Chapter 6

Heat Front Propagation

In the foregoing chapters on shear flow studies, generation of heat was observed at the particle level close to shear layers. It will be interesting to see if one can resolve the connection between such macroscopic shear flows and particle level heat generation. Here, we report using classical molecular dynamics simulations, the development and propagation of a nonlinear heat front in parallel shear flows of a strongly coupled Yukawa liquid. At a given coupling strength, a subsonic shear profile is superposed on an equilibrated Yukawa liquid and Kelvin Helmholtz (KH) instability is observed. Coherent vortices are seen to emerge towards the nonlinear regime of the instability. It is seen that while inverse cascade leads to a continuous transfer of flow energy towards the largest scales, at the smallest scale there is also a simultaneous transfer of flow energy into the thermal velocities of grains. The latter is an effect of velocity shear and thus leads to the generation of a nonlinear heat front. In the linear regime, the heat front is seen to propagate at speed much lesser than the adiabatic sound speed of the liquid. Spatio-temporal growth of this heat front occurs concurrently with the inverse cascade of KH modes.

6.1 Introduction

As is well known, complex plasmas can behave as essentially single phase systems when the grain-grain interactions dominate over the grain-plasma
interactions (Khrapak et al., 2004). Thus a near “exact” description of a complex plasma can be constructed by considering only the dust grains and assuming that the background plasma does not evolve in time. This allows the grain dynamics to be modeled by a Yukawa (screened Coulomb) potential (Equation 2.1). The resulting N body problem can then be numerically solved using a molecular dynamics (MD) simulation. In past, several authors have used such MD simulations to study transport phenomena (Saigo and Hamaguchi, 2002; Liu and Goree, 2005, 2008), phase transition (Hamaguchi et al., 1996, 1997; Ashwin and Ganesh, 2009) and collective behavior (Ohta and Hamaguchi, 2000b) in strongly coupled complex plasmas. There exists, however, a class of problems in complex plasmas where such a “first principles” study has so far, remained elusive. These are the “hydrodynamic instabilities”- a subject traditionally studied only through continuum methods. Recently, some of these hydrodynamic instabilities such as “shear flows” have been investigated at the most fundamental level of atomic motion by MD simulations of complex plasmas, for details, see chapter 3 and (Ashwin and Ganesh, 2010a,b, 2011b). In these works, it was noticed, that in addition to generation of coherent structures, shear flows also lead to “particle heat generation”. Such shear induced heat generation has been known to cause solid to liquid phase transition in soft materials (Ackerson and Clark, 1981; Delhommelle, 2004) and complex plasmas (Nosenko and Goree, 2004). Recently, shear induced melting has also been discovered in two-dimensional (2D) Yukawa crystals, where a melting front was seen to propagate at transverse sound speed (Feng et al., 2010). In the following section, we give details of the MD simulations carried out in the present chapter.

### 6.2 Molecular dynamics

In a typical large scale MD simulation like ours, one can control the grain-grain interactions using the switch ‘κ’ and obtain either ideal gas (κ → ∞) or Coulomb gas (κ → 0) behavior. We recall that the length, time and energy are normalized to a, $\Omega_{pd}^{-1}$ and $Q^2/(4\pi\varepsilon_0a)$ respectively. The dust plasma frequency is given by $\Omega_{pd} = [Q^2n/(4\varepsilon_0ma)]^{1/2}$, where $n$ and $m$ are...
the 2D dust number density and mass of the dust grain respectively. We take a total of $2.304 \times 10^5$ grains for the 2D Yukawa liquid and periodic boundary conditions are employed along $\hat{x}$ and $\hat{y}$. The number density $n$ of the Yukawa liquid is taken to be 1, which gives us a square region of size $L = 480$, centered at the origin $(0,0)$. The value of screening parameter $\kappa$ in our simulations is taken to be 0.5. The Yukawa liquid is first thermally equilibrated by connecting to a Gaussian thermostat (Evans et al., 1983) and letting it evolve canonically for $200\omega^{-1}_{pd}$. A standard leapfrog integrator with a time step $\Delta T = 0.01\omega^{-1}_{pd}$ is employed such that the fluctuation in total energy $\sim 10^{-5}\%$ without the thermostat over a typical run duration of $1000\Omega^{-1}_{pd}$. In the following section we report our results on Kelvin-Helmholtz instability due to a double step velocity profile.

