Soliton Gases and Generalized Hydrodynamics

Doyon, B.; Yoshimura, T.; Caux, J.-S.

DOI
10.1103/PhysRevLett.120.045301

Publication date
2018

Document Version
Final published version

Published in
Physical Review Letters

Citation for published version (APA):
https://doi.org/10.1103/PhysRevLett.120.045301
Introduction.—It is widely believed and acknowledged that the late-time and large-scale dynamics of interacting systems, whether quantum or not, is well described by hydrodynamics. The applicability of hydrodynamics encompasses a large number of many-body systems, from classical gases and interacting quantum field theories [1,2], where few hydrodynamic variables are necessary, to more exotic systems such as the classical hard-rod model [3]. Recently, the realm of hydrodynamics was extended to integrable quantum models by accounting for the infinity of conservation laws they admit [4,5]. On large (Eulerian) scales fluid cells are in generalized Gibbs ensembles (GGE) [6]. The theory describing this was dubbed generalized hydrodynamics (GHD). It has been very successful in many studies of quantum chains and field theory [7–11]. It is applicable [4] to the Lieb-Liniger model [12], and, thus, can describe the inhomogeneous dynamics in quasi-one-dimensional cold atom setups [13] such as in the celebrated quantum Newton cradle [14].

In this Letter, we show that the GHD equations also emerge as descriptions of classical gases. A special case of GHD reproduces the equations, mathematically derived by Boldrighini, Dobrushin, Sukhovin in 1983 [3], for a gas of hard rods on the line colliding elastically—a simple observation used in Ref. [15]. We show that a modification of the hard-rod dynamics leads to the general form of GHD found in integrable quantum systems. In the modified problem, pointlike “quasiparticles” are subject to velocity-dependent spatial shifts upon colliding, generalizing the velocity tracers in the hard rod problem. We show that this new classical gas is extremely easy to implement on the computer. This gives a “molecular dynamics” (MD) solver for GHD that is numerically efficient, that accounts for external forces, and that is flexible enough to offer the possibility of adding other effects such as integrability breaking, and viscosity. MD solvers are known for their usefulness in low-temperature Fermi liquids, strongly interacting gases and high-temperature or -density plasmas, see, e.g., Refs. [16–18]. The MD solver developed here offers better performance due to the stability of the integrable quasiparticles at the heart of the system’s dynamics. It is free from limitations on temperature, interaction strength, and density, only requiring Eulerian scales.

It is well known that velocity-dependent shifts occur in soliton scattering, and equations of the GHD form have in fact been found to describe classical soliton gases [19]. Wave packets of excitations in quantum models, although not strictly solitons, have also been observed to display such solitonlike features [20]. We identify the GHD of any quantum model with that of the gas of its solitonlike wave packets. This, we believe, is a remarkable quantum-classical correspondence. From the viewpoint of local averages in Eulerian hydrodynamics, all quantum effects can be accounted for by considering the two-body classical scattering of solitonlike wave packets.

Generalized hydrodynamics.—Hydrodynamics is a theory for the dynamics of weakly inhomogeneous, non-stationary states of many-body physics. It is based on local entropy maximization: local averages are related to each other in the same way they are in entropy-maximized homogeneous, stationary states, as per the equations of state. Eulerian hydrodynamics (that is, neglecting viscosity effects) is obtained by imposing the local conservation laws, and gives rise to a macroscopic dynamics for the local Lagrange parameters or any parametrization of the local
model within a force field as it applies, for instance, to the quantum Newton cradle setup [14]. Euler-type equations are often solvable by using appropriate molecular dynamics (MD). This requires finding a particle dynamics with the correct equations of state. As shown in Ref. [4], here the equations of state amount to the relation (2) between the effective velocity and the quasiparticle density. We now develop a family of classical gases which, at the Euler scale, reproduce exactly Eq. (2) and the equations of GHD, Eqs. (1) and (3).

