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Abstract. A combination of two stochastic hopping processes is studied on a one-dimensional chain. Firstly, the particles undergo asymmetric hops with different jump lengths and rates where the principle of detailed balance is violated. The second process favours the nearest neighbour hopping whenever the next nearest sites are occupied. Due to the competition of both processes the averaged density exhibits stable solitary excitations which are induced purely by the underlying kinetics and not by forces. The numerical results are supported strongly by an analytical approach based on a quantum formulation of the master equation. Already in the simplest approximation the averaged density satisfies the Korteweg–de Vries equation with additional dissipative terms, the influence of which is discussed by scaling arguments.

1. Introduction

Solitons are localized travelling waves that propagate with constant velocities and undistorted shapes. They exist in a broad spectrum of very different systems. Even though solitons were first observed by Russell in 1834. When a boat suddenly stopped, a lump of water formed at the front of the boat and moved forward with constant speed and shape. Applying hydrodynamics Korteweg and de Vries succeeded in deriving a famous equation named after both scientists (the KdV equation) for such shallow water waves. Moreover, solitons exist in plasmas [1], molecular systems [2], superfluids [3], laser pulses [4], magnetic systems [5], structural phase transitions [6], polymers [7], liquid crystals [8], fluid flows [9] as well as elementary particles [10]. Even solitary solutions are also observed in the sky as density waves in spiral galaxies, and the giant red spot in the atmosphere [11]. In a recent result it was shown that acoustic solitary waves could be produced by altering the propagation of sound through an air-filled tube [16]. The KdV equation also offers a variety of mathematical properties elaborated further in [12, 13]. An extension to a more general form is discussed in [14]. A review of the development is given by Lam [15].

Solitary excitations appear in systems which are characterized by non-trivial nonlinearities and dispersion relations. From a mathematical point of view solitons are special non-singular solutions of nonlinear partial differential equations. Physically, the underlying equations can be traced back to the action of forces. The KdV equation, for instance, is based on hydrodynamic equations and describes phenomena with weak nonlinearity and weak dispersion, including the mentioned waves in shallow water or magnetohydrodynamic waves in plasmas or certain kinds of photon excitations in crystals.

Contrary to all the previous studies we report on solitary excitations, the origin of which can be attributed to a statistical background. The system under consideration is far from thermodynamic equilibrium and is driven by local kinetic processes without any contact to a heat bath. The principle of detailed balance is broken due to a more refined random walk on

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a lattice. Our interest is focused on the following one-species process: each particle, situated at the lattice site i on a one-dimensional chain, hops with a constant rate D between site i and site $i - m$ with $m > 1$ by overjumping the intermediate sites. Simultaneously with that backward hopping across m bonds (we chose mostly $m = 3$), the particles are allowed to perform a forward jump with the m-fold rate mD between nearest neighbours. Obviously, the overjump process combined with the gradual hop visiting all the intermediate sites, leads to the violation of detailed balance, especially on a time scale of the order of the elementary hopping time τ and consequently on a small spatial scale. For the many-particle system it appears as a typical dispersion resulting in a local broadening of the characteristic motion. On the long time scale $t \gg \tau$ and consequently on the long spatial scale, the broken detailed balance due to the more complicated local kinetic processes should be irrelevant. The combination of the two random processes introduced is superimposed by an additional hopping process between nearest neighbours where the particles are subjected to a kinetically induced interaction in such a manner that the hopping attempt over one lattice unit l is realized only whenever the next nearest site is already occupied. That kind of an asymmetric process leads to a drift motion which is coupled to the density in a nonlinear manner.

Such a situation could be relevant for granular materials. Depending on the size of the materials, particles may perform local hopping processes in backward and forward directions with different rates. Furthermore, the transport should be influenced by a kinetically mediated attraction. A similar situation is realized when particles move on a ratchet. A gradual upward motion over several lattice sites is followed by a rapid downward fall, but different to our model, the particles move only in one direction. Moreover, the model could be interesting for traffic dynamics where cars fall back m sites and after that, they are able to overtake cars ahead only step by step. Even for a biological wandering motion the asymmetric behaviour could be relevant.