### 6.3 Kelvin Helmholtz instability

The initial equilibrium is a thermally equilibrated Yukawa liquid at a desired $\Gamma$ along the with the following step velocity profile superposed on grain velocities (only once at $t = 0$). Thus we have in Cartesian coordinates $(x, y)$:

$$
V_x = \begin{cases} 
+V_0, & |y| \geq L/4 \\
-V_0, & |y| < L/4 
\end{cases} \quad V_y = 0.0 \quad (6.1)
$$

where $V_0 = 1$ is the magnitude of imposed velocity. The adiabatic sound speed of the system on this scale is $c_s \approx 2.4$ and the thermal speed is about $v_{th} = \sqrt{2/\Gamma} \approx 0.13$, at $\Gamma = 120$. Hence, our profile $V_0$ is “subsonic” in nature. In Figure 6.1, we show time evolution of KH instability starting from an equilibrated liquid at $\Gamma = 120$ and shear profile (Equation 6.1). A grain at time $t = 0$ (when the shear is imposed) is colored blue if $|y| \geq L/4$, else colored green. One can clearly see the development of KH instability and the roll up of vortices in the nonlinear regime eventually leading to turbulent mixing of the liquid. In the following section we present the time evolution of local vorticity $\omega$ and local flow field $\mathbf{v}$. 
6.4 Vorticity field

The development of KH instability leads to a nonlinear regime which is characterized by the formation of vortices. In Figure 6.2, we show a snapshot at $t = 400$ with well developed vortices in the nonlinear regime. The magnitude of local vorticity ($\omega = \nabla \times \mathbf{v}$) is indicated on the vertical colorbar, where blue and red regions correspond to negative and positive values respectively. To construct local vorticity $\omega$, we first obtain the local velocity $\mathbf{v}$ by “fluidizing” grain velocities over a $45 \times 45$ grid. This amounts to a local averaging of grain velocities to obtain the fluid velocity at a grid point. The superposed white
Figure 6.2: Vorticity field \((\omega = \nabla \times \mathbf{v})\) for the entire system \([\pm 240, \pm 240]\) shown at time \(t = 400\) in the nonlinear regime. One can clearly see the developed vortices. Grain velocities in the region are fluidized through a \(45 \times 45\) grid to construct local vorticity. Blue and red regions correspond to negative and positive vorticity respectively and the color-map label shows the magnitude of local vorticity. Arrows indicating direction of local velocity are obtained by fluidizing the grain velocities over a \(60 \times 60\) grid. Arrow lengths give magnitude of local flow field qualitatively.

arrows showing the local flow direction are similarly obtained from a \(60 \times 60\) grid. In Figure 6.3, we show the time evolution of this vorticity field through a sequence of vorticity \((\omega)\) snapshots for the full system \((\pm 240, \pm 240)\). At late times \(t \geq 800\), one can clearly see the emergence of giant vortices due to inverse cascade of KH modes which is typical of 2D turbulence. In the following section, we present a discussion on the topology of this 2D turbulent field using the Okubo-Weiss criterion. The resulting Okubo-Weiss parameter \(Q\) can then be used to divide the turbulent field into either “rotation dominated” or “deformation dominated” regions.
Figure 6.3: Snapshots showing vorticity ($\omega = \nabla \times v$) contour plots for the full system ($\pm 240, \pm 240$). For details on extraction of $\omega$ and $v$, see Figure 6.2 caption.
6.5 Topology of turbulent mixing

