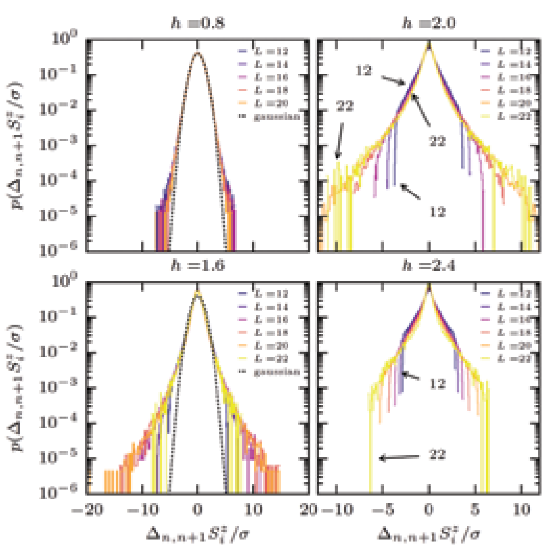

FIGURE 1: Probability distribution of the difference in local magnetization for states from the center of the spectrum of the random Heisenberg chain at disorder strength h. The distributions are normalized by their variance to compare their shapes for different chains of length L and their mean is zero. At weak disorder, the distributions are close to Gaussian and become increasingly non-Gaussian in the regime where transport is subdiffusive. The MBL critical point in this system is around h_c~3.7(1) [5].

many generic systems, noteworthy counterexamples have been discovered, one of which are many-body localized (MBL) systems [1], which violate ETH and do not thermalize.

MBL systems have been mostly explored in one dimension, due to the enormous computational complexity of the problem, caused by the exponential growth of the many-body Hilbert space, and the best-studied systems to date are interacting quantum spin chains with disorder (cf. e.g. [4,5]). In these, a transition between a thermal ETH phase and an MBL phase can be observed and the focus of our work lies in the transition and its vicinity to better understand how the thermalization mechanism breaks down at a critical strength of disorder. We use both concepts from ETH, mostly local operators like the local magnetization, and concepts from quantum information theory, like the entanglement entropy, to study the transition.

METHODS & RESULTS

We use state-of-the-art large-scale exact diagonalization techniques for the sparse Hamiltonian to obtain high energy eigenstates (cf. [5]), which are crucial for directly addressing the ETH. To leading order, local observables in the basis of eigenstates are required by the ETH to be diagonal matrices with Gaussian fluctuations around the mean (and around zero in the off-diagonal entries), whose variance vanishes exponentially with system size. We have studied the behavior of these matrix elements by a systematic study of the probability distributions of the local magnetization for various system sizes and strengths of disorder. This was achieved by calculating histograms of the matrix elements in the eigenbasis at zero energy transfer over a large number of eigenstates and realizations of disorder. Our main finding is that at weak disorder, the ETH ansatz is well-verified and the distributions are very close to a Gaussian distribution, whose variance scales with the exponential law in system size as predicted by ETH. However, at intermediate disorder, this is no longer true and the distributions become strongly non-Gaussian, while the variance of the distribution decreases slower than expected from ETH. In the MBL phase, ETH is violated and the variance of the (non-Gaussian) distributions does not decrease with system size, thus not leading to thermalization.

In ongoing work, we explore whether the deviation from the scaling of the variance from the ETH ansatz as well as the non-Gaussian distributions are linked to the subdiffusive transport, observed in the same parameter regime by previous studies [6, 7].

The MBL transition can also be addressed using concepts from quantum information theory, most prominently by the entanglement entropy (EE). The entanglement entropy can be viewed as the thermodynamic entropy of a subsystem if the rest of the system is considered to be the heat bath. This leads to the requirement from ETH, to the fact that thermodynamic entropies are extensive, and that if the system thermalizes, the EE has to scale by a volume law. Contrarily, in the MBL phase, this is explicitly broken and the EE displays an area law. We consider the transition between these two behaviors in our current work and develop a formalism based on general concepts (strong subadditivity of EE) that allows for a quantification of the EE scaling of single eigenstates in inhomogeneous systems. The erratic behavior of the EE as a function of subsystem size in disordered systems seems at first not to allow for such an analysis but we prove in [9] that in periodic chains, the EE is a concave function of subsystem size, if one averages over all cuts of the same length (cf. Fig. 2). By an extensive analysis of the probability distributions of the slope of this cut averaged EE as a function of subsystem size, we find that in the critical regime, a mixture of volume and area law states appears, which opens new questions about the nature of the MBL transition.