In order to make the argument clear, let us first recall how the classical hard rod model [1,3] connects with GHD; see Ref. [15]. Rods (nonintersecting one-dimensional segments) of a fixed length \( d \) move inertially at various velocities \( v \) on the infinite line, except for elastic collisions at which they exchange their velocities. The emergence of hydrodynamic equations on large scales in this model for a large class of initial conditions was rigorously demonstrated [3]. Let \( \rho(v) \) be the density of rods with velocity \( v (\rho_{cl}(v) dx dv) \) is the number of rod centers within the phase space element \( [x, x+dx] \times [v, v+dv] \). Then,

\[
\partial_t \rho_p(v) + \partial_x [v^{\text{eff}}(\theta) \rho_p(v)] = 0, \tag{1}
\]

where the effective velocity \( v^{\text{eff}}(\theta) \) solves

\[
v^{\text{eff}}(\theta) = v^{\text{gr}}(\theta) + \int d\alpha \frac{\varphi(\theta, \alpha)}{p^{\text{gr}}(\alpha)} \rho_{p}(\alpha)(v^{\text{eff}}(\alpha) - v^{\text{eff}}(\theta))
\]

(2)

(see the Supplemental Material [23] for the attractive regime).

Molecular dynamics: The classical flea gas.—The GHD equations are Euler-type hydrodynamic equations. An important problem in GHD is to numerically solve Eqs. (1) and (3). This is of particular interest for the LL model within a force field as it applies, for instance, to the quantum Newton cradle setup [14]. Euler-type equations are often solvable by using appropriate molecular dynamics (MD). This requires finding a particle dynamics with the correct equations of state. As shown in Ref. [4], here the equations of state amount to the relation (2) between the effective velocity and the quasiparticle density. We now develop a family of classical gases which, at the Euler scale, reproduce exactly Eq. (2) and the equations of GHD, Eqs. (1) and (3).

In order to make the argument clear, let us first recall how the classical hard rod model connects with GHD; see Ref. [15]. Rods (nonintersecting one-dimensional segments) of a fixed length \( d \) move inertially at various velocities \( v \) on the infinite line, except for elastic collisions at which they exchange their velocities. The emergence of hydrodynamic equations on large scales in this model for a large class of initial conditions was rigorously demonstrated [3]. Let \( \rho(v) \) be the density of rods with velocity \( v (\rho_{cl}(v) dx dv) \) is the number of rod centers within the phase space element \( [x, x+dx] \times [v, v+dv] \). Then,

\[
\partial_t \rho_p(v) + \partial_x [v^{\text{eff}}(\theta) \rho_p(v)] = 0, \tag{1}
\]

where the effective velocity \( v^{\text{eff}}(\theta) \) solves

\[
v^{\text{eff}}(\theta) = v^{\text{gr}}(\theta) + \int d\alpha \frac{\varphi(\theta, \alpha)}{p^{\text{gr}}(\alpha)} \rho_{p}(\alpha)(v^{\text{eff}}(\alpha) - v^{\text{eff}}(\theta))
\]

(2)

These are exactly the Eqs. (2) and (1), in the Galilean case \( v = \theta \), with a single unit-mass particle species, with negative differential scattering length \( \varphi(v, w) = -d \) (In the quantum context, this corresponds to a purely exponential scattering phase, \( S(\theta, \alpha) = e^{-id(\theta-\alpha)} \) [24]. In the large-\( c \) region of the repulsive LL model, one also finds constant \( \varphi(\theta, \alpha) \sim 2c/e \), but this would correspond to negative rod lengths \( d = -2c/e \) and \( v^{\text{eff}}(\theta) = v^{\text{eff}}(\theta) \). This simple observation suggests that if we allow the rods to collide more “softly,” so that \( d \) becomes velocity dependent, the hydrodynamics of the emerging gas might be identical to that of GHD. In a naive picture, neighboring rods of velocities \( v \) and \( w \) would exchange their velocities when their centers are at distance \( d(v, w) \), as if rods were elastically contractible. However, this dynamics causes difficulties with respect to many-body scattering and for negative or nonsymmetric lengths.