One can simplify the partition of a 2D turbulent field by distinguishing the contributions of rotation and deformation to the square of velocity gradient. This is done by writing,

\[ ||\nabla \mathbf{v}||^2 = \frac{1}{2}(\omega^2 + s^2) \]  \hspace{1cm} (6.2)

where \( \mathbf{v} \) is the Eulerian velocity field, \( \omega \) refers to the vorticity and \( s \) to the deformation, i.e

\[ \omega = \partial_x v_y - \partial_y v_x, \quad s^2 = s_1^2 + s_2^2, \quad s_1 = \partial_x v_x - \partial_y v_y, \quad s_2 = \partial_x v_y + \partial_y v_x \]  \hspace{1cm} (6.3)
Under the assumption that vorticity and strain (i.e. spatial derivatives of velocity) are slowly varying with respect to the vorticity gradient, the Lagrangian evolution of $\nabla \omega$ is then given by a linear differential equation whose solution is (Okubo, 1970; Weiss, 1991; Elhmaidi et al., 1993)

$$\nabla \omega \approx \exp(\pm \frac{1}{2}Q^{1/2}t)$$

where $Q = s^2 - \omega^2$. Even though Weiss approximation holds in the limit of vanishing viscosity, it has also been used by several authors in presence of finite viscosity (Rivera et al., 2001; Perlekar and Pandit, 2009). The Okubo-Weiss parameter $Q$ provides a simplified picture of 2D turbulence by an elementary partition of the field into two distinct domains, namely (a) “elliptic domains” ($Q < 0$), where rotation dominates deformation, $\omega^2 > s^2$, and (b) “hyperbolic domains” ($Q > 0$), where deformation dominates rotation, $\omega^2 < s^2$.

Figure 6.4 shows contour plots of $Q(x, y)$ at different times for the corresponding vorticity field shown in Figure 6.3. Based on the local value of $Q$, we identify three regions, namely (a) vortex cores, which are characterized by strong negative values of $Q$, (b) strain cells surrounding the vortex cores, which are characterized by large positive values of $Q$, and (c) the background, where $Q$ fluctuates between positive and negative values. Depending on the sign of $Q$, the background field may be further divided into non-coherent elliptic and hyperbolic patches. As the vortex cores show up in stark contrast to the background field, a $Q$ map is sometimes also used to count the number of vortices or coherent structures in the liquid. In the following section we present a quantitative analysis of inverse cascade of KH modes using Fourier transform of $\hat{y}$ averaged kinetic energy.

### 6.6 Inverse cascade of KH modes

To further characterize the KH instability in detail, we obtain the power spectrum of modes as follows: On the 2D simulation box, we construct a $(60 \times 60)$ grid and calculate the $\hat{y}$ averaged kinetic energy at various locations.
Figure 6.4: The field of Okubo-Weiss parameter $Q \times 10^{-3}$ at corresponding times for the vorticity field shown in Figure 6.3. The positive ("hyperbolic domain") and negative values ("elliptic domain") of $Q$ are indicated on the vertical colorbar.
6.6 Inverse cascade of KH modes

Figure 6.4: Continued

along \( \hat{x} \)

\[
\bar{E}_k(x) = \frac{1}{L} \int_{-L/2}^{L/2} E_k(x, y) dy
\]

(6.5)

where \( E_k(x, y) \) is the kinetic energy per grain at the grid location \( (x, y) \). By taking Fourier transform of this \( \hat{y} \) averaged kinetic energy \( \bar{E}_k(x) \), we get the power spectrum of modes as follows:

\[
E_k(m_n) = \int_{-\infty}^{\infty} \bar{E}_k(x) \exp \left( \frac{2\pi m_n x}{L} \right) dx
\]

(6.6)

where \( m_n \) is the mode number. In Figure 6.5, we show the power spectrum (normalized to the maxima) at similar times and quantitatively show inverse cascade of energy towards large scales (smaller \( m_n \)) which is typical
Figure 6.5: Power spectrum (normalized to the maxima) plotted at various times show the emergence of dominant mode $m_n = 1$ at late times. The initial excitation is random which is shown in the panel at $t = 20$. This inverse cascade of randomly excited modes to a dominant large scale structure ($m_n = 1$) at $t \sim 980$ is typical of 2D turbulence.

of 2D turbulence. This inverse cascade of KH modes is seen to concurrently evolve with the spatio-temporal growth of a nonlinear heat front, which is the subject matter of the following section.