Here we present the results of the numerical simulation originating from the elementary hopping processes introduced above. Moreover, we offer an analytical approach based on a master equation description as well as for systems with and without exclusion. From that point of view the feature of the dispersion relation, inherent for solitons, is manifested through the broken detailed balance. The nonlinearities are adopted by a kinetic interaction which favours a kind of attraction between the particles. In particular, due to such a facilitated process it results in a nonlinear coupling between the density gradient and the density itself. Systems, satisfying detailed balance or alternatively, without any kinetic interactions, do not reveal solitary excitations, i.e. only the combination of both competing effects leads to the suggested result.

2. Numerical simulation

Based on a conventional Monte Carlo algorithm the asymmetric dynamical rules can be used to simulate immediately the motion of the particles on the chain. A particle, randomly selected at the lattice site i, performs either a hopping process to the left-hand direction, overjumping m sites by that process, or it jumps to its nearest-neighbour site on the right-hand side. Whereas the probability for the first jump is λ, the second one is realized with probability $m\lambda$. Furthermore, the jumping probability will be enhanced by $m\lambda \rightarrow m\lambda(n_{i-1} + n_{n+2})$, whenever the left neighbour site $i - 1$ or the right neighbour site at $i + 2$ are already occupied. Here n_i is the occupation number at the corresponding site i. In particular, the occupation number becomes relevant when the exclusion principle is taken into account. In that case a hopping event is allowed only for $n_{i-m} = 0$ or $n_{i+1} = 0$. For an arbitrary occupation number per lattice site (Bose case) the occupation number of the final site of the jump is not relevant.

The simulation is performed on a chain of the length $L \simeq 10^3$ lattice sites with periodic boundary conditions. Initially, all particles are distributed in a random manner on the lattice. The averaged occupation number of the initial distribution depends on the position via the relation

$$\langle n_i \rangle = n_0 + h \exp\left\{-\frac{(x_i - L/2)^2}{2\sigma}\right\}.$$

Therefore, an initial excitation is created around $L/2$ with height h and width σ. The background occupation number n_0 is chosen as $n_0 = 0.2$ (Fermi case) and $n_0 = 20.0$ (Bose case).

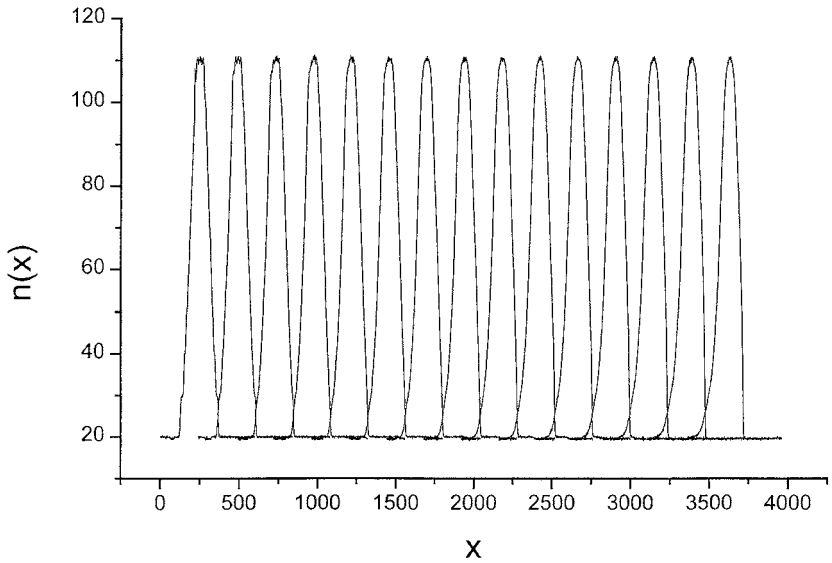

Figure 1. Time evolution of the averaged density without exclusion. The initial width is 250 lattice units. The time interval between two peaks corresponds to 10^6 elementary steps. The average is performed over 10^3 samples.

Both processes, the restricted hopping and the anisotropic overjumping events, lead in the case of bosons to the solitary excitations depicted in figure 1. Note that the form stable excitations appear only after averaging over an ensemble of equally prepared systems. Whereas each single event is subjected to stochastic dynamics the averaged density offers well defined solitons. To be more specific, the simulations shown in figure 1 are based on the dynamics characterized above where the initial width σ is approximately 250 lattice units. The nonlinear excitations are stable and the amplitude remains fixed during the whole process. In figure 2 we show likewise the simulation for a Bose system, however, with the initial width, smaller as before, of 50 lattice units. In that case the amplitude h is decreased slightly which will be discussed in the context of the analytical approach in the subsequent section. Figure 3 offers the result for the same model but with an exclusion principle, where all hopping attempts, leading to a double occupancy of a single lattice site, are rejected. Stable solitary excitations result with a rather constant amplitude after a relaxation process.

