Quantifying energetics and dissipation in magnetohydrodynamic turbulence

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ABSTRACT

We perform a suite of two- and three-dimensional magnetohydrodynamic (MHD) simulations with the ATHENA code of the non-driven Kelvin–Helmholtz instability in the subsonic, weak magnetic field limit. Focusing the analysis on the non-linear turbulent regime, we quantify energy transfer on a scale-by-scale basis and identify the physical mechanisms responsible for energy exchange by developing the diagnostic known as spectral energy transfer function analysis. At late times when the fluid is in a state of MHD turbulence, magnetic tension mediates the dominant mode of energy injection into the magnetic reservoir, whereby turbulent fluid motions twist and stretch the magnetic field lines. This generated magnetic energy turbulently cascades to smaller scales, while being exchanged backwards and forwards with the kinetic energy reservoir, until finally being dissipated. Incorporating explicit dissipation pushes the dissipation scale to larger scales than if the dissipation were entirely numerical. For scales larger than the dissipation scale, we show that the physics of energy transfer in decaying MHD turbulence is robust to numerical effects.

Key words: instabilities – magnetic fields – MHD – turbulence.

1 INTRODUCTION

The nature of magnetized gas in astrophysical systems is a long-standing problem. Linear analyses of various fluid configurations demonstrate that instabilities expected to be relevant in astrophysical contexts, such as the magnetorotational instability (MRI; Balbus & Hawley 1991) or the Kelvin–Helmholtz instability (KHI; e.g. Chandrasekhar 1961), can amplify the magnetic field and generate turbulence. However, the subsequent non-linear evolution into magnetohydrodynamic (MHD) turbulence is only accessible by appealing to numerical simulations.

Spectral energy transfer function analysis, first introduced by Kraichnan (1967), is a powerful diagnostic for quantifying energetics and dissipation in MHD turbulence. This diagnostic is able to determine precisely how energy is transferred across spatial scales as a function of both energy type (e.g. kinetic, magnetic, internal) and mediating force (e.g. compression, advection, magnetic tension, magnetic pressure). In addition to probing the energetics of MHD turbulence, the transfer function analysis allows for the scale-by-scale characterization of physical and numerical dissipation. Therefore, the transfer function analysis goes beyond the standard power spectrum diagnostic, which only provides information about the distribution of energy across spatial scales and says nothing about either the energy transfer mechanism or the scales on which energy exchange occurs.

Quantifying MHD turbulence with transfer function analysis experienced a recent revival with the advent of high-performance numerical simulations. Transfer function analysis has far-reaching astrophysical applications, including the turbulent solar dynamo (Pietarila Graham, Cameron & Schüssler 2010), accretion disc turbulence arising from the MRI (Fromang & Papaloizou 2007; Fromang et al. 2007; Simon & Hawley 2009; Simon, Hawley & Beckwith 2009; Davis, Stone & Pessah 2010) and ‘mesoscale’ magnetic structures that arise in local studies of accretion discs with large spatial domains (Simon, Beckwith & Armitage 2012). The transfer function diagnostic also provides a scale-by-scale look into the properties of energy dissipation distributions. For instance, applying a transfer function analysis to accretion disc atmospheric and coronal structure could reveal new insights into accretion power

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dissipation profiles, which have important consequences for the emergent spectra from black hole systems (e.g. Svensson & Zdziarski 1994; Merloni, Fabian & Ross 2000; Turner 2004; Blaes et al. 2006; Hirose, Krolik & Stone 2006; Salvesen et al. 2013).

The aim of this work is to explore the transfer function analysis in detail and further develop this diagnostic for MHD turbulence. Therefore, we seek a well-understood test problem that can generate an MHD turbulent state from generic initial conditions, but is free from potential complications such as strong magnetic field effects, supersonic motions and forcing of the turbulence. Motivated by these criteria, we elect to study the KHI, which is a well-posed linear instability commonly used in code testing (McNally, Lyra & Passy 2012).

Numerical methods are essential for understanding the non-linear development of the KHI. In two spatial dimensions (2D), hydrodynamic simulations of shearing flows by Norman & Hardee (1988) and Bodo et al. (1994, 1995) provided some of the first glimpses into the non-linear evolution of the KHI, followed by extensions into 2D/axisymmetric MHD by Frank et al. (1996), Jones et al. (1997), Jeong et al. (2000), Stone & Hardee (2000) and Palotti et al. (2008). Full three-dimensional (3D) numerical explorations of the KHI were conducted by Norman & Balsara (1993) and Basset & Woodward (1995) in the hydrodynamic limit and by Hardee, Clarke & Rosen (1997), Ryu et al. (2000) and Hardee & Rosen (2002) in full MHD. More recently, Marti, Perucho and Hanasz (2004), Perucho et al. (2004a, 2006), Perucho, Marti & Hanasz (2004b) and Radice & Rezzolla (2012) explored the KHI in relativistic hydrodynamics, while Zhang, MacFadyen & Wang (2009) and Beckwith & Stone (2011) discussed KHI development in relativistic MHD.

The majority of these numerical studies analysed KHI development through the measurement of instability growth rates, saturation behaviours and/or morphological consequences of instability. In this study, we provide a novel look at the development of the KHI by employing the spectral energy transfer function analysis. This approach provides us with insight into the details of the KHI physics that are not otherwise accessible and allows us to determine how integrated flow properties and morphology reflect the scale-dependent processes we identify. Additionally, we discuss how computational issues, such as numerical convergence and the effects of domain size, can be understood and evaluated in terms of KHI development. We will also explore numerical versus physical dissipation behaviours by comparing simulations of decaying MHD turbulence with and without dissipation in the same spirit as done previously for simulations of decaying hydrodynamic turbulence (e.g. Sytine et al. 2000).

While the KHI has important applications to subsonic, transonic, supersonic and relativistic astrophysics, we focus here on understanding the non-linear development and spectral structure of the KHI in the subsonic, weakly magnetized limit. The motivations for this choice are both simplicity and applicability. We wish to apply comprehensive analysis tools – particularly the transfer function analysis – to study the development of the KHI for a simplified case without the complications of additional physics like shock formation or the exchange between different fluid instabilities such as the family of current-driven instabilities (CDI; Begelman 1998). Particular attention is given to properly constructing an initial setup for the simulations and providing convincing evidence that the late-stage development is physical, rather than numerical, in origin. We aim for our numerical study of the KHI to be relevant and extendable to a broad range of astrophysical applications, such as the interplay between the KHI and CDI in jets, the nature of MHD turbulence arising from the KHI and dissipation profiles in accretion discs.

We organize this paper as follows. Section 2 provides descriptions of the ATHENA MHD code and the KHI problem setup. The methodology behind the spectral energy transfer function analysis we adopt is given in Section 3. In Section 4, we discuss the convergence of 3D KHI simulations, along with the inadequacy of 2D simulations. We next describe in Section 5 the evolution of the KHI simulations with a focus on the late-stage turbulent decay and the importance of energy transfer involving the magnetic energy reservoir. The inclusion of physical dissipation is explored in Section 6. Finally, Section 7 presents a summary and discussion of this work, followed by our conclusions in Section 8.

2 NUMERICAL DETAILS

We solve the equations of MHD using the ATHENA code (Stone et al. 2008), a second-order accurate Godunov flux-conservative code. ATHENA is an Eulerian code that solves the equations of compressible, adiabatic MHD in conservative form,

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) 
\]

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} = -\nabla \cdot \left[ \rho \mathbf{v} \mathbf{v} - \mathbf{B} \mathbf{B} + \left( P + \frac{1}{2} B^2 \right) \mathbf{I} - \tau \right] 
\]

\[
\frac{\partial E}{\partial t} = -\nabla \cdot \left[ (E + \frac{1}{2} B^2) \mathbf{v} - \mathbf{B} (\mathbf{B} \cdot \mathbf{v}) \right] 
\]

\[
\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}) + \eta \nabla^2 \mathbf{B} . 
\]

The notation is of familiar form, where \( \rho \) is the density, \( \mathbf{v} \) is the fluid velocity, \( P \) is the gas pressure, \( \mathbf{B} \) is the magnetic field and \( E \) is the total energy density defined by

\[
E = \frac{1}{2} \rho v^2 + \frac{1}{2} B^2 , 
\]

where \( \epsilon = P/(\gamma - 1) \) is the internal energy density for an ideal gas and \( \gamma \) is the adiabatic index, \( \mathbf{I} \) is the identity matrix operating on the total pressure, \( P + B^2/2 \). In the adopted notation, the magnetic field absorbs a factor of \( \sqrt{\mu_0/4\pi} \), where \( \mu_e = 1 \) is the assumed magnetic permeability. The MHD equations (1)–(4) are conservation equations describing, in order, the conservation of mass, momentum, total energy and magnetic flux. Equations (1)–(3) have the generic form of any conservation equation, where the time derivative of a conserved quantity is equal to the divergence of a flux, in the absence of any source/sink terms.

Viscosity enters the momentum equation through the stress tensor,

\[
\tau = \tau_{ij} = 2 \nu \rho \left[ \delta_{ij} - \frac{1}{3} (\nabla \cdot \mathbf{v}) \delta_{ij} \right] , 
\]

where the fluid is assumed to be isotropic, \( \nu \) is the kinematic viscosity, \( \delta_{ij} \) is the Kronecker delta function and the strain rate tensor is \( \epsilon_{ij} = \frac{1}{2} \left[ (\nabla \mathbf{v}) + (\nabla \mathbf{v})^T \right] \). Explicit dissipation enters the induction equation through the Ohmic dissipation term, \( \eta \nabla^2 \mathbf{B} \), where \( \eta \) is the resistivity. In our treatment of ideal MHD, we neglect dissipation terms such as viscosity (i.e. \( \nu = 0 \)), resistivity (i.e. \( \eta = 0 \)) and conduction. We investigate the addition of explicit dissipation

1 The ATHENA code and a repository of test problems are available online at https://trac.princeton.edu/Athena/
terms, following the implementation of Simon et al. (2009), and their effect on the KHI evolution in Section 6.

Gardiner & Stone (2005, 2008) describe the basic algorithms implemented in ATHENA with further details (implementation and multidimensional tests) given in Stone et al. (2008). Specifically, we use the dimensionally unsplit corner transport upwind integrator described by Stone et al. (2008) combined with the constrained transport (CT) method of Evans & Hawley (1988) to maintain the divergence-less nature of the magnetic field in multidimensions. ATHENA implements a variety of options for spatial reconstruction and solution of the Riemann problem. In this work, we use third-order spatial reconstruction in characteristic variables and the HLLC/HLLD Riemann solvers for hydrodynamic/MHD simulations. We avoid choosing the HLLE solver due to its highly diffusive behaviour (for further information, see Appendix A1). Toro (1999) and Leveque (2002) provide descriptions of the HLLC, HLLD and HLL Reimann solvers. In this work, we make extensive use of the conservation properties of ATHENA to examine exchange of energy between kinetic, magnetic and internal energy reservoirs.

2.1 Problem setup

The initial problem setup for numerical simulations of the KHI with ATHENA is shown schematically in Fig. 1. We consider a 3D Cartesian grid centred on \((x, y, z) = (0, 0, 0)\) with dimensions \(L_x = L_y = L_z = L = 1\) and periodic boundary conditions enforced in all directions. Counter-streaming flows are set up along the \(y\)-direction according to the velocity profile,

\[
v_y(z) = \begin{cases} 
U_0 \tanh \left( \frac{|z| - z_0}{a} \right), & |z| \geq z_0 \\
-U_0 \tanh \left( \frac{|z| + z_0}{a} \right), & |z| < z_0,
\end{cases}
\]

where \(2U_0 = 1\) is the magnitude of the relative shear velocity, \(z_0 = 0.25L\) specifies the location of the shear interfaces and \(a = 0.01L\) is a parameter describing the thickness of the shear layer.

