generalized vortex filaments.

Numerical calculations of specific heat and other cooperative variables in generalized vortex filament models from (A) require treating them as isolated systems in many applications. However, few simulation methods are available for studying isolated systems and corresponding microcanonical ensembles. To this end, a mathematical result in quantum field theory based on proposed work in project 1 was used to compute microcanonical partition functions and develop a meshless PIMC algorithm for vortex filaments.

3. *Phase transitions in fully 3D spin-lattice models for vortex-dominated flows.*

The objective partially accomplished is to develop a family of convergent 3D Eulerian lattice models for nearly inviscid macroscopic flows beyond the vortex filaments models in projects 1 and 2, with a view towards extending their validity to fully 3D problems. Current vortex filament models require the vortex lines to be nearly parallel - a substantial limitation. Discretization of the mechanical energy of macroscopic flows will be achieved by spatial decomposition based on a Voronoi cell - piecewise constant - approximation of the energy functional. It is believed that second order phase transitions and critical exponents are critical for understanding fully-developed

3D flows and predicting their specific heats in wide-ranging applications. The idea is to apply economical and readily available lattice Monte-Carlo methods combined with Renormalization Group (RG) techniques to proposed 3D Eulerian models to probe their cooperative behavior and collective / thermodynamic properties.

Further details on the objectives, significance, plan and broader impact of these projects are described in the following sections. Results from prior federally funded projects are given below.

1 Projects definition

The project is to develop a family of lattice models for 3D vortex-dominated flows and a computational approach based on Renormalization Group (RG) methods [] and Monte-Carlo (MC) simulations to calculate critical exponents and domain-wall structures in fully -3D macroscopic flows. However, few results are available for exploring the statistical mechanics of fully-3D flows beyond the validity of nearly parallel vortex-filaments models. New RG and MC techniques are needed here in addition to mean-field and exact-solution methods used in the statistical mechanics of quasi-2D flows.

It is widely believed and was checked in this project that second order phase transitions and universality of critical exponents characterize the cooperative phenomena of fully-developed 3D vortical flows. One of the first goals in this project was to establish that phase transitions in 3D fluid flows are second order ones by running extensive MC simulations near critical points of the 3D lattice models. The resulting map of the free-energy landscape will help in estimating rough exponents for the power laws obeyed by order parameters near phase transitions of the lattice.

Second order phase transitions where the order parameter is continuous in temperature at the critical point T_c are characterized by their critical exponents. Calculated by Renormalization Group techniques, they are in general independent of the short-range interactions in the system. Instead the critical exponents can be estimated from the spatial and spin dimensions of the lattice models and their interaction's long-range characteristics, that is, universality of the critical exponents.

The idea is to exploit the independence of critical exponents from short-range characteristics of the lattice models for 3D flows to estimate specific heat and relative size of vorticity supports across many flow geometries from effective spin dimensionality and other long-range characteristics of lattice interaction. Application specific details of the flows such as torque and pressure coupling at the boundary to energy and angular momentum reservoirs in the environment will determine precise values of critical temperatures and whether there is a phase transition. The latter quantities will be estimated by extensive MC simulations.

One specific aim accomplished was to apply the lattice approach to the concrete task of calculating specific heat and size of vorticity support in flows that are quasi-

2D with a view towards detailed comparisons between the lattice or Eulerian approach here and the meshless or Lagrangian approach in projects 1 and 2. Mean-field and exact solution methods can be used here in conjunction with MC simulations in light of the quasi-2D nature of the flows. Completion of this first task provided benchmarks and confidence in further development of the 3D lattice approach and its applications to fully - 3D vortical flows.

1.1 Project significance

Critical exponents and domain structures - important in the study of magnetic materials - is believed to be key also for the understanding of fully - 3D flows. Some early results based on the analogy between vortex filaments and polymers [] serve as valuable guides and benchmarks for the work in this proposal. These early results are rough and cannot be used to accurately predict critical temperatures, specific heats and size of vorticity supports. Indeed, the question of whether the phase transitions in fully -3D flows are second order remains open. And if phase transitions in 3D macroscopic flows are second order, it is not known how to estimate their critical exponents. The proposed project aims to take the initial steps towards solving these and other open problems in fully-developed 3D flows. It is anticipated that the methods and results developed in this project will help guide future experiments on improved measurements of two-point correlations and higher order structure functions of 3D flows. The success of lattice models for coupled barotropic and divergent shallow flows in predicting aspects of phase transitions in planetary atmospheres has been widely disseminated and recognized.