WHY BLUE WATERS

The numerical study of quantum many-body systems is an extremely hard problem that requires massive computational resources. Here, we consider disordered systems, which makes the problem harder by several orders of magnitude as one has to average over many configurations of disorder. The disorder corresponds basically to the effect of "dirt" on the system and is modeled by random potentials.

Solving the Schrödinger equation for one realization of such a dirty system already requires more than one node of Blue Waters for large systems and repeating this calculation for hundreds to thousands of configurations is only feasible on a massively parallel setup like Blue Waters.

PUBLICATIONS AND DATA SETS

Luitz, D. J., Long tail distributions near the many-body localization transition. *Phys. Rev. B* 93 (2016), 134201, DOI: 10.1103/PhysRevB.93.134201

Yu, X., D.J. Luitz, and B.K. Clark, Bimodal entanglement entropy distribution in the many-body localization transition, *arXiv*:1606.01260.

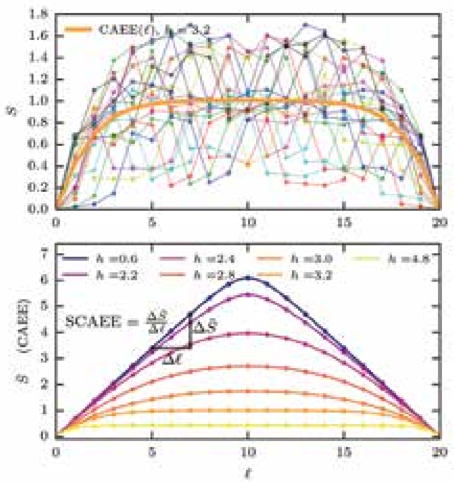

FIGURE 2: Top: Entanglement entropy as a function of subsystem size for one high-energy eigenstate of a random Heisenberg chain of length L=20 and at disorder strength h=3.2 for all possible left cut positions. The erratic behavior is completely removed by the average over all cut positions (CAEE). Bottom: Typical cut averaged EE curves for single eigenstates at various disorder strengths with well-defined slope (SCAEE).

DNS AND STOCHASTIC STUDY OF THE RELATIVE MOTION OF HIGH INERTIA PARTICLES IN ISOTROPIC TURBULENCE

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EXECUTIVE SUMMARY

The objective of our research is to investigate the role of turbulence in driving the relative velocities and positions of inertial particles in isotropic turbulence. First, we studied the effects of turbulence on the relative motion of high-inertia particle pairs in isotropic turbulence. Accordingly, we performed direct numerical simulations (DNS), as well as Langevin simulations (LS) based on a probability density function (PDF) kinetic model for pair relative motion. Recently, we developed a stochastic theory that derives closures in the limit of high Stokes number for the diffusivity tensor in the PDF equation for particle pairs. The diffusivity contained the time integral of the Eulerian two-time correlation of fluid relative velocities seen by pairs that are nearly stationary. The two-time correlation was determined analytically using the

approximation that the temporal change in the fluid relative velocities seen by a pair occurs principally due to the advection of smaller eddies past the pair by large scale eddies. Hence, two diffusivity expressions were obtained based on if the pair center of mass remained fixed during flow time scales, or moved in response to integral-scale eddies.