A continuous velocity profile is constructed across the shear layers, rather than a discontinuous interface, to ensure that the truncation error resulting from numerical diffusion of unresolved modes (i.e. short wavelength, large wavenumber) does not dominate the solutions (see Appendix A3). The linear growth rate of the KHI is proportional to the wavenumber; thus, an under-resolved shear layer will evolve unphysically into the non-linear regime. The hyperbolic tangent profile we adopt provides a sharp, yet smooth, transition while also introducing the length-scale, \(a\), to an otherwise scale-free problem. For a given grid resolution, \(N_x = N_y = N_z\), the shear layer is resolved by \(4a\sqrt{L}/L\) grid zones, which amounts to \(\sim 20\) resolution elements across the interface for the \(N = 512 \times 3D\) MHD simulation, which is the fiducial run for the majority of the analysis. The wavenumber corresponding to the full width of the shear layer is \(k_a = 2\pi/(4a) \approx 157\); therefore, to resolve modes that grow on the same spatial scale of the shear layer or smaller, the simulation resolution must be adequate, such that the Nyquist wavenumber, \(k_{Ny} = (N/2)(2\pi/L)\), exceeds \(k_a\).

The initial density profile is described by

\[
\rho(z) = \frac{1}{2} \left( \frac{\rho_1}{\rho_2} - 1 \right) \left| \tanh \left( \frac{|z| - z_0}{a} \right) - 1 \right| + 1,
\]

where \(\rho_1 = 2\) is the density of the central fluid slab and \(\rho_2 = 1\) is the density of the surrounding fluid. The contact discontinuity is smeared by the same hyperbolic tangent function applied to the velocity profile to ensure a resolved solution. Initially, the fluid slabs are in gas pressure equilibrium with \(P_0 = 1\) and adiabatic index, \(\gamma = 5/3\). A uniform magnetic field, \(B_0 = B_0 \hat{y}\), is aligned parallel to the shear flow with initial strength, \(B_0 = 0.02\), corresponding to the weakly non-linear regime, meaning that the magnetic field is weak and the flow is not linearly stable. In this regime, the instability is essentially hydrodynamic early on, and then enters the non-linear regime where secondary instabilities break up large-scale structures and magnetic energy is amplified due to twisting/stretching of magnetic field. After saturation, the flow enters a state of decaying MHD turbulence (for a discussion of different stability regimes of the magnetized KHI, see Ryu et al. 2000; Baty & Keppens 2002).

In order to provoke the onset of the KHI, at time \(t = 0\) we impose a small-amplitude, single-mode perturbation to the \(z\)-component of velocity of the form,

\[
v_z(x, y, z) = v_0 \sin(k_z x) \sin(k_y y) e^{-(k_z^2 + k_y^2)z^2/\sigma^2}.
\]

where \(v_0 = 0.01U_0\), \(k_z = k_y = 2\pi/L\) and \(\sigma = 0.1L\) describes the decaying behaviour of the perturbation along the \(z\)-direction. A full perturbation wavelength fits within the \(x\) and \(y\) computational box boundaries. Modes with wavelengths larger than the box scale, \(L\), are not captured.

Table 1 summarizes the set of initial parameters corresponding to each region defined in Fig. 1. All simulations used the

| Region | \(v_y\) | \(P_0\) | \(\rho\) | \(c_s\) | \(B_0\) | \(\rho_0\) | \(v_A\) | \(\sigma_A\) |
|--------|--------|-------|------|------|-------|--------|------|-------|
| 1      | −0.5   | 1     | 2    | 0.91 | 0.39  | 0.02   | 5000 | 0.014 | 35.4  |
| 2      | 0.5    | 1     | 1    | 1.29 | 0.55  | 0.02   | 5000 | 0.020 | 25.0  |

Figure 1. Schematic of the KHI problem setup for the ATHENA simulations. Each side of the computational box has length \(L\), with the origin at the centre, \((x, y, z) = (0, 0, 0)\). Periodic boundary conditions are adopted in all directions. Counter-streaming flows are initiated in the \(y\)-direction, each with speed \(U_0\) in the laboratory frame. A uniform pressure, \(P_0\), fills the box and a uniform magnetic field of strength \(B_0\) is established in the \(y\)-direction. The fluid densities are \(\rho_1\) and \(\rho_2\) in Region 1 and Region 2, respectively. Region 1 is bounded in the \(z\)-direction by \(-z_0 < z < z_0\) and Region 2 corresponds to \(z > |z_0|\), where the shear interfaces are located at \(\pm z_0\). Although not represented in the schematic, the density and velocity profiles across each shear layer are matched continuously by a hyperbolic tangent function, thus permitting the interfaces to be well resolved.
Table 2. Table of KHI simulations referred to in our study. From left to right, the columns give the simulation identification tag, grid resolution in each dimension, time at which the simulation was started from, size of the z-domain (in code units), initial magnetic field strength (in code units), kinematic viscosity coefficient relative to the fiducial value ($v_{\text{id}} = 2.6 \times 10^{-5}$), and Ohmic resistivity coefficient relative to the fiducial value ($\eta_{\text{id}} = 1.7 \times 10^{-5}$).

| ID$^a$ | $N$ | $t_{\text{start}}$ | $L_z$ | $B_0$ | $v/v_{\text{id}}$ | $\eta/\eta_{\text{id}}$ |
|-------|-----|-------------------|-----|------|-----------------|-----------------|
| 3M1024 | 1024 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 3M512 | 512 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 3M256 | 256 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 3M128 | 128 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 2M16384 | 16384 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 2M8192 | 8192 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 2M4096 | 4096 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 2M2048 | 2048 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 3M1024 | 1024 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 3M512 | 512 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 3M256 | 256 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 3M128 | 128 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 2M16384 | 16384 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 2M8192 | 8192 | $t_0$ | 1 | 0.02 | 0 | 0 |
| 2M4096 | 4096 | $t_0$ | 1 | 0.02 | 0 | 0 |

$^a$The ID tag generally follows a straightforward, three-part naming convention. The first number indicates the dimensionality (i.e. 2D or 3D), the letter denotes the gas dynamics used (i.e. M for MHD or H for hydrodynamics) and the trailing number specifies the grid resolution in each direction.

$^b$The shear layer in this simulation was discontinuous, corresponding to the $z$ configuration depicted in Fig. 1. A start time of $t_0$ means the simulation started from the initial KHI configuration, the starting time of the simulation evolved from $t_0$ to the point in the saturated state when the magnetic energy peaked and was then restarted with non-ideal MHD terms introduced.

$^c$Simulations 3M512x2 and 3M512x4 have $N_z = 1024$ and 2048, respectively.

$^d$A start time of $t_0$ means the simulation started from the initial KHI configuration depicted in Fig. 1. A start time of $t_{\text{peak}}$ means the ideal MHD simulation evolved from $t_0$ to the point in the saturated state when the magnetic energy peaked and was then restarted with non-ideal MHD terms introduced.

$^e$A start time of $t_0$ means the simulation started from the initial KHI configuration depicted in Fig. 1. A start time of $t_{\text{peak}}$ means the ideal MHD simulation evolved from $t_0$ to the point in the saturated state when the magnetic energy peaked and was then restarted with non-ideal MHD terms introduced.

$\Delta k$ is constant. To avoid double counting, the spectral energy contained within a shell of thickness $2\Delta k$, $\Delta E(k)$, is computed as the sum total energy contained within a shell that is of interest, rather than merely the spectral shape. To improve statistics and aid in interpretation, the energy power spectra are integrated over concentric spherical shells of thickness, $\Delta k L_{\text{H}}/(2\pi) = 1$, as shown schematically in Fig. 2. This yields the differential power contained within a shell,

$$\frac{dE(k)}{dk} = \frac{\Delta E(k)}{\Delta k}. \tag{14}$$

Figure 2. Schematic representation of how differential spectral energy density is spherically integrated over concentric $k$-shells of constant thickness, $\Delta k$. For a given spectral energy density, $E(k)$, the differential spectral energy density, $\Delta E(k_{i+1/2})$, is computed as the sum total energy contained within a shell of inner boundary $k_i$ and outer boundary $k_{i+1}$, where $\Delta k = k_{i+1} - k_i$ is constant. To avoid double counting, the spectral energy contained at the outer boundary of a shell [i.e. $E(k_{i+1})$ for $\Delta E(k_{i+1/2})$] is omitted, while the energy at the inner boundary is taken to be inclusive. Spectral energy is integrated over shells of thickness $\Delta k L_{\text{H}}/(2\pi) = 1$ from $k_{\text{min}} L_{\text{H}}/(2\pi) = 0$ to $k_{\text{max}} L_{\text{H}}/(2\pi) = k_{\text{N}} L_{\text{H}}/(2\pi) = N/2$. Plots of energy power spectra show the differential spectral energy density contained within a $k$-shell, $dE(k)/dk = \Delta E(k)/\Delta k$. 

3 SPECTRAL ANALYSIS

Throughout this work, we use energy power spectra to examine at which scales the majority of the magnetic energy is generated and how the spectral shape of the different energy reservoirs (i.e. kinetic, magnetic and internal) evolves. The kinetic, magnetic and internal energy power spectra, also referred to as spectral energy densities, are defined as

$$E_k(k) = \frac{1}{2} \left( \bar{w}(k) \cdot [\rho \bar{v}]^T(k) \right) \tag{10}$$

$$E_M(k) = \frac{1}{2} \left( \bar{B}(k) \cdot \bar{B}^T(k) \right) \tag{11}$$

$$E_i(k) = \frac{\rho}{\gamma - 1}, \tag{12}$$

where $k = |k| = \sqrt{k_x^2 + k_y^2 + k_z^2}$, an asterisk superscript denotes a complex conjugate and $\hat{F}(k)$ indicates the Fourier transform of the quantity $f(x)$.

$$\hat{F}(k) = \int \int \int f(x) e^{-i k \cdot x} d^3x. \tag{13}$$

No normalization is performed, as the magnitude of energy transfer is of interest, rather than merely the spectral shape.
centred on half-integer values of wavenumber $k$. Sometimes we will have cause to perform a shell-averaged normalization of spectral energy density (see Section 6) according to

$$\frac{dE(k)}{dk} = \left[ \int k^2 \frac{dE(k)}{dk} dk \right]^{-1} \frac{dE(k)}{dk},$$

(15)

where the angled bracket convention, $dE(k)/dk$, indicates that a shell average was performed on the spectral energy density.