1.2 Projects plan and approach

It is believed that critical exponents and domain structures are key for the study of fully developed 3D flows but few results are available to characterize them. Some form of lattice, particle or spectral discretization is required for feasible computation of the critical exponents because of technical obstacles involved in working with path-integrals based on the continuous form of the flow energy. A fully-3D lattice approach will remove many restrictions of the quasi-2D meshless Lagrangian models in projects 1 and 2 such as the requirement of nearly-parallel vortex lines. RG techniques that integrate out the short range behaviour and rescale the interaction without solving the full path-integrals are critical to the success of this approach because there are still no exact solutions to this family of 3D lattice models. Unlike quasi-2D problems, the mean-field approximation is not known to be valid for fully - 3D vortex dominated flows. But RG methods alone are not enough in view of the dependence of phase transitions and critical temperatures on short range characteristics and boundary conditions of the lattice where the flows are coupled to rigid or elastic boundaries. Monte-Carlo simulations will be used together with RG to obtain complete solutions.

For the purpose of investigating cooperative phenomena in fully-3D vortex-dominated flows, we developed a family of spin-lattice models for the 3D kinetic energy of macroscopic flows based on a magnetic- variable formulation for the 3D Euler's equation [Chorin]. Defining the magnetic variable to be $\mathbf{M} = \mathbf{u} + \nabla\phi$ where $\mathbf{u}$ is the 3D velocity and ϕ is a scalar gauge field, the usual 3D kinetic energy can be written as

$$H = \frac{1}{2}\int_V d\mathbf{x}\int_V d\mathbf{x}' \ \left\{\mathbf{M}(\mathbf{x})\cdot\mathbf{M}(\mathbf{x}')g(|\mathbf{x}-\mathbf{x}'|) + (\mathbf{M}(\mathbf{x})\cdot\nabla)\left(\mathbf{M}(\mathbf{x}')\cdot\nabla'\right)\Psi(|\mathbf{x}-\mathbf{x}'|)\right\} \tag{1}$$

where g is a real-valued function of the separation between $\mathbf{x}$ and $\mathbf{x}'$, ∇' denotes grad with respect to $\mathbf{x}'$ and $\Delta\Psi = g$ in domain V. A lattice approximation for kinetic energy H based on a piecewise constant spatial discretization of the magnetic variable, i.e., $\mathbf{M}(\mathbf{x}) = \mathbf{M}_j = \mathbf{M}(\mathbf{x}_j)$ if $\mathbf{x}\in\mathbf{D}(\mathbf{x}_j)$ on Voronoi cells $\{\mathbf{D}(\mathbf{x}_j)|\mathbf{x}_j\in V, j=1,...,N\}$, is given by

$$H_N = \frac{1}{2}\sum_{j=1}^{N}\sum_{k=1}^{N}\{\mathbf{m}_j\cdot\mathbf{m}_k g(|\mathbf{x}_j-\mathbf{x}_k|) + (\mathbf{m}_j\cdot\nabla)(\mathbf{m}_k\cdot\nabla)\Psi(|\mathbf{x}_j-\mathbf{x}_k|)\}$$

with $\mathbf{m}_j = h^3\mathbf{M}_j$ and h is the mesh size.

The reason for using a Voronoi decomposition that is based on an irregular (and randomized) mesh instead of a regular lattice such as the cubic lattice is to avoid any contamination of their thermodynamic properties by artificial lattice effects. The point is that while second order critical phenomena does not depend on short - range properties of the lattice interactions, they may be affected by the type of 3D mesh used. Mesh effects on lattice models for 3D flows are undesirable because the original macroscopic flow is continuous.

The natural choice of the delta function, $g = \delta$ in H_N gives the following 3D lattice model ($d = 3$)

$$H_N = \sum_{j=1}^{N}|\mathbf{m}_j|^2 - \sum_{j<k}^{N}\left\{\frac{\mathbf{m}_j\cdot\mathbf{m}_k}{|\mathbf{x}_j-\mathbf{x}_k|^3} - \frac{3\mathbf{m}_j\cdot(\mathbf{x}_j-\mathbf{x}_k)\mathbf{m}_k\cdot(\mathbf{x}_j-\mathbf{x}_k)}{|\mathbf{x}_j-\mathbf{x}_k|^5}\right\}$$

with spins $\mathbf{m}_j$ of dimensionality $n = 3$ at nodes $\mathbf{x}_j\in V$. The first sum $\sum_{j=1}^{N}|\mathbf{m}_j|^2$ looks like a typical positive-definite quadratic term for the kinetic energy of a gas of particles. Keep in mind however that the whole H_N represents the total kinetic energy of macroscopic flows in lattice form. The second sum in H_N is just the dipolar coupling energy and has r^{-3} decay rate, properties that will be key in estimating the critical exponents. It follows from results in [] that dipolar interactions generate domain walls - non-uniform structures near phase transitions that arise when symmetry breaks in different ways across the ordered phase. These sheet - like structures - ubiquitous in magnetic materials and astrophysics - are believed to be important also in the study of fully-developed, well-mixed fluid flows.