A quantitative analysis of the aforementioned stochastic theory is performed through a comparison of the particle pair statistics obtained using LS with those from DNS. LS consists of evolving the Langevin equations for pair separation and relative velocity, which is statistically equivalent to solving the Fokker-Planck form of the pair PDF equation. LS of particle pair dispersion were performed using three closure forms of the diffusivity—i.e., one containing the time integral of the Eulerian two-time correlation of the seen fluid relative velocities, and two analytical diffusivity expressions. In the first closure form, the two-time correlation was computed using DNS of forced isotropic turbulence laden with stationary particles. The three diffusivities are extensively analyzed to quantify the effects of the approximations made in deriving them. Pair relative-motion statistics obtained from the three sets of Langevin simulations are compared with the results from the DNS of (moving) particle-laden forced isotropic turbulence for St_η = 10, 20, 40, 80 and Re_λ = 76, 131. Here, St_η is the particle Stokes number based on the Kolmogorov time scale, and Re_λ is the Taylor micro-scale Reynolds number.

INTRODUCTION

The turbulence-driven relative motion of high-inertia particles is relevant in astrophysical scenarios, such as the interstellar medium, protoplanetary disks, and the atmospheres of planets and dwarf stars. Specifically, the "sticking" of dust particles in protoplanetary disks is believed to be the mechanism for planetesimal formation. An intriguing question that astrophysicists are investigating concerns the effects of turbulence on the dispersion, sedimentation, collisional coalescence and fragmentation of dust grains. The viscous relaxation times, τ_v, of these particles are significantly large, with estimated St_η ~ 10-100, where $St_\eta = \tau_v/\tau_\eta$ is the Stokes number based on the Kolmogorov time scale τ_η.

The two principal quantities describing the relative motion of inertial particles in a turbulent flow are the radial distribution function (RDF), which is a measure of the particle spatial clustering, and the PDF of pair relative velocities, which quantifies the particle encounter rate. The RDF and the relative velocity PDF are both key inputs to the particle collision kernel and depend sensitively on the Stokes number. Both statistics can be determined through DNS of particle-laden turbulent flows. However, DNS suffers from the well-known computational limitation on the Reynolds numbers that can be achieved. This drawback of DNS is one of the motivating factors for developing PDF equation-based stochastic models for particle-laden turbulent flows.

We developed a stochastic theory for the relative velocities and positions of high-inertia pairs in forced isotropic turbulence [1]. The theory involved deriving a closure for the diffusivity tensor characterizing the relative-velocity-space diffusion current in the PDF kinetic equation of particle-pair separation and relative velocity. Since we had considered the St_r >> 1 limit, the pair PDF equation is of the Fokker-Planck form (St_r is the Stokes number based on the time-scale τ_r of eddies whose size is of the order of pair separation r). Using the diffusivity formulation, one can perform Langevin simulations of pair relative velocities and positions, which is equivalent to simulating the Fokker-Planck equation.

In this context, the current study has two main objectives. First, we perform a quantitative analysis of the three forms of the diffusivity derived in [1]. The insights gained will help us understand the implications of the approximations made in deriving the diffusivities, as well as guide future improvements to the theory. The second objective is to compute the relative motion statistics of particle pairs using both DNS and Langevin simulations (LS), and compare the corresponding results.

METHODS & RESULTS

DNS of forced isotropic turbulence were performed using a discrete Fourier-expansion- based pseudospectral method. Simulations were performed over a cubic domain of length 2π discretized using N^3 grid points, with periodic boundary conditions. The fluid velocity is advanced in time by solving the Navier-Stokes equations in rotational form, as well as the continuity equation for an incompressible fluid. Direct evaluation of the non-linear convective terms in the Navier-Stokes equations is computationally intensive. Hence, a pseudospectral approach is adopted wherein the non-linear terms are first computed in physical space, and then transformed into the spectral space. P3DFFT library [2] was used to carry out the transforms between physical and spectral spaces.

RDF is a well-established measure of particle clustering. In figure 1, the RDF is presented as a function of St_η at four separations r/η = 6, 12, 18, and 24 (η is the Kol-mogorov length scale). LS results are compared with the data from the DNS performed in [3] DNS and [4]. The Février et al. [3] data were for Re_λ = 69, while the current DNS data are for Re_λ = 76. There is excellent agreement between the LS RDF and the two sets of DNS RDFs at all four separations, particularly for St_η > 10. The [4] theory significantly over predicts the RDFs for high Stokes numbers at all separations.