Power spectra describe the distribution of energy across spatial scales; however, such distributions provide no clear way of determining how the energy transfers between scales and different forms (e.g. between magnetic and kinetic energies). Transfer function analysis, first introduced by Kraichnan (1967), allows for the scale-by-scale quantification of energy transfer between reservoirs and identification of the mechanism responsible for the energy exchange. The mechanics of deriving the transfer functions are given in Appendix B, with an outline of the derivations and an explanation of notation given here. In this, we closely follow the approach and interpretation of Pietarila Graham et al. (2010), who rigorously developed a transfer analysis for compressible MHD in the context of the small-scale solar turbulent dynamo. We specialize to the case of the KHI by decomposing the velocity field into contributions from the shearing flow and turbulent fluctuations (Fromang & Papaloizou 2007; Fromang et al. 2007; Simon et al. 2009),

$$\mathbf{v} = \mathbf{v}_{sh} + \mathbf{v}_t,$$

(16)

where $\mathbf{v}_t$ is the turbulent velocity field and $\mathbf{v}_{sh}$ is the background flow field, defined as

$$\mathbf{v}_{sh} = \mathbf{v}_{sh}(z) = \frac{\hat{y}}{L_z} \int \int v_{sh}(x,y,z) dx dy.$$

(17)

Inserting the decomposed velocity field into the momentum, energy and induction equations, taking the Fourier transform and performing the appropriate dot product (see Appendix B), the complete transfer function equations for kinetic, magnetic and internal energies are

$$\frac{dE_K(k)}{dr} = T_{IKC}(k) + S_{IKC}(k) + T_{KKA}(k) + X_{KKA}(k)$$

$$+ T_{KBT}(k) + S_{KBT}(k) + T_{KBMP}(k) + S_{KBMP}(k)$$

$$+ T_{KQC}(k) + S_{KQC}(k) + X_{KQC}(k) + D_K(k),$$

(18)

$$\frac{dE_M(k)}{dr} = T_{BBA}(k) + S_{BBA}(k) + T_{KBRT}(k) + S_{KBRT}(k)$$

$$+ T_{KBMP}(k) + D_M(k),$$

(19)

$$\frac{dE_I(k)}{dr} = T_{KLA}(k) + S_{KLA}(k) + T_{KJC}(k) + D_I(k),$$

(20)

where the notation is time evolution equations of spectral energy densities. Fourier transforms are computed according to equation (13) using a fast Fourier transform algorithm. The shear layer is not driven and is continually decaying; thus, the energy densities in the saturated state are not in a steady state and time derivatives are calculated explicitly.

Following Pietarila Graham et al. (2010), we interpret the transfer function $T, S, X_{XYF}(k)$ as measuring the net energy transfer rate from all scales of reservoir X to scale k of reservoir Y, where the energy exchange is via the force F. The net energy transfer from reservoir X into reservoir Y at scale k is positive (negative) for $T, S, X_{XYF}(k) > 0 (< 0)$. The available energy reservoirs are kinetic (K), magnetic (M) and internal (I). The mediating forces (F) depend on the exact form of each transfer function, but in general these forces are compressive motions (C), advection (A), magnetic tension (T) and magnetic pressure (P). Energy transfer due to purely turbulent motions, $\mathbf{v}_t$, is denoted by $X_{XYF}(k)$, the background shear flow, $\mathbf{v}_{sh}$, by $S_{XYF}(k)$ and some hybrid cross-term involving both $\mathbf{v}_t$ and $\mathbf{v}_{sh}$ by $X_{XYF}(k)$. Finally, the terms $D_K(k), D_M(k)$ and $D_I(k)$ in equations (18)–(20) are simply the residuals of the time derivative of spectral energy density and the sum of all transfer functions, resulting in a measure of numerical dissipation rate as a function of scale (Fromang & Papaloizou 2007; Fromang et al. 2007; Simon et al. 2009).

All transfer functions are spherically integrated over shells of constant thickness $\Delta k L_k/(2\pi) = 1$ and then plotted as $k \cdot (d T_{XYF}(k)/dk)$ versus log(k) so that the peak in the spectrum corresponds to the wavenumber containing the most power (Zdziarski & Gierliński 2004). We choose to time average the transfer functions over the same intervals shown in the energy power spectral analysis of Fig. 10. This improves statistics across all k and allows us to make robust statements regarding energy exchange during different stages of the KHI evolution.

4 CONVERGENCE

In the absence of explicit dissipative terms in the conservation equations (1)–(4), the effective (i.e. numerical) dissipation present in the simulation is governed by the choice of grid resolution. The numerical dissipation, expressed in units of diffusivity as $(\Delta x)^2/\Delta t$, decreases with improved grid resolution for a fixed timestep. As grid resolution elements become finer, small-scale structures are preserved that would otherwise be smeared out by under-resolved simulations whose numerical dissipation scale is too large to capture said structures. Small-scale structures can drive energy exchange and morphological evolution, particularly in the non-linear and turbulent regimes. Therefore, establishing a converged solution is paramount for a physical interpretation of the simulation results.

Convergence, in the formal sense, refers to an unchanging power spectrum across all scales when resolution is increased. However, this is unattainable in inviscid turbulent simulations. Expecting an exact point-to-point match of a quantity between different grid resolutions is inappropriate in the non-linear regime given the turbulent nature of the problem at hand and the presence of numerical dissipation. Instead, we refer to convergence in the sense that quantities integrated over the entire volume do not change appreciably for a factor of 2 increase in $N$, the grid resolution in each dimension. This definition we adopt is colloquially referred to as virtual convergence and is demonstrated as an effective diagnostic in practice (e.g. Palotti et al. 2008; Lemaster & Stone 2009).

Convergence of the linear growth stage of the KHI can be assessed through the volume-averaged root mean square (rms) velocity transverse to the shear layer, $(\mathbf{v}_z^2)^{1/2}$ (e.g. Frank et al. 1996). In this work, angled brackets surrounding a quantity denote volume averages, where the volume average of quantity $Q(x,y,z)$ is given by

$$\langle Q \rangle = \frac{1}{L_x L_y L_z} \int \int \int Q(x,y,z) dx dy dz.$$

(21)

When considering the volume average of a vector quantity, such as the magnetic field, $\mathbf{B}$, we consider the magnitude of that vector quantity, $B = |\mathbf{B}| = (B_x^2 + B_y^2 + B_z^2)^{1/2}$, and take its volume average.

Fig. 3 shows $(\mathbf{v}_z^2)^{1/2}$ for the runs 3M128, 3M256, 3M512 and 3M1024, where the initial value is dictated by the perturbation of the equilibrium configuration. The linear growth phase of the KHI corresponds to the exponentially increasing portion of $(\mathbf{v}_z^2)^{1/2}$. We
choose to parametrize time in terms of the linear growth e-folding time, \(\tau \simeq 0.16\). We evaluate \(\tau\) over the exponentially increasing portion of \((v_z^2)^{1/2}\) according to \((v_z^2)^{1/2} = A e^{\tau / \tau}\), where A is the initial rms transverse velocity and \(\tau\) is time in code units. Although \(\tau\) is decreasingly relevant as the flow becomes turbulent, it is physically motivated and well defined during the linear growth. Fig. 3 shows that the linear growth phase converges even at the lowest 3D resolution considered here, \(N = 128\). The linear growth phase of the instability terminates at \(\tau \simeq 20\), following which \((v_z^2)^{1/2}\) saturates and then decays for \(\tau \gtrsim 30\). During this phase of the evolution, \((v_z^2)^{1/2}\) exhibits non-monotonic behaviour with resolution. As a result, we conclude that \((v_z^2)^{1/2}\) is not a sufficient diagnostic to determine convergence in the non-linear regime. From here onwards, we take convergence to mean in the virtual sense described above.

Fig. 4 shows the time evolution of the volume-averaged magnitude of the magnetic field for sets of 3D MHD simulations at various grid resolutions. This figure serves as a convergence study of the KHI simulations in the non-linear regime, with convergence obtained at \(N = 512\). That is, the difference in evolution of magnetic energy in the non-linear regime of interest (i.e. \(\tau \gtrsim 50\)) between the \(N = 512\) and 1024 simulations is at the 1 per cent level. Based on Fig. 4 and the discussion presented above, we conclude that the decay of turbulence in the non-linear regime is driven by physical, rather than numerical processes. This will be confirmed by the transfer function analysis of Sections 5.3 and 6. We therefore treat \(N = 512\) as our fiducial resolution and the 3M512 run as our fiducial simulation.

By contrast, 2D MHD simulations of the KHI do not exhibit convergence in the non-linear regime. Fig. 5 shows the same quantity as in Fig. 4, but for a series of 2D simulations of the KHI at resolutions up to \(N = 16,384\), with little indication of convergence in the non-linear regime. This is evidenced by the absence of both a consistent peak in the magnetic field and a single sustained value at late times. A more detailed comparison of the evolution of the 2D and 3D KHI is found in Fig. 6, which shows the time evolution of the volume-averaged internal, kinetic and magnetic energies, each normalized by the volume-averaged total energy. Inspecting Fig. 6, the evolution of the energetics in the 2D system shows substantial differences from the 3D case. In particular, the 2D flow is more efficient than the 3D flow at generating magnetic energy from the linear growth e-folding time, \(\tau\), as computed from the fiducial 3M512 simulation.
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available kinetic energy and this magnetic energy is less efficiently dissipated into heat in the 2D case. Internal energy is the dominant energy component and increases throughout the simulation because there is no cooling prescription.

Figure 6. Time evolutions of the volume-averaged quantities: internal energy, \( \langle E_I \rangle \) (top panel), kinetic energy, \( \langle E_K \rangle \) (middle panel) and magnetic energy, \( \langle E_M \rangle \) (bottom panel). All volume-averaged energies are shown relative to the total volume-averaged energy in the computational box, \( \langle E_{\text{tot}} \rangle \). Shown are results for KHI simulations 3M1024 (black dotted lines), 3M512 (black solid lines), 3H512 (red solid lines), 2M8192 (black dashed lines) and 2H8192 (red dashed lines). Magnetic energy is more efficiently generated from the available kinetic energy and less efficiently dissipated for the 2D KHI.

Further evidence of the differences in behaviour of the 2D and 3D KHI can be found through comparison of Figs 7 and 8. These figures show the time-averaged spectral distributions of the magnetic and kinetic energies in the three- and two-dimensional simulations, respectively, compensated by \( k^{4/3} \) to enable visual comparison. Fig. 7 shows that, for the 3D simulations, the spectral distribution of these quantities follows a \( k^{-4/3} \) power law for \( kL/(2\pi) \gtrsim 3 \), over all the resolutions considered. The main effect of increasing resolution is to move the dissipation scale to progressively smaller scales, from \( kL/(2\pi) \sim 10 (N = 128) \) to \( kL/(2\pi) \sim 50 (N = 512) \). As evidenced by Fig. 8, the behaviour of the 2D simulations is different.

Figure 7. Time-averaged, one-dimensional spectral energy densities for simulations 3M128 (dash–dotted lines), 3M256 (dashed lines) and 3M512 (solid lines). Time averages are performed over the non-linear turbulent decay interval, \([t_{\text{peak}}, t_f]\). Top panel: kinetic energy power spectra, \( E_K(k) \). Bottom panel: magnetic energy power spectra, \( E_M(k) \). Spectral energy densities are compensated by a factor of \( k^{4/3} \). Consistent behaviour in both \( E_K(k) \) and \( E_M(k) \) is seen in the non-linear turbulent decay regime across the resolutions studied, with an inertial range emerging at intermediate scales for the 3M512 simulation. The effect of increasing resolution is to shift the dissipation scale to smaller scales (i.e. higher \( k \)).

5 EVOLUTION

Here, we explore in detail the evolution of the non-driven KHI with a focus on the properties of the non-linear MHD turbulent regime. We start with simple volume-averaged quantities to characterize global properties and morphology (Section 5.1) and then use spectral energy densities to quantify the distribution of energy across spatial scales (Section 5.2). Increasing the utility of our analysis diagnostic, we take advantage of the spectral energy transfer function analysis to probe deep into the physics of decaying MHD turbulence (Section 5.3) and later we apply this tool to study dissipation (Section 6). The transfer function diagnostic allows for an in-depth quantification of MHD turbulence in general and here we demonstrate its power by focusing on a well-studied problem – the KHI.

\(^2\) By ‘inverse cascade’ we mean that energy in the magnetic reservoir is initially spectrally dominated at small scales and evolves to become primarily distributed on large scales. We do not mean to imply a dynamo process by using this phrase.
computational box at $t_0 = 0$. The KHI continues to develop into the non-linear stage by $t = t_{G(1/3)}$, at which time two primary commensurate features have been established along each interface with multiple mini-vortices arising from secondary instabilities. The non-linear evolution continues and produces finger-like strands of density, magnetic field and pressure by $t = t_{G(2/3)}$ (not shown in Fig. 9). When the magnetic field reaches its peak amplitude at $t = t_{\text{peak}}$, the shear layer is nearly shredded beyond recognition into turbulence with evidence for the single-mode form of the initial perturbation also nearly erased. At this point in time, the magnetic energy production mechanism (i.e. a driven shear layer) is absent and the magnetic field begins to decay as the fluid motions remain turbulent and the fluid is well mixed. Subsequent evolution of the system to late times is characterized by gradual decay of magnetic energy.