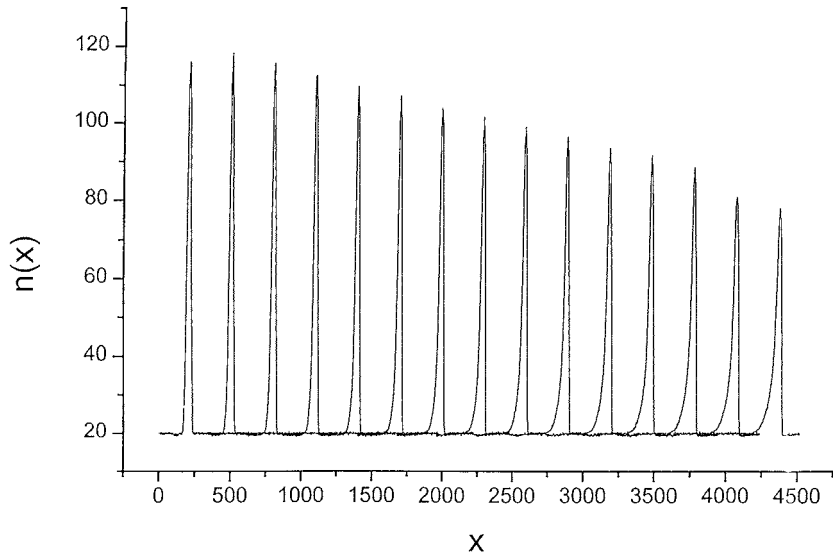

Figure 2. The same system as shown in figure 1, but with an initial width of 50 lattice units.

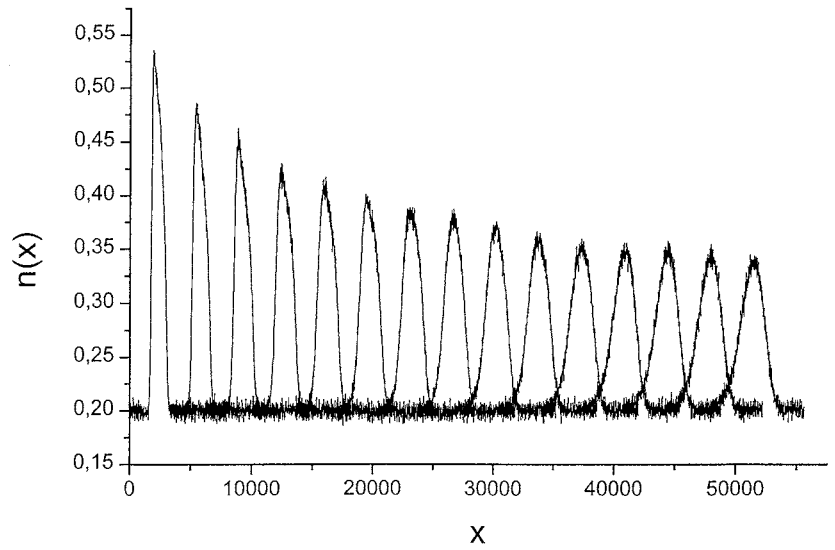

Figure 3. Time evolution of the averaged density with exclusion. The time interval between two peaks corresponds to 4×10^6 elementary steps, The average is performed over 10^4 samples. The solitary excitation becomes asymptotically form stable.

3. Analytical approach

Now we present an analytical treatment of the mentioned problem. To that end we adopt a coarse-grained point of view. At any instant of time the system is considered to be in a random configuration characterized by the occupation numbers $\boldsymbol{n} = n_1, n_2, \ldots$ at the lattice sites. A

complete description is provided by the probability $P(\boldsymbol{n}, t)$, the time evolution of which should obey the master equation [17]

$$\partial_t P(\boldsymbol{n}, t) = L' P(\boldsymbol{n}, t). \tag{1}$$

The evolution operator L' will be specified by the dynamical rules considered above. Introducing the state vector $|F(t)\rangle$ which is related to the probability distribution function $P(\boldsymbol{n}, t)$ according to $P(\boldsymbol{n}, t) = \langle \boldsymbol{n}|F(t)\rangle$ the master equation can be rewritten in an equivalent form [18]

$$\partial_t |F(t)\rangle = L|F(t)\rangle. \tag{2}$$

Here, we have introduced a complete set of basic-vectors $|\boldsymbol{n}\rangle$ composed of second quantized operators. The evolution operator L can be mapped onto the operator L' appearing in the master equation. Such an approach had been introduced by Doi [18] using Bose operators (cf also [19]). A generalization to Pauli–operators had been proposed [20–23], for recent reviews see [24–26].