### 6.7 Development and growth of heat front

At the smallest scales, particle heat generation due to velocity shear leads to the development of a heat front. The propagation of this heat front is elucidated through a time sequence of $\Gamma$ contour plots as shown in Figure 6.6. A typical instantaneous plot of $\Gamma(x, y)$ field is obtained as follows:

$$\Gamma(x, y, t) = \frac{1}{\sum_i N \frac{1}{2} (\vec{v}_i - \bar{\vec{v}})^2}$$

(6.7)
Figure 6.6: $\Gamma$ contour plots at different times showing the spatio-temporal growth of heat front (Ashwin and Ganesh, 2011a). It is easily seen that the development of heat front follows the spatial profile of coherent structures as seen in Figure 6.3.
where \( v_i \) is the velocity of \( i^{th} \) grain in the bin at location \((x, y)\) on the \(45 \times 45\) grid. \( N \) and \( \bar{v} \) are the total number of grains and average velocity in the specified bin. The spatio-temporal growth of heat front reveals particle heat generation - an effect of velocity shear. In Figure 6.6, we see the spreading of hot regions due to particle heat generation. At \( t = 20 \), this hot region is confined close to the shear layer at \( y = \pm 120 \). In the nonlinear regime, a spatial growth ("widening") of this hot region continues due to velocity shear close to vortex boundaries. Interestingly, while part of flow energy is transferred towards the largest possible length scale due to inverse cascade (see Figure 6.3 and 6.5), at the smallest scale there is also a simultaneous transfer of this flow energy into thermal velocities of grains.

The temporal evolution of thermal kinetic energy of the liquid can be obtained by constructing a spatial average of instantaneous \( \Gamma(x, y, t) \) as follows:

Figure 6.6: Continued
6.7 Development and growth of heat front

Figure 6.7: Plot of $\langle \Gamma \rangle_{xy}$ at different times for the full system $(\pm 240, \pm 240)$. The rise in thermal kinetic energy (fall in $\Gamma$) is easily seen from this figure.

Figure 6.8: Profiles of the coupling parameter as function of $y$ at $x = 0$: $\Gamma(y)_{x=0}$ at different times. The initial state is a uniform $\Gamma = 120$. These profiles show the propagation of heat front corresponding to the first three panels of Figure 6.6. Dashed lines show the location of initial shear layer at $y = \pm 120$. 
Figure 6.9: Time evolution of “full width half maxima” (FWHM) of \( \Gamma(y)_{x=0} \) in the linear regime. Dashed line shows a linear fit having slope \( v_{hf} \approx 0.34 \), which is the propagation speed of the heat front.

Figure 6.10: Time evolution of spatially averaged density variation normalized to initial background density \( (n_0) \). It is clearly seen that the peak density variation is around 4% which is observed close to \( t \sim 800 \). At such late times, inverse cascade has already resulted in the formation of large scale coherent structures in the liquid [see Figure 6.3]
6.7 Development and growth of heat front

\[
\langle \Gamma \rangle_{xy}(t) = \frac{1}{L^2} \int \int \Gamma(x, y, t) dx dy \tag{6.8}
\]

where \( \langle \ldots \rangle_{xy} \) correspond to instantaneous spatial average over the entire 2D system. In Figure 6.7, we show a plot showing the time evolution of \( \langle \Gamma \rangle_{xy} \). The generation of heat in the system is evident from the fall of \( \langle \Gamma \rangle_{xy} \) in time. It should be noted that the total energy of the 2D Yukawa liquid