5.2 Spectral energy densities

The time-averaged kinetic and magnetic energy power spectra computed over these same time intervals from the fiducial simulation are shown in Fig. 10. Table 3 provides the spectral slopes for the intermediate scales, $5 \leq kL/(2\pi) \leq 30$, corresponding to each time-averaging interval in Fig. 10. This figure shows that magnetic energy is concentrated in small spatial scales as the KHI begins to develop from the linear to saturated state (i.e. from $t = t_{0.05}$ to $t = t_{\text{peak}}$). As the volume-averaged magnetic field is amplified and peaks, magnetic energy at small scales (i.e. large $k$) grows with a fixed slope, while the spectral shape at small $k$ flattens. By contrast, during this phase of the non-linear evolution, kinetic energy contained on large scales, $kL/(2\pi) \lesssim 30$, retains the same spectral slope and magnitude, while the majority of the kinetic energy amplification occurs on small spatial scales, $kL/(2\pi) \gtrsim 30$, due to the development of small-scale vortices. Once the peak magnetic energy is reached, magnetic energy on large scales decays more gradually than that on small scales, causing the magnetic energy spectrum to steepen. Conversely, kinetic energy on large scales decays more rapidly than that on small scales, causing the kinetic energy spectrum to flatten.

The bottom panel of Fig. 10 makes the comparison of the spectral evolution of magnetic and kinetic energies explicit. As the KHI develops from the linear regime towards the turbulent regime, the $E_M(k)/E_k(k)$ spectrum tends to increase and level off with increasing $k$. This behaviour was also observed in the relativistic MHD KHI simulations of Zhang et al. (2009). The equipartition point of magnetic and kinetic energies slides towards larger scales for the entirety of the evolution, until magnetic energy dominates over kinetic energy across nearly all scales at the termination of the simulation. Although the individual kinetic and magnetic energy spectra are decreasing in amplitude after $t = t_{\text{peak}}$, the equipartition point continues to shift towards lower $k$.

5.3 Spectral energy transfer function analysis

The time-averaged transfer functions associated with energy exchange with the magnetic energy reservoir are shown in Fig. 11 and provide a quantification of magnetic energy sources/sinks as a function of scale $k$. Only the transfer functions associated with turbulent motions (i.e. the $\nu_i$ piece of the velocity decomposition) are plotted, as we found that the transfer functions associated with pure shear (i.e. $S_{XYF}$) and cross-terms (i.e. $X_{XYF}$) are negligible players in energy transfer in comparison.

We first consider energy transfer during the stages of the KHI development leading up to saturation (i.e. from $t = t_{0.05}$ to $t = t_{\text{peak}}$).
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Figure 9. 2D slices taken in the $yz$-plane at $x = 0.5L$ from the 3M512 simulation at times $t_{G1/3}$ (first row), $t_{\text{peak}}$ (second row) and $t_f$ (third row). From left to right, the columns show the gas density, $\rho$, magnetic field strength relative to the initial value, $B/B_0$, logarithm of the vorticity magnitude, $\log(|\nabla \times v|)$, and logarithm of the current density magnitude, $\log(|\nabla \times B|)$. The bracketed numbers above each column mark the [minimum, maximum] parameter values for the linear-scale colour bar used to plot the respective quantity in all rows of the column. By the saturation time, $t_{\text{peak}}$, the initial shear layer is destroyed and the flow enters a state of decaying turbulence.

The dominant growth mechanism of magnetic energy at large and intermediate scales is due to turbulent motions twisting/stretching magnetic field lines [i.e. $T_{\text{BKT}}(k) < 0$ and $T_{\text{KBT}}(k) > 0$]. Transfer inside the magnetic energy reservoir by turbulent velocities [i.e. $T_{\text{BBA}}(k)$] is responsible for an inverse cascade of magnetic energy. Work done against magnetic pressure gradients by turbulent compressive motions [i.e. $T_{\text{BBP}}(k)$ and $X_{\text{BBP}}(k)$] is negligible in comparison to other magnetic transfer mechanisms. Although not plotted, we inspected the kinetic energy transfer functions and found the following behaviour. The dominant contribution to large-scale kinetic energy growth between $t = t_{10\%}$ and $t = t_{\text{peak}}$ is from advection\(^3\) within the kinetic energy reservoir [i.e. $T_{\text{KKA}}(k)$ and $X_{\text{KKA}}(k)$]. Ancillary contributions come from both compressible turbulent motions within the kinetic energy reservoir [i.e. $T_{\text{KKC}}(k)$ and $X_{\text{KKC}}(k)$] and transfer from the internal energy reservoir by compression [i.e. $T_{\text{IKC}}(k)$ and $S_{\text{IKC}}(k)$]. Meanwhile, energy is being transferred out of the kinetic energy reservoir on these large scales into the magnetic energy reservoir by turbulent fluid motions twisting/stretching the magnetic field [i.e. $T_{\text{BKT}}(k) < 0$]. The small-scale growth of kinetic energy during this time is overwhelmingly dominated by the same magnetic tension force\(^4\) acting on turbulent motions that causes kinetic energy loss on large scales. To summarize the KHI evolution...

\(^3\) Here, and henceforth, ‘advection’ is used to refer to the transfer of energy between scales but within the same form. For example, the ‘advection’ of kinetic energy from large to small scales.

\(^4\) Here, and henceforth, ‘tension’ is used to describe the restoring force directed along the radius of curvature that is exerted by bent magnetic field lines. We do not mean to imply that the magnetic field is always putting tension on the fluid.
leading up to saturation, we find that the magnetic field grows first at small scales and then cascades to larger scales, which is evidence for an inverse cascade operating in the KHI. The dominant energy exchange mechanism involves turbulent fluid motions interacting with magnetic tension.
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Figure 12. Time-averaged, one-dimensional spectral energy transfer functions associated with energy transfer into/out of the magnetic energy reservoir for the 3M512 simulation for the time-averaging interval \([t_{\text{peak}}, t_{i}]\). The fluid is in a state of decaying turbulence over this interval in time. The lines shown here are a representation of the data from the solid lines and dotted lines in Fig. 11, but placed on the same scale to allow for relative comparisons. The transfer functions shown are \(T_{\text{BBA}}(k)\) (solid line), \(T_{\text{BKT}}(k)\) (dotted line), \(T_{\text{KBT}}(k)\) (dash-dotted line), \(T_{\text{BKP}}(k)\) (short-dashed line) and \(T_{\text{KBP}}(k)\) (long-dashed line). Energy transfer is dominated by exchanges within the magnetic energy reservoir [i.e. \(T_{\text{BBA}}(k)\)] and transfer mediated by magnetic tension [i.e. \(T_{\text{BKT}}(k)\) and \(T_{\text{KBT}}(k)\)]. Magnetic pressure effects are small in comparison due to the weakly compressive nature of the subsonic and sub-Alfvenic flow studied here.

We now turn our attention to times after \(t = t_{\text{peak}}\), where the fluid is in a turbulent state and energy decays away by numerical dissipation. From \(t = t_{\text{peak}}\) onwards, when the simulation box is fully turbulent and the shear layer is destroyed, a transition occurs where the subsequent evolution of the kinetic energy spectrum over all scales is determined primarily by interactions with the magnetic energy reservoir. Fig. 12 shows the energy transfer between magnetic energy transfer functions in the time-averaged decay stage from \(t = t_{\text{peak}}\) to \(t = t_{i}\). As before, exchanges within the magnetic energy reservoir and transfer mediated by magnetic tension dominate the magnetic energetics, with exchange by magnetic pressure gradients being negligible across all scales. Magnetic energy is supplied by large-scale, \(kL/(2\pi) \lesssim 10\), kinetic energy loss due to turbulent fluid motions working against the magnetic tension force, as evidenced by negative values of \(T_{\text{BKT}}(k)\) on large scales. The positive values of \(T_{\text{KBT}}(k)\) on intermediate scales peaking at \(kL/(2\pi) \approx 80\) indicate that magnetic energy is also being placed into intermediate-scale kinetic energy by the reversal of the process just described. Note that the transfer function \(T_{\text{BKT}}(k)\) reveals that a significant amount of energy is being exchanged, but one cannot say on what scales it is distributed in the magnetic energy reservoir. Presumably, some of this large-scale kinetic energy is transferred into large-scale magnetic energy. The kinetic energy reservoir contributes a modest amount of intermediate/small-scale magnetic energy via work done on the magnetic field by fluid motions, as shown by positive values of \(T_{\text{KBT}}(k)\). Most of the small-scale magnetic energy comes from turbulent transfer within the magnetic energy reservoir from large to small scales (i.e. \(T_{\text{BBA}}\) transitions from negative to positive values going from large to small scales). Thus, Fig. 12 tells a story of a mechanism for ongoing large-scale magnetic energy production and a turbulent cascade from large to small scales within the magnetic energy reservoir. This small-scale energy is exchanged forwards and backwards with the kinetic energy reservoir and is gradually dissipated, allowing the magnetic field to keep a relatively sustained value in the absence of a driven shear layer.

Finally, we perform an inventory of energy transfer operating in the KHI over the late-time turbulent decay stage from \(t_{\text{peak}}\) to \(t_{i}\) for the fiducial simulation 3M512. Separately collecting the positive and negative contributions from each transfer function involved with exchange with the magnetic energy reservoir allows one to determine the total magnetic energy gain and loss rates due to energy exchanges,

\[
\frac{dE_{M}^{+}}{dt} = \int [T_{\text{BKT}}^{+}(k) + T_{\text{KBT}}^{+}(k) + T_{\text{KBP}}^{+}(k) + T_{\text{BKP}}^{+}(k)] \, dk
\]

(22)

\[
\frac{dE_{M}^{-}}{dt} = \int [T_{\text{BKT}}^{-}(k) + T_{\text{KBT}}^{-}(k) + T_{\text{KBP}}^{-}(k) + T_{\text{BKP}}^{-}(k)] \, dk
\]

(23)

The ± notation in the superscript indicates whether the positive (i.e. \(\geq 0\)) or negative (i.e. \(< 0\)) component of the transfer function should be taken. We find a time-averaged magnetic energy gain rate of \((dE_{M}^{+}/dt) = 4.4 \times 10^{-3}\) and loss rate of \((dE_{M}^{-}/dt) = -2.3 \times 10^{-3}\). This gives a time-averaged net magnetic energy gain rate due to energy transfer with the magnetic energy reservoir of \((dE_{M}^{\text{tot}}/dt) = 2.1 \times 10^{-3}\), all in code units. Note that the transfer functions describing the magnetic energy cascade [i.e. \(T_{\text{BBA}}(k)\) and \(S_{\text{BBA}}(k)\)] are not included in this inventory because they cannot contribute to overall magnetic energy gain or loss.

Table 4 lists the relative contributions of each transfer function involved in magnetic energy gain and loss rates (see equations 22 and 23) averaged from \(t_{\text{peak}}\) to \(t_{i}\). Stretching and twisting of magnetic field lines by the turbulent velocity field [i.e. \(T_{\text{BKT}}(k)\) and \(T_{\text{KBT}}(k)\)] is the dominant exchange mechanism at work during late times, accounting for 83 and 81 per cent of energy transfer leading to magnetic energy gain and loss, respectively. Magnetic pressure is a negligible contributing transfer mechanism for the subsonic and sub-Alfvenic flows we consider.