Using the state function $\langle s| = \sum \langle \boldsymbol{n}|$ and the relation $\langle s|L = 0$, the evolution equation for an arbitrary operator B can be written as

$$\partial_t \langle B\rangle = \langle s|[B, L]|F(t)\rangle. \tag{3}$$

It should be noted that all the dynamical equations governed the classical problem are determined by the commutation rules of the underlying operators and the structure of the operator L.

For the processes used in the simulations the evolution operator consists of two parts $L = L^{(m)} + L^{(r)}$ where the first one describes the overjumping attempts

$$L^{(m)} = D \sum_i \left(a^\dagger_{i-m} a_i - n_i + m\left(a^\dagger_{i+1} a_i - n_i\right)\right). \tag{4}$$

The index i runs over the whole lattice, and the index m is fixed. Mostly, we are interested in the case $m = 3$. The first term describes the hopping process between lattice site $i - m$ and site i. A particle is annihilated at i and recreated at site $i - m$. The second term in $L^{(m)}$ with the rate mD represents the shorter forward jumps visiting the intermediate sites. Obviously, the principle of detailed balance is violated by such a complex process.

The evolution operator $L^{(r)}$ is related to hops under constraints. This means that a particle moves stochastically from lattice site i to site $i+1$ whenever that site $i+1$ and, moreover, site i are already occupied. These processes model a kind of kinetic monitored attraction, because the jump of the particle is facilitated by the occupation number of the site to which the particle intends to jump or on the site from which the particle jumps,

$$L^{(r)} = \mu \sum_i \left[a^\dagger_{i+1} a_i - n_i\right][n_{i+1} + n_i]. \tag{5}$$

We should stress again, that each single hopping event is a complete stochastic process, whereas the resulting evolution equation for the density is an averaged equation over all realizations. Assuming Bose commutation rules and applying equation (3) one verifies for the averaged density

$$\partial_t \langle n_r\rangle = D[\langle n_{r+m}\rangle - \langle n_r\rangle + m(\langle n_{r-1}\rangle - \langle n_r\rangle)] + \mu[\langle n_{r-1}(n_r + n_{r-1})\rangle - \langle n_r(n_{r+1} + n_r)\rangle]. \tag{6}$$

This equation is characterized by dispersion originated by the m-fold jumps and by nonlinearities traced back to the facilitated hopping. Using the simplest decoupling

approximation of the nonlinear part we derive from equation (6) an evolution equation for the averaged density in a continuous representation ($m = 3$)

$$\partial_t n = n_{xx} - n_{xxx} - nn_x - \tfrac{3}{8}(n_x^2 + nn_{xx}) \tag{7}$$

where $n(x,t)$ denotes $\langle n_r(t)\rangle$. The involved factorization of the density correlation function is a reasonable approximation in the case of a high averaged density n. It seems to be the better the higher the occupation number per lattice site. This suggestion is likewise confirmed by the numerical simulations. The prefactors of the first three terms are chosen to be one which can be reached by an appropriate rescaling of the density $n \to -\frac{9D}{4\mu}n$, the spatial coordinate $x \to -\frac{2l}{3}x$ and the time $t \to \frac{2}{27D}t$. The last equation is the Korteweg–de Vries equation well known in hydrodynamics with an additional diffusive n_{xx}-term and further dissipative terms, which are attributed to the statistical consideration of the problem.