\[
E = 0.5 \left[ \sum_i N v_i^2 + \sum_{i \neq j}^{N} \frac{1}{r_{ij}} \exp(-\kappa r_{ij}) \right] \tag{6.9}
\]

remains conserved up to \( 10^{-5}\% \) throughout the simulation (not shown here). To further elucidate this spatio-temporal growth of heat front, we obtain the profile of \( \Gamma \) as a function of \( y \) at \( x = 0 \) and plot this at various times (see Figure 6.8). One can clearly see the propagation (“widening”) of heat front starting from a thermally equilibrated background at \( t = 20 \). To aid the reader, we have shown the location of initial shear layer \( (y = \pm 120) \) with vertical dashed lines.

The propagation speed of the heat front can be obtained by from the time evolution of “full width half maxima” (FWHM) of \( \Gamma(y)_{x=0} \) in the linear regime (see Figure 6.9). The dashed line shows a linear fit, the slope of which gives the propagation speed \( v_{hf} \) of the heat front. In our normalized units \( v_{hf} \approx 0.34 \), which is much lesser than the adiabatic sound speed \( c_s \approx 2.4 \) at background \( \Gamma = 120 \). As shown in Figure 6.6, beyond this linear regime, structures begin to develop in the heat front and it no longer remains symmetric about \( \hat{x} \) or \( \hat{y} \). As time evolves and the heat front propagates nonlinearly, one can clearly see the local modulation of grain number density \( n(x, y) \). The deviation from incompressibility can be quantified by taking a spatial average of density variation normalized to background density \( n_0 = 1 \) (in normalized units \( n_0 = 1 \)) as follows:

\[
\left\langle \left| \frac{\Delta n}{n_0} \right| \right\rangle_{xy}(t) = \frac{1}{L^2} \int \int \left| \frac{n_0 - n(x, y, t)}{n_0} \right| dx dy \tag{6.10}
\]
Figure 6.11: Snapshots of density profile $n(x, y)$ for the full system $(\pm 240, \pm 240)$ shown at different times. As the heat front evolves (see Figure 6.6), hot zones expand in size and push grains into nearby cooler zones. This is evident from the reduced densities in hotter zones compared to cooler zones.
In Figure 6.10, we plot the time evolution of $\langle |\Delta n| \rangle_{xy}$ and see that the peak value of density variation is around 4% at $t \sim 800$. At such late times, large scale coherent structures “vortices” have already been formed due to inverse cascade [see Figure 6.3]. The development of heat front and its spatio-temporal growth is also manifested in Figure 6.11, where we show the time evolution density contour plots. One can clearly see the development of both low and high density zones as the time evolves. These zones are the manifestations of onset of hot and cool regions respectively. This is because these hot zones push the particles towards comparatively cooler zones.

6.8 Summary

For the first time, using large scale MD simulations, we have reported, the coevolution of inverse cascade and spatio-temporal growth of a heat front in
parallel shear flows of strongly coupled Yukawa liquids. At a given coupling strength, a subsonic shear profile is superposed on an equilibrated Yukawa liquid and KH instability is observed. The onset of nonlinear regime of the instability is observed by emergence of coherent vortices. The characterization of these coherent vortices is done through grain color coding, contour plots of vorticity $\omega$ and Okubo-Weiss parameter $Q$. Inverse cascading of KH modes towards the largest scales is shown quantitatively. Concurrently, it is seen that shear flows lead to generation of heat at the smallest scales (“particle level”) resulting into the formation of a heat front. The spatio-temporal growth of this heat front is elucidated through the contour plots of inverse temperature $\Gamma$ and grain density $n$. It is seen that the heat front propagates at speeds much lesser than the adiabatic sound speed of the system for the initial equilibrium chosen. It will be interesting to perform the present shear flow studies at supersonic speeds, a subject which we defer for future work. In the following chapter, we present a summary of the work done in this thesis.