To understand the two-way energy flow into/out of the magnetic energy reservoir, we consider the total time-averaged magnetic energy exchange rate, \((dE_{M}^{\text{tot}}/dt) = |(dE_{M}^{+}/dt)| + |(dE_{M}^{-}/dt)|\), and construct a schematic diagram in Fig. 13 that tracks the contributions of each transfer function to \((dE_{M}^{\text{tot}}/dt)\). Fig. 13 illustrates that the kinetic energy reservoir interacts with the large-scale field and injects energy into the magnetic energy reservoir. This energy cascades down to smaller scales and is exchanged backwards and forwards with the kinetic energy reservoir, before ultimately being dissipated. The turbulent cascade from large to small scales [i.e. \(T_{\text{BBA}}(k)\)] operates on 61 per cent of \((dE_{M}^{\text{tot}}/dt)\), making the cascade within the magnetic energy reservoir an effective mechanism for breaking down magnetic structures.

Simultaneously with the magnetic energy reservoir exchange described by the transfer functions are net magnetic energy loss rates resulting from both the decaying nature of the MHD turbulence (i.e. \(dE_{M}/dt)\) and numerical dissipation of magnetic energy.
Table 4. Percentage breakdowns of the contributions to the magnetic energy gain and loss rates by transfer function. The leftmost column shows the time-averaged magnetic energy transfer rate, where the superscripts denote + for gain and — for loss. The rightward columns list the percentage contribution from each transfer function involved in magnetic energy exchange. Notably, energy transfer mediated by turbulent motions (i.e. the \( v_i \) component of \( \mathbf{v} \) interacting with the magnetic tension force) is the primary player in energy exchange with the magnetic energy reservoir.

| Transfer rate     | \( \langle dE_M^T/dt \rangle \) | \( \langle dE_M^B/dt \rangle \) | \( \langle dE_M^{TB}/d\tau \rangle \) | \( \langle dE_M^{KS}/d\tau \rangle \) | \( \langle dE_M^{TB}/d\tau \rangle \) | \( \langle dE_M^{TB + KS}/d\tau \rangle \) |
|-------------------|------------------------------|------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| (per cent)        | (per cent)                   | (per cent)                   | (per cent)                      | (per cent)                      | (per cent)                      | (per cent)                      |
| \( T_{BKT} \) (3%) | 53.9                         | 7.4                          | 29.0                            | 6.8                             | 0.5                             | 2.4                             |
| \( S_{BKT} \) (3%) | 69.5                         | 0.6                          | 11.7                            | 0.0                             | 5.0                             | 4.6                             |
| \( T_{KBRT} \) (4%) |                             |                              |                                 |                                 |                                 |                                 |
| \( S_{KBRT} \) (24%) |                             |                              |                                 |                                 |                                 |                                 |

Figure 13. Diagram showing the contributions from transfer functions to the two-way energy exchange between the kinetic and magnetic energy reservoirs at late times. Percentages in parentheses indicate the amount of energy exchange into that reservoir as described by the associated transfer functions, relative to the time-averaged total energy exchange rate, \( \langle dE_M^T/dt \rangle \), over the time interval \([t_{peak}, t_f]\). The dominant scales (i.e. small, large, all) across which the energy transfer operates are indicated for each exchange path. For instance, transfer of large-scale kinetic energy into the magnetic energy reservoir by twisting/stretching of magnetic field by fluid motions (i.e. \( T_{BKT} < 0 \) and \( S_{BKT} < 0 \)) is responsible for 40 per cent of the total energy exchange. The line styles are chosen to overlap with those of Fig. 12. Magnetic tension is the dominant transfer mechanism for exchanges into/out of the magnetic energy reservoir. The kinetic/magnetic energy reservoir interactions result in a net magnetic energy gain rate. This energy then cascades from large to small scales and is further exchanged forwards and backwards with the kinetic energy reservoir until it is ultimately dissipated.

6 DISSIPATION

The extremely large Reynolds numbers that characterize astrophysical flows suggest that it is appropriate to carry out numerical simulations of the same flows in the inviscid, flux-freezing regime, where explicit dissipation terms are omitted from the momentum and induction equations. In nature, however, astrophysical flows have some small, but finite amount of viscosity and resistivity, which violates the assumption of an inviscid, flux-frozen flow. In a turbulent flow, such as that considered here, it is these dissipation terms that mediate the dissipation of small-scale turbulent structures and conversion of magnetic and kinetic energies contained in these structures into thermal energy. When performing calculations in the inviscid, flux-freezing regime, simulators hope that the details of dissipation, which are provided by the algorithm, have little influence on large to intermediate scales. If dissipation does influence these scales, simulators hope that the details of the numerical dissipation are sufficiently similar to physical dissipation such that the simulation remains an accurate representation of the physical system. This non-trivial issue regarding the validity of relying on numerical dissipation to adequately capture the behaviour of physical dissipation in simulations is what we address in this section.

Fig. 14 shows shell-averaged (see Section 3) spectral energy densities obtained from simulations of decaying turbulence arising from the KHI with explicit dissipation added to the momentum and induction equations. Specifically, we include the effects of kinematic shear viscosity and Ohmic resistivity. The data of the convergence study presented in Fig. 7 are also shown in Fig. 14 for comparison. The simulations with explicit dissipation were initialized from the fiducial MHD simulation, 3M512, at \( t = 6 \). We found that kinematic shear viscosity and Ohmic resistivity coefficients, \( v = 3.25 \times 10^{-5} \) and \( \eta = 2.125 \times 10^{-6} \) (Pm = \( \nu/\eta \) = 1.53, simulation 3M512D \( t_{peak} \)), produced a small, but non-negligible change in the magnetic and kinetic spectral energy densities over the time interval \( t_{peak} \) to \( t_f \) compared to the fiducial simulation. The dissipation coefficients were then increased by a factor of 2 (at fixed magnetic Prandtl number, Pm, and initialized from \( t = 6 \) of...
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3M512) until the magnetic and kinetic spectral energy densities provided a close match to those obtained from simulation 3M256. This occurs for simulation 3M512D_{fid}^{1/2}, where \( v_{\text{fid}} = 2.6 \times 10^{-3} \) and \( \eta_{\text{fid}} = 1.7 \times 10^{-5} \) (where subscript ‘fid’ denotes that we treat these as our fiducial values), a factor of 8 increase over the dissipation coefficients found to match 3M512. This result suggests that the numerical dissipation in the KHI problem is determined by the order of spatial reconstruction. To demonstrate that this scaling holds generally for \( \textsc{athena} \)-run KHI models would require an ensemble of 3D simulations including dissipation, which is beyond the scope of this work.

Fig. 15 examines the convergence of the simulations using the fiducial dissipation coefficients, where the data from the ideal MHD convergence study presented in Fig. 7 are included for comparison. At resolutions lower than \( N = 512 \) (i.e. \( N = 128, 256 \)), we find that numerical dissipation plays an increasingly important role. In particular, there is a close correspondence across all scales between the simulations at \( N = 128 \) with \( 3M128D_{1/2}^{\nu} \) and without \( 3M128D_{1/2}^{\nu} \) contributions from explicit dissipation, indicating that solutions at this resolution are dominated by effects due to numerical dissipation. The \( N = 256 \) case with the fiducial dissipation coefficients, \( 3M256D_{1/2}^{\nu} \), matches the large-scale behaviour of 3M28 and the small-scale behaviour of 3M256. As noted previously, the \( N = 512 \) case with the fiducial dissipation coefficients, \( 3M512D_{1/2}^{\nu} \), provides a close match to results obtained for 3M256 at all scales. The primary difference from 3M256 is a small power deficit for 3M512D_{1/2}^{\nu}. All simulations are compensated by \( k^{4/3} \). Numerical dissipation becomes a more dominant contributor to the total dissipation with decreasing numerical resolution.

\[ \langle k \rangle \]
The dissipation scale refers to the approximate turnover scale where the dissipation rate is such that it is comparable to the transfer function, \( k \eta \nu / 1 \). This scale is often associated with a peak in the dissipation transfer function, \( D(k) \), and is influenced by the numerical dissipation rate, \( \eta \), and the viscosity, \( \nu \), of the fluid. At scales around the dissipation scale, \( kL/(2\pi) \sim 30 \), due to power being transferred over to smaller scales, \( kL/(2\pi) \sim 100 \), where there is a slight power excess. We regard the simulation using the fiducial dissipation coefficients as being converged at \( N = 512 \) for two reasons. First, we already demonstrated that simulations conducted in ideal MHD are converged at this resolution (see Section 4), implying that numerical dissipation plays a small role in simulations at this resolution. Secondly, for simulations incorporating physical dissipation terms, convergence implies that the dissipation scale is determined by the dissipation terms themselves rather than numerical effects. Therefore, we can conclude that the dissipation scale associated with \( \nu_{\text{fid}}, \eta_{\text{fid}} \) is resolved at \( N = 512 \).

With these arguments in mind, Fig. 16 compares transfer functions associated with energy exchange with the magnetic energy reservoir for simulations 3M512D\(_{16}^\nu\) and 3M256, time averaged over the interval \([t_{\text{peak}}, t_f]\). At large spatial scales, \( k \leq 5 \), the transfer functions for 3M512D\(_{16}^\nu\) and 3M256 are well matched. At intermediate scales, \( 5 \leq k \leq 30 \), the transfer functions are well matched for transfer within the magnetic energy reservoir through advection, \( T_{\text{BBA}}(k) \), and transfer from magnetic energy to kinetic energy through tension forces, \( T_{\text{BKT}}(k) \). By contrast, we see greater transfer from kinetic to magnetic energy through tension, \( T_{\text{BKT}}(k) \), at these intermediate scales for 3M512D\(_{16}^\nu\) than for 3M256. At small scales, \( k \geq 30 \), we see that peaks in the transfer functions are shifted to smaller scales in 3M512D\(_{16}^\nu\), as compared to 3M256, as a consequence of the higher numerical resolution in this simulation. Finally, at all scales, the effect of dissipation is to reduce the (already small) contribution of energy transfer through compressive motions, \( T_{\text{KBT}}(k) \) and \( T_{\text{KBP}}(k) \). Overall, these results demonstrate the robustness of the physics of energy transfer within decaying MHD turbulence to the effects of numerical dissipation at scales larger than the dissipation scale.