A similar approach can be used for a hard-core exclusive interaction where different to the previous case a spin-$\frac{1}{2}$ representation should be used. In terms of Pauli operators the threefold-jump evolution operator, see equation (4), now reads

$$L^{(3)} = D\sum_i \left(a^\dagger_{i-3}a_i - (1-n_{i-3})n_i + 3\left[a^\dagger_{i+1}a_i - (1-n_{i+1})n_i\right]\right). \tag{8}$$

Here, the underlying operators fulfil the commutation rule $[a_i, a_j^\dagger] = (1-2n_i)\delta_{ij}$. The resulting evolution equation for the density always leads to a modified KdV equation with a similar structure to equation (7). There also appear dissipative terms, the influence of which will be estimated by using scaling arguments. To this end let us introduce dimensionless variables by rescaling the continuous form of equation (6): $n \to \alpha n$, $t \to \beta t$ and $x \to \gamma x$. The conventional KdV equation yields $|\beta^{-1}| \simeq t_K^{-1} \equiv |Dl^3\gamma^{-3}| + |\mu l\alpha\gamma^{-1}|$. Physically, t_K denotes the characteristic time scale for the propagation of a soliton based on the pure KdV equation. Using the same arguments for the whole equation (6) we obtain the more general estimation

$$|\beta| = \frac{t_K}{1 + t_K/t_D + t_K/t_{Di}}. \tag{9}$$

Here, $t_D = |\gamma^2/(Dl^2)|$ is a typical diffusion time, and $t_{Di} = |\gamma^2(\mu l\alpha)^{-1}|$ denotes a typical time scale over which the energy can be dissipated. From equation (9) one observes a slowing down of the characteristic time for propagation of a soliton due to dissipation and diffusion given by $|\beta| < t_K$. Such a retardation leads to a broadening of the soliton width and to the decrease of its amplitude as observed by the numerics (see figures 2 and 3). Due to the fact that the dissipation time scale t_{Di} decreases with increasing numbers of particles in a cell nl, the energy dissipation occurs at a small time scale $t_K \gg t_{Di}$ in dense systems. Hence, such systems are dominated by the dissipation $|\beta| \simeq t_{Di}$. Consequently, a soliton excitation will be presumably suppressed completely. When the diffusion time is much smaller than the propagation time for solitons $t_D \ll t_K$, the system reveals a purely diffusive behaviour where the time scale is given by $|\beta| \simeq t_D$. In that case solitary excitations are also suppressed. Only whenever both time scales t_D and t_{Di} are simultaneously large in comparison with t_K, is the behaviour of the system dominated by the travelling of solitons as has been realized by the simulations. Physically it means that solitary modes can be excited within the framework of a statistical approach when diffusive and dissipative processes are only relevant in the long-time limit. However, on a reasonable time scale solitons are produced in a self-organized manner after averaging over an ensemble. Based on scaling arguments we find that both conditions $t_K \ll t_D$ and $t_K \ll t_D$ are simultaneously fulfilled

for $\mu\alpha\gamma/(Dl) \gg 1$ and $\gamma/l \gg 1$. The condition $\alpha \simeq D/\mu$ means that $t_D \simeq t_{Di}$. When both scales are large and of the same order then the propagation of a soliton is realized. It seems that for a sufficiently extended excitation $\gamma \gg l$ dissipation will occur only in the long-time limit. Obviously that case is even realized within the simulations (cf figures 1 and 2).

4. Conclusions

In the present paper we have considered a system with competing kinetic processes. A random hopping process with different jump lengths and rates into the left- and right-hand directions (the product of both quantities is fixed) breaks the principle of detailed balance and consequently, the underlying equation evolves a dispersive part and additional dissipative ones. Furthermore, the hopping process between nearest neighbours is supported by the occupation of the corresponding sites in the environment. This fact gives rise to nonlinearities because both the density of the hopping particles and the density of the particles in the environment contribute to the jumping process. Although each individual process is random, stable solitary excitations result without any tuning from the outside. The soliton appears self-organized after a statistical averaging over different configurations. The simulation, performed on a simple chain, demonstrates the occurrence of solitons induced by the underlying kinetics and not by forces. Alternatively to the Monte Carlo simulation, we have studied the problem using the master equation. Applying a second quantized formulation we succeeded in deriving a nonlinear partial differential equation of Korteweg–de Vries type which is supplemented by the inclusion of diffusive and dissipative terms, attributed to the statistical consideration. The dissipative term leads the solitary excitation, the amplitude of which decreases slightly in the direction of propagation. This decreasing amplitude is also manifested in the numerical approach. However, the simulation offers form stable excitations on a rather long time scale. Note, that the soliton appears after averaging over several stochastic processes. Collective random processes are able, obviously, to organize their motion in such a manner that the excitation reveals an undistorted or only slightly distorted shape as was demonstrated by the simulations. Moreover, the numerical findings could be supported strongly by an analytical approach based on a probabilistic approach.

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