Consider instead a velocity tracer, following the center of a rod of velocity \( v \). This is a pointlike quasiparticle, with trajectory that of a free particle except for jumps by a distance \( d \) at rod collisions. Here rod collisions occur when the positions \( x_1 < x_2 \) of two quasiparticles satisfy \( x_2 - x_1 = d \) and their velocities \( v_1 > v_2 \), and at this instant \( x_1 \mapsto x_1 + d \) and \( x_2 \mapsto x_2 - d \). Crucially, this means that every crossing of two quasiparticles’ trajectories comes with such trajectory shifts, and this within microscopic time. In fact, any dynamics with this property, independently of the microscopic details of the trajectory shifts, leads to the same hydrodynamics. We may thus modify the
dynamics by proclaiming collisions to occur at \( x_2 = x_1 \), at which the involved quasiparticles instantaneously jump, like fleas, by a distance \( d \). The jump is “forward”: the quasiparticle on the left (right) jumps towards the right (left). This is easily generalizable to velocity-dependent jump lengths: a quasiparticle of velocity \( v \) that enters in collision with one of velocity \( w \) jumps by \( d(v, w) \), forward if positive, backward if negative. Importantly, the jump lengths may be positive or negative, and need not be symmetric with respect to exchange of velocities. A jump is an infinitely fast displacement, during which more collisions can occur, occasioning new jumps in a chain reaction that reorganizes the quasiparticles’ positions in the local neighborhood. This is the classical “flea gas”; see the Supplemental Material [23] for a precise, somewhat subtle algorithm.

We now argue that this reproduces GHD. We are looking for the effective velocity \( v_{\text{eff}}(v) \) of a test quasiparticle of velocity \( v \), defined through the actual distance \( \Delta x = \Delta t v_{\text{eff}}(v) \) that it travels in a macroscopic time \( \Delta t \). The gas is characterized by the density \( \rho_{\text{cl}}(w) \), and by standard arguments the continuity Eq. (5) holds. The quantity \( \Delta x \) results from the total linear displacement at velocity \( v \), given by \( \Delta x v \), along with the accumulation of jumps the quasiparticle undergoes as it travels through the gas. The oriented distance jumped due to hitting a quasiparticle that has velocity \( w \) is \( \text{sgn}(v - w) d(v, w) \). The average number of quasiparticles of velocity between \( w \) and \( w + dw \) that has been crossed, is the total number \( dw \rho_{\text{cl}}(w) \Delta x \) present within the length \( \Delta x \), times the probability \( \Delta t / \Delta x \times |v_{\text{eff}}(v) - v_{\text{eff}}(w)| \) that the test particle crosses such a quasiparticle in time \( \Delta t \). Assuming that the effective velocity is monotonic with \( v \) (see the Supplemental Material [23]), the total jumped distance is obtained by integrating the product of these: \( \int dw d(v, w) \rho_{\text{cl}}(w) \Delta x |v_{\text{eff}}(v) - v_{\text{eff}}(w)| \). Equating the total jumped distance plus the total linear displacement with \( \Delta x = \Delta t v_{\text{eff}}(v) \), we obtain

\[
v_{\text{eff}}(v) = v + \int dw d(v, w) \rho_{\text{cl}}(w) [v_{\text{eff}}(v) - v_{\text{eff}}(w)].
\]

This is readily generalizable to many species, with, in Eq. (7), velocity parameters \( v, w \) replaced by doublets \( v = (v, \alpha), w = (w, b) \), and the driving velocity value \( v \) replaced by \( v^\gamma(v) \). We recover Eq. (2) by reparametrization. It is clear that, if an external potential \( V(x) \) affects the velocities \( v \) of the quasiparticles of the flea gas so that there is an acceleration \( dv/dt = -\partial_x V/m \), the continuity equation (3) holds.

**Domain of validity.**—As any molecular dynamics, the flea gas reproduces the GHD equations only at the gas’s Euler scale. Two sets of lengths determine this scale: (i) the interparticle length \( 1/\rho = \int d\rho_{\text{cl}}(v) \), and (ii) the jump distance \( d(\theta, \alpha) \). We expect the Euler scale to be reached when these two lengths are much smaller than the variation length—the typical length over which \( \rho \) varies. In this case, particles locally maximize entropy, as jumps do not send them away from their fluid cell and many jumps occur within a fluid cell. The flea gas cannot solve GHD away from such conditions. Of course, GHD only applies under similar conditions; for instance, in quantum models, variation lengths must be much bigger than the scattering length, determined by \( \phi(\theta, \alpha) \).