The transfer functions associated with explicit dissipation take the form (see Appendix B)

\[
T_r(k) = \frac{\nu}{2} \left( \frac{1}{\rho} \left[ (\nabla \cdot \tau)^* \right](k) + \nabla \cdot (\nabla \cdot \tau)^*(k) \right) \tag{24}
\]

\[
T_\eta(k) = \eta \left( \hat{B} \cdot (\nabla^2 \hat{B})^*(k) \right). \tag{25}
\]

These are plotted in Fig. 17 for simulations 3M256 and 3M512D\(_{16}^\nu\). Note that for ideal (i.e. inviscid, \( \nu = 0 \) and non-resistive, \( \eta = 0 \)) MHD simulations, such as 3M256, the physical dissipation transfer functions \( T_r(k) \) and \( T_\eta(k) \) do not contribute to the overall energy transfer inventory, but are instead computed for the sake of establishing ‘effective’ quantities. The effective dissipation transfer function data of 3M256 adopt \( \nu_{\text{fid}} \) and \( \eta_{\text{fid}} \) to enable comparison with \( T_r(k) \) and \( T_\eta(k) \) from 3M512D\(_{16}^\nu\). Also shown in Fig. 17 for both simulations are the quantities \( D_r(k) \) and \( D_\eta(k) \). These numerical dissipation rates are derived by calculating the residual between the terms in equations (18) and (19) [including \( T_r(k) \) and \( T_\eta(k) \)]
for 3M512D[\text{\textsuperscript{\text{H}}}] and the total dissipation rates (\(\xi_k(k)\) and \(\xi_M(k)\)) for simulation 3M512D[\text{\textsuperscript{\text{H}}}] . The total kinetic and magnetic energy dissipation rates are expressed as

\[
\xi_k(k) = T_k(k) + D_k(k) 
\]

(26)

\[
\xi_M(k) = T_M(k) + D_M(k). 
\]

(27)

Fig. 17 shows that the spectral distribution of \(T_k(k)\) and \(T_M(k)\) is very similar between the two simulations for scales larger than the dissipation scale and that the spectral distribution of numerical dissipation in 3M256 is very close to that expected from physical dissipation close to the grid scale (i.e. small scales). A further point comes from comparing physical and numerical dissipation in simulation 3M512D[\text{\textsuperscript{\text{H}}}]. For this simulation, physical dissipation, \(T_k(k)\), dominates over numerical dissipation, \(D_M(k)\), for the magnetic energy dissipation terms by a factor of \(\sim 100\) for \(2 \leq kL/(2\pi) \approx 30\). However, the same is not true for the kinetic energy dissipation terms, where physical dissipation, \(T_k(k)\), and numerical dissipation, \(D_k(k)\), are relatively comparable to within a factor of \(\sim 2\) over this range of scales. Similar levels of numerical and physical kinetic energy dissipation could be due to the computation of derivatives that are required for the viscous stress tensor, \(\tau\), and the associated divergence, \(\nabla \cdot \tau\). The same considerations do not apply for the addition of Ohmic diffusion to the induction equation due to the use of the CT algorithm for these terms, which may explain why physical magnetic energy dissipation greatly exceeds numerical magnetic energy dissipation on scales larger than the dissipation scale.

7 SUMMARY AND DISCUSSION

We performed a suite of 2D and 3D simulations of the KHI in the weakly magnetized, subsonic regime with a non-driven shear layer, focusing on the results of a high-resolution 3D MHD simulation. The problem setup, though simple and straightforward, was scrutinized in detail, paying particular attention to dimensionality (2D versus 3D), convergence and properly resolving the shear layer in order to make a convincing argument for the physical nature of the KHI development beyond the linear growth. After establishing the basic evolution of energetics using volume-averaged energies and time-averaged energy power spectra, we took advantage of the energy conserving nature of \textsc{athena} to investigate the spectral structure of the KHI development into MHD turbulence using the spectral energy transfer function analysis. We then extended this analysis to characterize both numerical and physical dissipation in \textsc{athena}. Here, we discuss our results.

Two-dimensional MHD simulations of the KHI (e.g. Frank et al. 1996; Jones et al. 1997; Jeong et al. 2000; Bucciantini & Del Zanna 2006) are attractive due to their ability to achieve high resolution relative to their 3D counterparts. However, a demonstration of convergence of the resulting turbulent flow is required to justify 2D studies of MHD turbulence arising from the KHI. We observe well-converged solutions of the initial growth of the 2D KHI at the moderate resolution \(N = 512\), which justifies the linear growth stage of the 2D KHI as a highly reliable, robust test for code verification as suggested by McNally et al. (2012). However, the saturated state and level of magnetic energy sustainment fail to converge even out to the extremely high 2D resolution \(N = 16384\), as evidenced by both the time evolution of the volume-averaged magnetic field strength (see Fig. 5) and the changing shape of spectral energy densities with resolution (see Fig. 8). In stark contrast to the 2D case, 3D simulations of the KHI reliably converge at a resolution \(N = 512\) over the full course of evolution out to the turbulent and decaying stages.

Time evolutions of volume-averaged energetics and slices of the simulation volume reveal a decline in kinetic energy and growth of magnetic energy to a saturated level, at which time the shear layers are almost completely disrupted. The subsequent evolution leads to turbulence with a sustained, but gradually decaying, magnetic field. This general evolution is also observed in relativistic MHD simulations of the KHI when the driving mechanism is switched off (Bucciantini & Del Zanna 2006; Zhang et al. 2009; Drake & MacFadyen 2011). These studies adopt either a discontinuous shear layer, use a Riemann solver of type HLLE or both. We find that the decline in kinetic energy during the non-linear growth and generation of a sustained magnetic field is robust to the details of the initial setup and Riemann solver used (see Appendix A). We confirm the results of the relativistic MHD study of the KHI of Beckwith & Stone (2011) in the Newtonian regime using a linearized Riemann solver. While the generic result of the appearance of a saturated state is unaffected, we caution against using a setup with an unresolved interface and/or the HLLE Riemann solver for quantitative studies of the KHI.

The spectral distributions of kinetic and magnetic energies for 3D KHI simulations at late times follow an approximate \(k^{-4/3}\) power law on intermediate scales, \(5 \leq kL/(2\pi) \approx 30\), remaining unaltered for all resolutions considered (see Fig. 7). A spectral slope \(\alpha_{\text{K}}^{-4/3}\) over intermediate scales also appeared in the strong-field-driven supersonic MHD turbulence studies of Lemaster & Stone (2009) for 3D resolutions of \(N = 512\) and 1024. The effect of increasing numerical resolution is to move the dissipation scale to smaller scales. The magnetic-to-kinetic energy spectral equipartition point shifts to larger scales throughout the simulation evolution (see Fig. 10). Performing a study of relativistic, ideal MHD turbulence arising from the KHI, Zhang et al. (2009) claim that this observed evolution of the \(E_M(k)/E_K(k)\) equipartition point indicates that the kinematic viscous dissipation is more efficient than the magnetic resistive dissipation. However, this conjecture was not based on a direct study of dissipation. Fig. 18 shows the ratio of total magnetic to kinetic energy dissipation rates in the turbulent regime for simulations with (3M512D[\text{\textsuperscript{\text{H}}}]) and without (3M256, 3M512) explicit dissipation included. Fig. 18 demonstrates that magnetic energy dissipation actually exceeds kinetic energy dissipation across the majority of scales, \(k \gtrsim 10\). Therefore, the shift in the \(E_M(k)/E_K(k)\)

\[
\frac{E_M(k)}{E_K(k)} 
\]

Figure 18. Ratio of total (i.e. numerical + physical, if applicable) magnetic to kinetic energy dissipation rates for simulations 3M512 (solid line), 3M256 (dashed line) and 3M512D[\text{\textsuperscript{\text{H}}}].
equi-partition point in Fig. 10 is instead a consequence of the exchange of large-scale kinetic energy into the magnetic energy reservoir mediated by turbulent motions acting against magnetic tension (i.e. fluid motions twisting/stretching magnetic field lines). This is evidenced by the dominating negative values of the transfer function $T_{BK}(k)$ in Figs 11 and 12. Therefore, large-scale kinetic energy loss to the magnetic energy reservoir, rather than competing dissipation rates, is the true mechanism behind the shift in the $E_{sk}(k)/E_{k}(k)$ equi-partition point to large scales as the KHI evolves non-linearly. Transfer function analysis resolved this ambiguity and this example illustrates that the transfer function diagnostic is a powerful tool for studying how energy is transferred across scales and forms.

Spectral energy transfer analysis allows for both the scale-by-scale quantification of energy transfer between reservoirs and identification of the mechanism responsible for the energy exchange. This information is inaccessible from power spectra alone. As the KHI develops to a saturated state, the growth of magnetic energy is dominated by the magnetic tension force interacting with turbulent motions and an inverse cascade is observed. This means that magnetic energy is initially concentrated on small scales and then evolves to a spectrum dominated on large scales (see Fig. 11). At late times following saturation when the fluid is in a decaying turbulent state, we find no evidence for dynamo operation for a single-fluid treatment. This is contrary to claims from simulations of decaying turbulence arising from relativistic MHD KHI studies (Zhang et al. 2009). Kinetic energy contained in turbulent fluid motions is transferred to magnetic energy, primarily mediated by interactions with the magnetic tension force, and a turbulent cascade from large to small scales operates within the magnetic energy reservoir. This small-scale magnetic energy is interchanged forwards and backwards with the kinetic energy reservoir and is eventually dissipated, allowing the magnetic energy to decay. For the subsonic and sub-Alfvénic relative flow considered in this work, compressible effects are of ancillary importance in energy transfer.

By their nature, numerical simulations exhibit dissipative behaviour due to finite numerical resolution. Even in instances where physical dissipation terms are explicitly included in the solution of the MHD conservation equations, numerical dissipation is still present at some level. We found that the most important effect of increasing numerical resolution for ideal MHD simulations was to move the dissipation scale to progressively smaller scales. While energy dissipation in ideal MHD simulations occurs preferentially on the grid scale, physical dissipation should act across all scales. Therefore, determining the extent to which numerical dissipation affects MHD turbulence when physical dissipation is present is non-trivial. We found that when the numerical resolution was held fixed, the location of the dissipation scale moves to larger spatial scales when physical dissipation is incorporated (3M512D$^{a}_{15}$) compared to the corresponding ideal MHD simulation (3M512). This result indicates that it is the dissipation terms that determine the dissipation scale, rather than numerical effects. The physical dissipation scale is considered to be resolved when the dissipation scale (i.e. the turnover in the power spectrum at large $k$) moves to larger spatial scales than in the case without explicit dissipation terms included. In this sense, the effective resolution of the simulation, by which we mean the location of the dissipation scale, is reduced by construction. Furthermore, when physical dissipation is introduced, the magnitude of numerical dissipation is diminished and the spectral characters of the transfer functions (i.e. general shapes and relative proportions) involved in exchange with the magnetic energy reservoir are well matched to their ideal MHD counterparts. These observations indicate the robustness of the physics of energy transfer in decaying MHD turbulence to the effects of numerical dissipation, at least for scales larger than the dissipation scale where numerical effects do not dominate.

8 CONCLUSIONS

We list our conclusions here followed by some astrophysical implications of this work.

(i) 3D KHI simulations converge – in the virtual meaning (see Section 4) – across all stages of evolution. The main effect of further increasing numerical resolution is to push the numerical dissipation scale to smaller spatial scales without changing the shape of the power spectrum.

(ii) For subsonic, weakly magnetized, decaying turbulence arising from the non-driven KHI, the spectral distributions of kinetic and magnetic energy for 3D simulations follow an approximate $k^{-4/3}$ power law on intermediate scales.

(iii) Spectral energy transfer function analysis is a powerful diagnostic for quantifying energetics and dissipation in MHD turbulence.

(iv) At late times corresponding to decaying MHD turbulence, energy is injected into the magnetic reservoir as a result of kinetic energy interactions with the large-scale magnetic field. This magnetic energy turbulent cascades down to smaller scales and is exchanged backwards and forwards with the kinetic energy reservoir, before ultimately being dissipated.

(v) Incorporating explicit dissipation terms reduces the importance of numerical dissipation and moves the dissipation scale to larger spatial scales. For the levels of physical dissipation considered, introducing dissipation terms does not grossly alter the overall shape of the kinetic and magnetic energy power spectra.

(vi) The nature of numerical dissipation does not affect the physics of energy transfer within decaying MHD turbulence at scales larger than the dissipation scale, as evidenced by comparing the relative strengths of the transfer functions and dissipation rates.

Our investigation of the subsonic KHI in the weak magnetic field limit and the generalized spectral energy transfer function techniques we exploit serve as a launching point for future studies of MHD turbulence and the extension to more targeted astrophysical applications of the KHI.

In addition to serving as a direct examination of KHI physics, this work provides a valuable baseline for investigations of shear layers in astrophysical systems also subject to the family of CDI. Such systems could potentially feature either sharp shear layers, such as those explored by Baty & Keppens (2002) or Mizuno, Hardee & Nishikawa (2011), or more gradual profiles, such as those examined analytically by Nalewajko & Begelman (2012). Regardless of the details, it should be possible to compare growth rates of systems unstable to the KHI and CDI to both analytic estimates of linear growth and those rates measured empirically in this work. This will enable differentiation between CDI (O’Neill, Beckwith & Begelman 2012) and KHI contributions (this work) to energy evolution in these systems. Furthermore, one could compare the non-linear evolution of turbulence examined here to similar turbulence that develops in joint KHI/CDI systems to determine how turbulent spectra, energy partitioning and saturation levels differ between the two scenarios.