Investigation of the cooperative properties of H_N will be based on Gibbs' canonical and microcanonical ensembles with suitable choice of constraints such as the square-norm $Q_N = \sum_{j=1}^{N}|\mathbf{m}_j|^2$ of the spins and helicity $\Gamma_N = \sum_{j=1}^{N}\mathbf{m}_j\cdot(\nabla_L\times\mathbf{m}_j)$ where

$\nabla_L \times$ is a suitable lattice version of the curl operator in 3D. The canonical partition function is

$$Z_N^c(\beta, \mu) \propto \sum_{\mathbf{m}} e^{-\beta H_N} e^{-\mu \Gamma_N}$$

where the sum in Z_N^c is taken over all allowed microstates $\mathbf{m} = \{\mathbf{m}_j, \, j = 1, ..., N\}$. A significant point here is that in putting the whole H_N conjugate to inverse temperature β, we have already included a canonical constraint on Q_N in the Gibbs canonical formulation. The Gibbs' microcanonical partition function is

$$Z_N^{mc}(E, K) \propto \sum_{\mathbf{m}} \delta(H_N - E)\delta(\Gamma_N - K).$$

The dipolar coupling form of the second sum in H_N can be exploited to estimate mean values of pairwise products of the spin magnitudes, their relative angles and orientations between spins and the vector separating them by using adaptatons of the RDC - residue dipolar coupling- methods[] in NMR spectroscopy for measuring separations between molecules or parts of long chains, their relative orientations as well as the orientations of bonds with an external magnetic field. The 3D lattice models we formulated have fixed nodes, that is, the separations and orientations of the vectors between spins are fixed quantities, which increases further the effectiveness of these modified RDC methods.

Together with MC simulation - in the form of so-called RG - Monte-Carlo methods - this approach is the basis of much of the proposed work here. With a view towards applying this method to quasi-2D geophysical and astrophysical fluid flows, and for the sake of brevity and concreteness, we will outline the RG method using a simplified energy functional rather than the more complicated energy H in (1). [**?**]: The total energy of macroscopic flow is

$$H = \int d^d\mathbf{x} \, \left\{ \alpha \sum_{l=1}^{n} \sum_{j=1}^{d} |\partial_j \psi_l(\mathbf{x})|^2 + V\left(\sum_{l=1}^{n} \psi_l^2\right) \right\}$$

where the n real-valued scalar fields $\psi_l(\mathbf{x})$ represent generalized velocity potentials, spatial dimension $d = 3$, and $V\left(\sum_{i=1}^{n} \psi_l^2\right)$ is the available potential energy in power series form - $\frac{\partial V(\cdot)}{\partial(\cdot)}$ is a constant - such as those in the quasi-geostrophic model of stratified flows [pedlosky]. The partition function is

$$Z = \int \prod_{l=1}^{n} d\psi_l \; e^{-\beta H[\psi]}.$$

Rewriting the potentials $\psi_l(\mathbf{x}) = L^{-d/2} \sum_{|\mathbf{k}|<\Lambda} \exp(i\mathbf{k} \cdot \mathbf{x})\hat{\psi}_{l\mathbf{k}}$ in Fourier form with lattice cutoff Λ, complex coefficients $\hat{\psi}_{l\mathbf{k}}$ and total volume of system $\int d^d\mathbf{x} = L^d$, and separating the small from the large scales, $|\mathbf{k}| < \Lambda/s$ where s is a real number greater than 1, we get

$$\begin{aligned} Z &= \int \prod_{l=1}^{n} \prod_{|\mathbf{k}|<\Lambda} d\hat{\psi}_{l\mathbf{k}} e^{-\beta H[\hat{\psi}]} = \int \prod_{l=1}^{n} \prod_{|\mathbf{k}|<\Lambda/s} d\hat{\psi}_{l\mathbf{k}} e^{-\beta \hat{H}[\hat{\psi}]} \\ e^{-\beta \hat{H}[\hat{\psi}]} &= \int \prod_{l=1}^{n} \prod_{|\mathbf{k}|\geq\Lambda/s} d\hat{\psi}_{l\mathbf{k}} e^{-\beta \hat{H}[\hat{\psi}]}. \end{aligned}$$