**Numerical checks.**—We have numerically simulated the classical gas corresponding to the LL model (4) with \( c = 1, m = 1 \). Besides being a model of experimental interest, the GHD of the LL model was studied in Ref. [4] at length, allowing benchmarking of the MD developed here. All verifications are done well within the strong coupling regime, far from either the Tonks-Girardeau or the free boson points. First, we have verified the form of the effective velocity by evaluating explicitly, in a homogeneous stationary gas with LL coupling parameter \( \gamma = mc^2 \approx 1.1 \), the total displacement of a test quasiparticle divided by the time spent, and comparing with the result of solving numerically the integral equation (2). See Fig. 1(a); the agreement is excellent. Second, we have implemented a domain wall initial condition in the LL model, and checked that its dynamics reproduces the self-similar solution derived in Ref. [4]. See Fig. 1(b), as well as Fig. 2 in the Supplemental Material [23]. Again, these provide convincing evidence of the validity of the MD. Finally, we have implemented the “breathing motion” of the LL model occurring after a sudden change of frequency

\[\text{FIG. 1.} \text{ GHD for the LL model with } m = 1, c = 1 \text{ is simulated using the classical flea gas. (a) Truncated Gaussian distribution } \rho_{\text{cl}}(v) = 0.5e^{-v^2} \chi(-3 < v < 3). \text{ Effective velocity evaluated using } \approx 1500 \text{ trajectories over a time of } 1200 \text{ (blue); using the formula (2) (red). (b) Density profile from domain wall initial condition, initial left and right temperatures 10 and 1/3, respectively, at times } t = 10, 30, 50, \text{ and } 70. \text{ Simulation with } \approx 2400 \text{ quasiparticles (initial baths of lengths 1000, open boundary condition) averaged over 1000 samples (blue); exact self-similar solution (red).}\]
of a harmonic confining potential. This has been studied experimentally, with TDMRG and with conventional hydrodynamics; see Ref. [25]. As found in Ref. [11], GHD supersedes conventional hydrodynamics at nonzero temperature, and thus it is important to test the MD solver’s validity in this case. The initial state, at temperature $T = 1$, is evolved within a wider harmonic potential. As expected, the density expands and contracts almost periodically (with observed period slightly smaller than that of the evolution potential, as the interaction slows down the particles; see Fig. 3 in the Supplemental Material [23]). We have simulated this setup using the flea gas, and directly verified the conservation equations (3), integrating over cells in phase space-time. Without changing scattering and interparticle lengths, we have considered setups with 120 and 1200 particles. These have widely different variation lengths, affecting the accuracy of the hydrodynamic approximation. With a gas of as little as 120 particles, we found Eq. (3) to be satisfied to 0.2%–0.9%, and with 1200 particles, 0.08%–0.16%. The accuracy is higher in central cells, away from the boundary of the density support where hydrodynamics is expected to fail. This quantifies the accuracy of the hydrodynamic approximation, and provides precise tests of how MD solves the GHD equations within force fields. See the Supplemental Material [23] for details.

Quantum-classical dictionary.—The GHD equations were derived in quantum integrable models using quantum integrability. There is thus a quantum-classical dictionary, such as Eqs. (8) and (9). Further elements of the dictionary are as follows. Consider the “free space fraction” $\rho_{\text{free}}(v) = 1 - \int dwd(v,w)\rho_{\text{cl}}(w)$. In the hard rod gas, this is the fraction of a unit length where there is no rod at all. In the general case, that available omitting the distances jumped if forward, or adding them if backward; in the latter, the effect of quasiparticle scattering is to increase the space available. We recognize the free space fraction as, up to a factor, the quantum density of states $\rho_{\text{cl}}(\theta)$ [21], $\rho_{\text{free}}(\theta) = 2\pi\rho_{\text{cl}}(\theta)/p'(\theta)$. The occupation function $n(\theta) = \rho_{\text{cl}}(\theta)/\rho_{\text{cl}}(\theta)$ plays an important role in GHD, being the normal mode of the hydrodynamics [4,5]. We find that $n(\theta)p'(\theta)d\theta/(2\pi)$ equals the number of quasiparticles per unit length of free space $\rho_{\text{cl}}(v)dv/\rho_{\text{free}}(v)$. The classical picture also helps understand the effective velocity. Let us write it as $v_{\text{eff}}(v) = \langle \dot{v}^{\text{MD}}(v) - \int dwd(v,w)\rho_{\text{cl}}(w)\rangle/\langle 1 - \int dwd(v,w)\rho_{\text{cl}}(w) \rangle$, and consider $d(v,w) < 0$. The gas slows down a test quasiparticle with respect to its “center of momentum,” as it is affected by backwards jumps at collisions. There is thus a friction effect—the denominator—and a drag effect—the second term in the numerator, which were numerically noticed in Ref. [4] when studying steady states. Finally, note that the flea gas is invariant under simultaneous scaling of space, time, and jump lengths; in the quantum problem a physical length scale arises due to $\hbar$ in the differential scattering phase.