The transfer function machinery developed and used here can be applied to other astrophysically relevant systems. In particular, consider the Simon et al. (2012) simulations of magnetized...
accretion discs in the ‘mesoscale’ regime (i.e., scales much larger than a vertical scaleheight but much less than the disc radius). These simulations show that as larger disc scales are captured within the domain, turbulence driven by the MRI (Balbus & Hawley 1998) develops structures on these larger scales at the expense of small-scale structures. This behaviour is indicative of either an inverse cascade of energy or direct communication between small scales and large scales. In either case, applying our transfer function analysis to these mesoscale simulations will lead to a better understanding of energy flow in MRI turbulent discs.

While astrophysical scenarios often lend themselves nicely to powerful computational studies, various obstacles (e.g. numerical convergence, multitude of important physical processes, wide range in physical and temporal scales) force numerics to omit certain physics. When restricted to the ideal (i.e. inviscid and non-resistive) MHD limit, one often conjectures that numerical dissipation behaves sufficiently similarly to physical dissipation, even in situations where dissipation may be an important physical process for the problem at hand. For instance, dissipation of turbulence arising from the MRI is an important problem in compact object accretion disc physics, yet these studies are commonly performed in the ideal MHD limit. As an example, attempts to model the effect of the vertical dissipation profile on the emergent accretion disc spectrum are very important for understanding observations of X-ray binaries (Turner 2004; Blaes et al. 2006; Hirose et al. 2006). A reasonable question to ask is whether numerical dissipation leads to unwanted numerical artefacts in the absence of physical dissipation. Our work demonstrates that the details of numerical dissipation do not affect the physics of KHI-produced MHD turbulence on scales larger than the dissipation scale. Therefore, studies of ideal MHD turbulence conducted with codes comparable to Athena are not plagued by numerical effects due to the nature of numerical dissipation.

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APPENDIX A: NUMERICAL ISSUES

Here, we address some of the numerical issues in the KHI simulations with the ATHENA code in order to justify our particular setup.

A1 Riemann solvers

The available suite of Riemann solvers implemented in ATHENA for approximating physical fluxes across cell interfaces are the Roe, HLLD and HLLE solvers for MHD and the exact, Roe, HLLC and HLLE solvers for hydrodynamics (for descriptions of Riemann solvers, see Toro 1999 and Leveque 2002). Waves travelling between grid cells are dispersive and wave propagation can be visualized as a Riemann `fan', with the fastest moving `leftward' and `rightward' waves defining the fan edges and an ensemble of intermediate-speed waves composing the fan. The HLLD and HLLC solvers consider many intermediate-speed waves when computing fluxes, while the HLLE solver omits these waves and only accounts for the fastest waves propagating in each direction. Unlike the HLL family of Riemann solvers, the Roe solver constructs the exact solution to a linearized form of the equations at the cell interfaces.

Fig. A1 shows the comparison of Riemann solver performance in ATHENA for the two-dimensional KHI in hydrodynamics and MHD. Note that the simulations shown in Fig. A1 are equivalent to the 2H2048 and 2M2048 runs, except with different choices for the Riemann solver – these additional simulations are not listed in Table 2. While all solvers capture similar linear growth rates as measured from the magnetic energy evolution, the HLLE solver diverges from Roe and HLLD during the onset of the non-linear evolution. Specifically, magnetic energy in the HLLE run saturates at a level approximately 30 per cent less than that of the Roe solver and spends a much longer time at a saturated state prior to entering the decay phase of the instability. Such diffusive behaviour in the HLLE solver has been reported in other contexts (Mignone, Ugliano & Bodo 2009; Beckwith & Stone 2011; O’Neill, Beckwith & Begelman 2012), all of which suggest that previous investigations of the magnetized KHI that rely on the HLLE solver (e.g. Bucciantini & Del Zanna 2006; Zhang et al. 2009) may suffer from similar effects. In our KHI simulations, we use the HLLC and HLLD solvers exclusively for hydrodynamics and MHD, respectively, with the h1allwave configure option turned on to include the full interpolated Riemann fan.

A2 Linear growth

To demonstrate that our computational setup indeed produces sensible linear growth of the KHI, we compared the development of a simple, equal density realization of the KHI simulated with ATHENA to estimates of linear growth provided in Chandrasekhar (1961) and Miura & Pritchett (1982). The expression in Chandrasekhar (1961) describes the growth of an infinitesimally sharp shear layer in an incompressible, weakly magnetized fluid as $\Gamma \sim k U_0$ (using our notation), which corresponds to a value of $\Gamma \sim 3$ in our code units. The growth rates in Miura & Pritchett (1982) are more applicable to our setup in that they incorporate a finite-width shear layer and compressibility, but unfortunately rely on the approximation that the modes are short in wavelength compared to the box size, which is not satisfied for our $k = 2\pi/L$ perturbations. The maximum growth rate from Miura & Pritchett (1982) most appropriate for our setup is $\Gamma \sim 7$, which is considerably faster than that of Chandrasekhar (1961) because it occurs on a much smaller physical scale. Empirically, our fastest growth rates are measured to be $\Gamma \sim 5$, which falls comfortably between the two estimates. Furthermore, when we conducted KHI test cases featuring perturbations considerably smaller in scale than $L$, we found growth rates more comparable to those in Miura & Pritchett (1982). We therefore conclude that the linear development of the KHI in our simulations is consistent with theoretical expectations for the instability.

Figure A1. Comparison of Riemann solver performance in 2D KHI simulations with resolution $(N_x \times N_y) = (2048 \times 2048)$ computed with the ATHENA code. Top panel: time evolution of volume-averaged kinetic energy, $\langle E_K \rangle$, relative to the volume-averaged total energy in the computational box, $\langle E_{tot} \rangle$, for hydrodynamic simulations performed with the exact (green line), HLLC (black line), HLLE (red line) and Roe (blue line) solvers. The evolution of $\langle E_K \rangle$ is essentially independent of the chosen solver in hydrodynamical simulations. Bottom panel: time evolution of volume-averaged magnetic energy, $\langle E_M \rangle$, multiplied by a factor of 5 (solid lines) and volume-averaged kinetic energy, $\langle E_K \rangle$ (dashed lines), each relative to $\langle E_{tot} \rangle$, for MHD simulations performed with the HLLD (black line), HLLE (red line) and Roe (blue line) solvers. The saturation level of $\langle E_M \rangle$ for the run adopting the HLLE solver is $\sim 30$ per cent below that of the runs that used the HLLD and Roe solvers.
A3 Discontinuous versus resolved shear layers

An inadequately resolved shear interface may result in the accumulation of numerical truncation error, causing unphysical realizations of the subsequent evolution. To quantify the degree to which the energetics are affected by the presence of an unresolved shear layer, we repeated the 3M512 simulation with the hyperbolic tangent interfaces for velocity and density replaced by jump discontinuities,

\[ v_y(z) = \begin{cases} U_0, & |z| \geq z_0 \\ -U_0, & |z| < z_0 \end{cases} \quad (A1) \]

\[ \rho(z) = \begin{cases} 1, & |z| \geq z_0 \\ 2, & |z| < z_0 \end{cases} \quad (A2) \]

We refer to this simulation as 3M512J, where the J refers to the jump discontinuities in velocity and density across the shear interfaces. Fig. A2 compares the time evolution of the volume-averaged rms velocity transverse to the shear layers, \( \langle v_y^2 \rangle^{1/2} \), for the cases of resolved (solid line) and discontinuous (dotted line) interfaces. The initial onset of instability for 3M512J occurs sooner than that in 3M512 because the accumulation of truncation errors at the interface permits perturbations at smaller scales (i.e. faster growth rates) than those would be available for a finite-width shear layer. Despite the triggering of the KHI from an unresolved interface, the ultimate saturation and late-time evolution of 3M512J remain similar to that of 3M512.

A4 Extending the domain transverse to the shear layer

The choice of periodic boundary conditions was motivated by its ease of implementation and its attractive consequence of energy conservation within the domain. As the KHI evolves to the non-linear regime, propagating waves and fluid that exit through one boundary will re-enter through the opposite boundary and interact with the flow. A potential concern is that cross-boundary interactions do not grossly affect the asymptotic shape of the decay phase even if they do adjust its levels.

APPENDIX B: DERIVATION OF SPECTRAL ENERGY TRANSFER FUNCTIONS

Spectral energy transfer analysis was first introduced in the incompressible limit by Kraichnan (1967). Transfer analysis is a well-developed tool for studying MHD turbulence in the incompressible (Debliquy, Verma & Carati 2005; Verma, Ayyer & Chandra 2005) and compressible (Fromang & Papaloizou 2007; Fromang et al. 2007; Simon et al. 2009; Pietarila Graham et al. 2010) limits. Transfer theory was outlined for compressible MHD in Pietarila Graham et al. (2010), which was a generalization of the incompressible treatment of Alexakis, Mininni & Pouquet (2005). Here, we expand on the transfer analysis of Pietarila Graham et al. (2010) by incorporating a decomposed velocity, thus separating the transfer mechanisms involving the velocity field into components due to the background shear flow and turbulent motions. This allows one to distinguish between energy transfer arising due to turbulence and that due to the background flow.

The basic philosophy behind deriving the transfer functions is to start by taking the complex conjugate of the Fourier transform of the conservation equations to obtain time evolution equations of energy densities in Fourier space. The Fourier transformed conservation equations are then dotted with the Fourier transform of the appropriate quantity. The result is the time derivative of a spectral energy density being equated to many individual terms. These terms are the transfer functions and describe energy transfer from one energy reservoir to another, mediated by a force. In what follows, we derive the magnetic, kinetic and internal energy transfer functions, each in turn.