The integration over small scales $|\mathbf{k}| \geq \Lambda/s$ for $\hat{H}[\hat{\psi}]$ will be carried out using the method of steepest descent: After some lengthy algebra based on the substitutions, $\Phi_{\mathbf{k}} = \sum_{l=1}^{n} |\hat{\psi}_{l\mathbf{k}}|^2$ and $\bar{\psi}_l(\mathbf{x}) = \sum_{|\mathbf{k}|<\Lambda/s} \exp(i\mathbf{k}\cdot\mathbf{x})\hat{\psi}_{l\mathbf{k}}$, and changing variables of integration in Z from $d\hat{\psi}_{l\mathbf{k}}$ to $d\Phi_{\mathbf{k}}$, i.e., for each $\mathbf{k}$,

$$\prod_{l=1}^{n} dRe\hat{\psi}_{l\mathbf{k}}\ dIm\hat{\psi}_{l\mathbf{k}} = A\Phi_{\mathbf{k}}^{n-1} d\Phi_{\mathbf{k}},$$

where A is the surface area of an $n-sphere$, we get

$$H[\hat{\psi}] = \alpha \sum_{|\mathbf{k}|<\Lambda/s} |\mathbf{k}|^2 \Phi_{\mathbf{k}} + \alpha \sum_{|\mathbf{k}|\geq\Lambda/s} |\mathbf{k}|^2 \Phi_{\mathbf{k}} + \int d^d\mathbf{x}\ V\left(\sum_{l=1}^{n} \bar{\psi}_l^2 + L^{-d} \sum_{|\mathbf{k}|\geq\Lambda/s} \Phi_{\mathbf{k}}\right)$$

and the integral over small scales $|\mathbf{k}| \geq \Lambda/s$ becomes

$$e^{-\beta \hat{H}[\hat{\psi}]} \propto \int \prod_{|\mathbf{k}|\geq\Lambda/s} \Phi_{\mathbf{k}}^{n/2} d\Phi_{\mathbf{k}} \exp\left\{-\alpha\beta \sum_{|\mathbf{k}|\geq\Lambda/s} |\mathbf{k}|^2 \Phi_{\mathbf{k}} - \beta \int d^d\mathbf{x}\ V\left(\sum_{l=1}^{n} \bar{\psi}_l^2 + L^{-d} \sum_{|\mathbf{k}|\geq\Lambda/s} \Phi_{\mathbf{k}}\right)\right\}.$$

In the large n steepest-descent method, the saddle- point equation - for each small scale $\mathbf{k}$ -

$$0 = \frac{\partial}{\partial \Phi_{\mathbf{k}}}\left\{\frac{1}{2} n \log \Phi_{\mathbf{k}} - \alpha\beta|\mathbf{k}|^2 \Phi_{\mathbf{k}} - \beta \int d^d\mathbf{x}\ V\left(\sum_{l=1}^{n} \bar{\psi}_l^2 + L^{-d} \sum_{|\mathbf{k}|\geq\Lambda/s} \Phi_{\mathbf{k}}\right)\right\}$$

gives the main contribution to $e^{-\beta \hat{H}[\hat{\psi}]}$ at the saddle-point,

$$\begin{aligned} \Phi_{\mathbf{k}}' &= \frac{1}{2} n \left\{\alpha\beta|\mathbf{k}|^2 + \beta \int d^d\mathbf{x} \frac{\partial V}{\partial Y} \frac{\partial}{\partial \Phi_{\mathbf{k}}}\left(\sum_{l=1}^{n} \bar{\psi}_l^2 + L^{-d} \sum_{|\mathbf{k}|\geq\Lambda/s} \Phi_{\mathbf{k}}'\right)\right\}^{-1} \\ &= \frac{1}{2} n \left\{\alpha\beta|\mathbf{k}|^2 + \beta \frac{\partial V}{\partial Y}\right\}^{-1} \end{aligned}$$

after using the power series form of the potential energy $V(Y)$.

This consitutes half of the RG procedure and the other half which consists of re-scaling the remaining (large-scales) modes to obtain a renormalized energy H' that looks like the original H but with different values of parameters is straightforward in principle but too lengthy to include here. The renormalized H' gives rise to a mapping in parameter space which is associated with a RG-flow - the fixed points of this flow are critical points and the eigenvalues of the linearized RG-flow give the critical exponents for the cooperative phenomena of the 3D lattice models of macroscopic flows.

2 Broader Impact

The proposed projects involved the collaboration and input from Dr. Bryan Taylor FRS, Drs. Hermann Clerxc and Gertjan van Heijst at Eindhoven, the Netherlands and Dr. Marie Farge's group at CNRS France. International collaborations with former M.Sc student Syed M. Assad from Singapore, and collaborations with former PhD students Dr. Joseph Nebus and Dr. Tim Andersen will continue from projects funded currently by ARO and DOE.

3 Papers from This DOE Project

1 Statistical equilibrium of the Coulomb / Vortex gas in the unbounded two-dimensional plane (with S.M. Assad), Discrete and Cont. Dyn. Sys. B, 5(1), 1-14, 2005.

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