Soliton gases.—The above intriguing quantum-classical correspondence might be explained in terms of soliton gases. In classical soliton scattering, two solitons retain, asymptotically, their form and their speeds, the only change being in shifts of their trajectories. These shifts are velocity dependent, and thus the flea-gas dynamics is similar to that of classical soliton scattering. Indeed, it turns out that equations of the GHD form, without force fields, were already found in recent studies of gases of solitonic modes of classical field theory [19]. In these studies an effective velocity emerges that is determined by the soliton’s scattering shifts $d(v,w)$ as per Eq. (7). The integrability of the resulting equations was investigated; see also Ref. [26].

Why do gases of classical solitons have the same Euler hydrodynamics as that of quantum models? In the quantum context, it is known that quasiparticle excitations have solitonlike features. This was recently made numerically explicit by forming wave packets of quasiparticle excitations in the Heisenberg quantum chain [20]. It was seen that the trajectory shifts are given by the differential scattering phase of the quantum model. This exactly agrees with the relation (9) that we derived between the shift $d(v,w)$ and the differential scattering phase $q(\theta,\alpha)$. Wave packets in quantum models are, however, not solitons: in the example of Ref. [20], for instance, they do not keep their shape but rather spread with time, as do wave packets of free fields. But this effect is subleading: at the Euler scale, only the scattering shifts play a role. This explains why the Euler hydrodynamics of true classical solitons is the same as that of quantum models upon identifying the solitonlike features of quantum excitations, and is expected to be general. That quantum gases can be seen as the gas of their classical solitonlike wave packets gives, we believe, new insight into the large-scale dynamics of quantum models. It is also in agreement with the picture according to which multiparticle scattering processes are sequences of well separated two-body scattering processes, at the basis of the (generalized) thermodynamic Bethe ansatz [21].

Conclusion.—We have developed a classical gas dynamics that reproduces, at the Euler scale, the equations of GHD for arbitrary differential scattering phase. This gives an efficient way of simulating full space-time dependent profiles solving GHD. It complements the exact “solution by characteristics” found in Ref. [9] and numerical methods [10,11]. It is the first numerical procedure applicable in general states to the experimentally relevant case of the LL model in force fields. With the numerical technique developed here, the quantum Newton cradle setup [14] is now accessible, which it will be important to analyze.

We have explained the ensuing quantum-classical dictionary, and how quantum models relate to the gases of their solitonlike excitation wave packets. The connection between GHD and soliton gases has far-reaching implication. For instance, the integrable structures of soliton gases [19] can now be used in quantum models, and may have
connections with the solution by characteristics [9]. The GHD equation, including for force fields, was only derived in quantum models [7]; it would be interesting to understand its meaning in classical soliton gases. The large-deviation theory of classical gases is also a problem of interest, especially its relation with that of quantum problems (see, e.g., Ref. [27]). Soliton gases may be seen as wide generalizations of the semiclassical picture proposed in Ref. [28], and may lead to efficient ways of evaluating correlations in certain regimes.

Viscosity or other higher-derivative effects in the quantum problems will have many sources, including the finite scattering length taken into account by the classical gas, but also wave packet spreading. By appropriately modifying the classical algorithm, it might be possible to phenomenologically account for such corrections to GHD, as well as for integrability-breaking processes, which would otherwise be extremely difficult to numerically implement. We believe these constitute very exciting research directions.

We thank Robert Konik and Herbert Spohn for useful discussions. Hospitality is acknowledged as follows: all authors thank SISSA and ICTP, Trieste (visits and workshop “Entanglement and non-equilibrium physics of pure and disordered systems.”), B.D. and T.Y. thank City University New York (workshop “Dynamics and hydrodynamics of certain quantum matter.”), T.Y. thanks Tokyo Institute of Technology (Japan) and B.D. thanks the support from the Takenaka Scholarship Foundation. J.-S. C.’s work is part of the Delta-ITP consortium, a program of the Netherlands Organization for Scientific Research (NWO) that is funded by the Dutch Ministry of Education, Culture and Science (OCW).