The primitive form of the induction equation is

\[ \frac{dB}{dt} = \nabla \times (v \times B), \quad (B1) \]

where \( B \) is the magnetic field and \( v \) is the fluid velocity field. We decompose the velocity field into a turbulent velocity, \( v_t \), and a shear velocity, \( v_{sh} \), according to

\[ v = v_{sh} + v_t, \quad (B2) \]

where

\[ v_{sh} = v_{sh}(z) \hat{y} = \frac{\hat{y}}{L_x L_y} \int v_y(x, y, z) \, dx \, dy. \quad (B3) \]
Replacing the velocity field in equation (B1) with the decomposed velocity defined by equation (B2), taking the complex conjugate of the Fourier transform, where the Fourier transform of a quantity \( f(x) \) is given by

\[
\tilde{F}(k) = \iiint f(x)e^{-ik \cdot x} \, dx,
\]

and dotting the result with \( \tilde{B}(k) \), we obtain the equation representing the transfer of magnetic energy in \( k \)-space,

\[
\frac{dE_M(k)}{dt} = T_{BBA}(k) + S_{BBA}(k) + T_{KBT}(k) + S_{KBT}(k)
+ T_{KBP}(k) + D_M(k).
\] (B5)

The left-hand side is the time derivative of the spectral magnetic energy density, where

\[
E_M(k) = \frac{1}{2} \tilde{B}(k) \cdot \tilde{B}^*(k).
\] (B6)

The terms on the right-hand side of equation (B5) are the magnetic energy transfer functions. We first describe the transfer function notation and then identify each term explicitly. Transfer functions with the notation \( T_{XY}(k) \) depend only on turbulent velocities, \( \nu \), those with notation \( S_{XY}(k) \) depend only on the background shear velocity, \( \nu_s \), and those with notation \( X_{XY}(k) \) have a mixed velocity dependence. As described by Pietarila Graham et al. (2010), the transfer function \( T, S, X_{XY}(k) \) measures the net energy transfer rate from all scales of reservoir X to scale k of reservoir Y, where the energy exchange is mediated by the force F. The net energy transfer from reservoir X into reservoir Y at scale k is positive (negative) for \( T, S, X_{XY}(k) > 0 \) \( < 0 \). In other words, energy is lost by reservoir X and gained by reservoir Y at scale k for \( T, S, X_{XY}(k) > 0 \) and vice versa for \( T, S, X_{XY}(k) < 0 \). The available energy reservoirs are kinetic (K), magnetic (M) and internal (I). The cascade of magnetic energy to other scales from within the magnetic energy reservoir is described by the terms

\[
T_{BBA}(k) = -\tilde{B}(k) \cdot [(\nu \cdot \nabla) \tilde{B}]^*(k)
\] (B7)

\[
S_{BBA}(k) = -\tilde{B}(k) \cdot [(\nu_s \cdot \nabla) \tilde{B}]^*(k).
\] (B8)

The transfer of energy from the kinetic energy reservoir to the magnetic energy reservoir by turbulent (\( T \)) and shearing (\( S \)) fluid motions that twist and stretch field lines are

\[
T_{KBT}(k) = \tilde{B}(k) \cdot [(\nabla \cdot \nu) \tilde{v}]^*(k).
\] (B9)

\[
S_{KBT}(k) = \tilde{B}(k) \cdot [(\nabla \cdot \nu_s) \tilde{v}]^*(k).
\] (B10)

Magnetic energy transfer from the kinetic energy reservoir by compressive motions via the magnetic pressure force is given by

\[
T_{KBP}(k) = -\tilde{B}(k) \cdot [\tilde{B} \cdot (\nabla \cdot \nu_s)]^*(k),
\] (B11)

where there is no \( S_{KBP}(k) \) transfer function with a background shear velocity dependence because

\[
\nabla \cdot \nu_s = \frac{d\nu_s(z)}{dy} = 0.
\] (B12)

Formally, the magnetic energy transfer function expression (equation B5) is analytically exact in the omission of the numerical magnetic energy dissipation term, \( D_M(k) \). However, numerical schemes have dissipative effects. Therefore, any inequality that arises from comparing the time derivatives of spectral energy densities on the left-hand side to the sum of the transfer function terms on the right-hand side is folded into \( D_M(k) \), which is a measure of the numerical magnetic dissipation. The other transfer function equations will have associated numerical dissipation terms as well.

The kinetic energy transfer functions are derived in a similar fashion as was done for the magnetic energy transfer functions. Starting from the primitive form of the momentum equation,

\[
\frac{\partial \nu}{\partial t} = -\rho (\nu \cdot \nabla) \nu - \nabla P + (\nabla \times B) \times B,
\] (B13)

and the conservative form of the momentum equation,

\[
\frac{\partial (\rho \nu)}{\partial t} = -\nabla \cdot \left[ \rho \nu \nu - BB + \left( P + \frac{1}{2}B^2 \right) I \right],
\] (B14)

the velocities in each of these equations are decomposed according to equation (B2). Here, \( \rho \) represents the mass density, \( P \) is the pressure and \( I \) is the identity matrix. The complex conjugate of the Fourier transform of equation (B13) is dotted with \( \rho \nu \) and the complex conjugate of the Fourier transform of equation (B14) is dotted with \( \nu \). Combining these two resulting equations yields the expression representing the transfer of kinetic energy in \( k \)-space,

\[
\frac{dE_K(k)}{dt} = T_{KKC}(k) + S_{KKC}(k) + T_{KKA}(k) + X_{KKA}(k)
+ T_{BKT}(k) + S_{BKT}(k) + T_{KBP}(k) + S_{KBP}(k)
+ T_{KK}(k) + S_{KK}(k) + X_{KK}(k) + D_K(k).
\] (B15)

where the spectral kinetic energy density is defined by

\[
E_K(k) = \frac{1}{4} \left( \tilde{\nu}(k) \cdot [\rho \tilde{\nu}]^* (k) + [\rho \tilde{\nu}] (k) \cdot \tilde{\nu}^*(k) \right).
\] (B16)

The transfer functions describing the exchange of kinetic energy from within the kinetic energy reservoir by compressible motions due to turbulence and background shear are

\[
T_{KKC}(k) = -\frac{1}{2} \left( \tilde{\nu}(k) \cdot [\nu_s (\nabla \cdot \rho \tilde{\nu})]^* (k) \right)
\] (B17)

\[
S_{KKC}(k) = -\frac{1}{2} \left( \tilde{\nu}(k) \cdot [\nu_s (\nabla \cdot \rho \tilde{\nu})]^* (k) \right),
\] (B18)

respectively. The corresponding cross-term transfer function is

\[
X_{KKC}(k) = \frac{1}{2} \left( \tilde{\nu}(k) \cdot [\nu_s (\nabla \cdot \rho \tilde{\nu})]^* (k) \right) + \tilde{\nu}(k) \cdot [\nu_s (\nabla \cdot \rho \tilde{\nu})] (k)
\] (B19)

The transfer of energy within the kinetic energy reservoir by advection is described by the transfer functions,

\[
T_{KKA}(k) = \frac{1}{2} \left( [\rho \tilde{\nu}] \cdot [\nu_s (\nabla \cdot \nu)]^* (k) \right)
\] (B20)
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Generally speaking, the transfer functions involving mixed velocity terms, which are denoted by $X_{XYF}(k)$, are not intuitively graspable. However, these cross-terms only appear for the transfer functions describing the energy cascade within the kinetic energy reservoir by compressive motions and advection. Energies transferred from the magnetic energy reservoir to the kinetic energy reservoir by fluid motions via the magnetic tension force are
\begin{equation}
\frac{d}{dk} B_{1} = \frac{1}{2} \left\{ \frac{1}{\rho} \nabla \cdot (B \cdot \nabla) B \right\} (k) + \frac{1}{2} \left\{ \frac{1}{\rho} \nabla B^2 \right\} (k) + \nabla \cdot \left\{ (B \cdot \nabla) B \right\} (k),
\end{equation}
(B22)

and by compressive turbulent fluid motions via the magnetic pressure force are
\begin{equation}
\frac{d}{dk} B_{2} = \frac{1}{2} \left\{ \frac{1}{\rho} \nabla \cdot (B \cdot \nabla) B \right\} (k) + \frac{1}{2} \left\{ \frac{1}{\rho} \nabla B^2 \right\} (k) + \nabla \cdot \left\{ (B \cdot \nabla) B \right\} (k).
\end{equation}
(B23)

Finally, the transfer functions describing energy exchange from the internal energy reservoir to the kinetic energy reservoir by compressive motions are
\begin{equation}
T_{KKC}(k) = -\frac{1}{2} \left\{ \frac{1}{\rho} \nabla \cdot (B \cdot \nabla) B \right\} (k) + \frac{1}{2} \left\{ \frac{1}{\rho} \nabla B^2 \right\} (k) + \nabla \cdot \left\{ (B \cdot \nabla) B \right\} (k).
\end{equation}
(B24)

Again, following the same procedure as for deriving the magnetic and kinetic energy transfer functions, we start with the internal energy equation
\begin{equation}
\frac{\partial P}{\partial t} = -\nabla \cdot P + \gamma P \nabla \cdot v,
\end{equation}
(B28)

where $\gamma$ is the adiabatic index. Decomposing the velocity in this equation according to equation (B2) and multiplying the complex conjugate of the Fourier transform by $\hat{P}(k)$, the equation describing the transfer of internal energy in $k$-space becomes
\begin{equation}
\frac{dE_{I}(k)}{dt} = T_{KIA}(k) + S_{KIA}(k) + T_{KIC}(k) + D_{I}(k).
\end{equation}
(B29)

The internal energy density in $k$-space is defined as
\begin{equation}
E_{I}(k) = \hat{P}(k) \gamma - \frac{1}{\gamma - 1}.
\end{equation}
(B30)

and the transfer functions associated with energy exchange from the kinetic energy reservoir to the internal energy reservoir by advection and compressive motions are
\begin{equation}
T_{KIA}(k) = -\frac{1}{\gamma - 1} \sqrt{\hat{P}(k)} \left\{ \frac{1}{\sqrt{\hat{P}}}(v_{i} \cdot \nabla) P \right\} (k),
\end{equation}
(B31)

\begin{equation}
S_{KIA}(k) = -\frac{1}{\gamma - 1} \sqrt{\hat{P}(k)} \left\{ \frac{1}{\sqrt{\hat{P}}}(v_{i} \cdot \nabla) P \right\} (k),
\end{equation}
(B32)

\begin{equation}
T_{KIC}(k) = \frac{\gamma}{\gamma - 1} \sqrt{\hat{P}(k)} \left\{ \frac{1}{\sqrt{\hat{P}}} \nabla \cdot (\hat{P} \cdot v_{i}) \right\} (k).
\end{equation}
(B33)

The transfer function analysis presented above can be extended to the case of a viscous and resistive fluid. We derive these additional dissipation transfer function terms following the procedure outlined in Fromang & Papaloizou (2007) and Simon et al. (2009).

Turning our attention first to the induction equation, the inclusion of Ohmic resistivity introduces the term, $\eta \nabla^2 B$, to the right-hand side of equation (B1), where $\eta$ is the resistivity. Taking the complex conjugate of the Fourier transform for this Ohmic dissipation term and dotting it with $\hat{B}(k)$ yields
\begin{equation}
T_{\eta}(k) = \eta \left\{ \hat{B}(k) \cdot \left[ \nabla^2 B \right] (k) \right\}.
\end{equation}
(B34)

Incorporating viscosity would add the terms $(\nabla \cdot \tau)/\rho$ and $(\nabla \cdot \tau)$ to the right-hand sides of equations (B13) and (B14), respectively, where the stress tensor for an isotropic fluid is
\begin{equation}
\tau_{ij} = 2\mu \left\{ \varepsilon_{ij} - \frac{1}{3} (\nabla \cdot v) \delta_{ij} \right\},
\end{equation}
(B35)

where $\mu$ is the dynamic viscosity, $\delta_{ij}$ is the Kronecker delta function and the strain rate tensor is given by
\begin{equation}
\varepsilon_{ij} = \frac{1}{2} \left[ (\nabla v) + (\nabla v)^T \right].
\end{equation}
(B36)

One can show that
\begin{equation}
\nabla \cdot \tau = \mu \nabla \cdot \left\{ \left[ (\nabla v) + (\nabla v)^T \right] - \frac{2}{3} (\nabla \cdot v) \delta_{ij} \right\} = \mu \left[ \nabla^2 v + \frac{1}{3} (\nabla \cdot v) \right].
\end{equation}
(B37)
The dynamic viscosity is related to the kinematic viscosity, \( \nu \), by 
\[ \nu = \frac{\mu}{\rho}. \]
Taking the complex conjugate of the Fourier transform of the viscous term and dotting the conservative form with \( \hat{\mathbf{v}}(k) \) and the primitive form with \( [\rho \mathbf{v}](k) \) gives the transfer function describing the viscous dissipation,

\[
T_v(k) = \frac{\nu}{2} \left( [\rho \mathbf{v}] \cdot \left( \frac{1}{\rho} \mathbf{V} \cdot \mathbf{r} \right)^\ast \mathbf{v} - \mathbf{v} \cdot (\mathbf{V} \cdot \mathbf{r})^\ast \right) (k). \tag{B38}
\]

Note that due to the non-linear nature of the resistive and viscous terms, we choose not to decompose the velocity field in the definitions of \( T_\eta(k) \) and \( T_v(k) \) in order to simplify their interpretations.