WHY BLUE WATERS

Direct numerical simulations are the most accurate numerical approach to resolve all the temporal and length scales in a turbulent flow. However, DNS of particle-laden turbulent flows are computationally intensive and requires running code using tens of thousands of cores. Also, each DNS run is expected to generate several terabytes of data. Due to these CPU time and storage requirements, Blue Waters is the **ideal platform** to achieve our objective and proved to be an invaluable resource in computing key inputs to our stochastic theory. For instance, the theory requires as an input the two-time Eulerian correlations of fluid relative velocities seen by particle pairs. Evaluation of the two-time correlation for nearly half a trillion pairs is a highly computationally intensive process. We were only able to compute this quantity because of the Blue Waters access, where we ran the code on 20,000 cores.

PUBLICATIONS

Dhariwal, R., Sarma L. Rani, and D. L. Koch, Analysis and comparison with DNS of a stochastic model for the relative motion of high-stokes-number particles in isotropic turbulence. *68th Ann. Mtg. APS DFD*, Boston, MA, 2015.

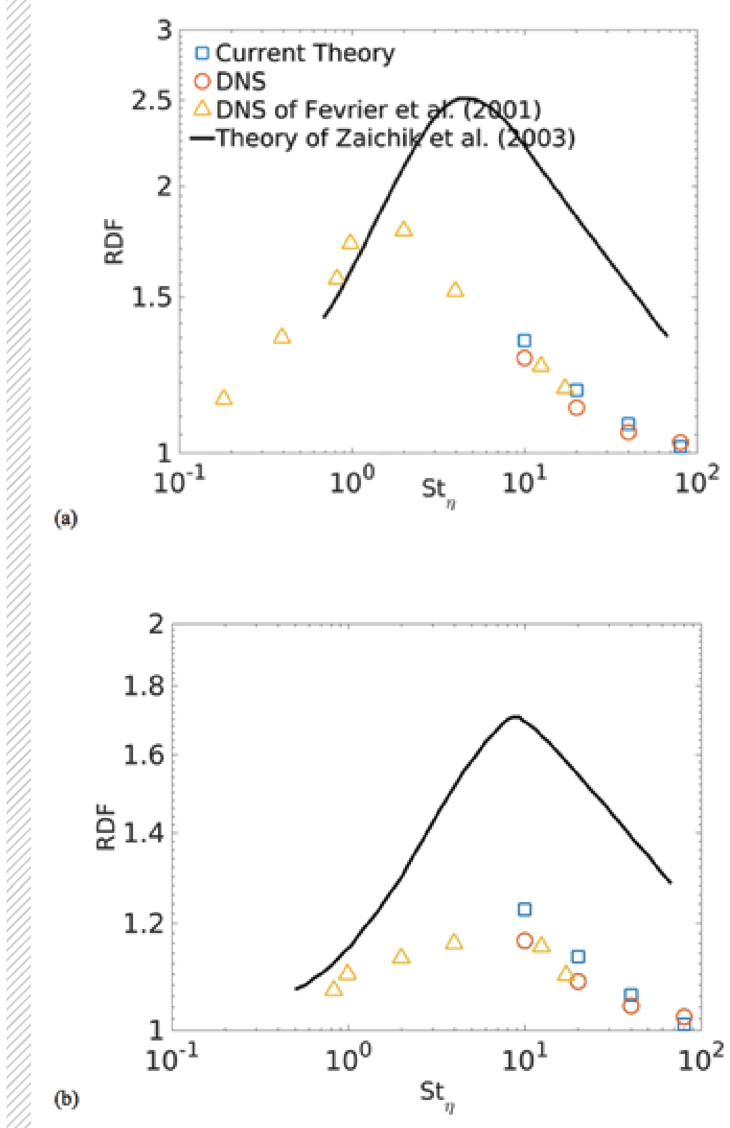

FIGURE 1: Radial distribution function (RDF) versus St_η at specific radial separations: (a) r/η = 6, and (b) r/η = 18. In each plot, squares and circles represent data from CF1 and current DNS at Re_λ = 76; triangles represent DNS data at Re_λ = 69 taken from [3]. Solid line represents data from [4] theory for Re_λ = 69.