Effects of Collectively Induced Scattering of Gas Stream by Impurity Ensembles: Shock Wave Enhancement and Disorder-Stimulated Nonlinear Screening

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We report on specific effects of collective scattering for a cloud of heavy impurities exposed to a gas stream. Formation is presented of a common density perturbation and shock waves, both generated collectively by a system of scatterers at sudden application of the stream-inducing external field. Our results demonstrate that (i) the scattering of gas stream can be essentially amplified, due to nonlinear collective effects, upon fragmentation of a solid obstacle into a cluster of impurities (heterogeneously fractured obstacle); (ii) a cluster of disordered impurities can produce considerably stronger scattering accompanied by enhanced and accelerated shock wave, as compared to a regularly ordered cluster. We also show that the final steady-state density distribution is formed as a residual perturbation left after the shock front passage. In particular, a kink-like steady distribution profile can be formed as a result of shock front stopping effect. The possibility of the onset of solitary diffusive density-waves, reminiscent of precursor solitons, is shown and briefly discussed.

Gas stream scattering by an impurity cloud often leads to pronounced collective effects. This can be manifested by formation of common perturbation “coat” around a cloud of scatterers or common wake, localization of gas particles (blockade effects), induced correlations and formation of nonequilibrium (dissipative) structures in the ensemble of impurities. This type of phenomena are intrinsic in various physical systems, including examples from hydrodynamics [1, 2], dusty plasmas [3], quantum liquids or Bose condensates [10, 11], and can exhibit unusual behavior such as non-Newtonian wake-mediated forces [3–5, 7, 12–15] that is characteristic of diffusive or dissipative systems. Spatiotemporal characteristics of medium perturbations are mostly determined by the mechanism of energy losses specific to each particular system and by the properties of medium itself, e.g., nonlinearity of associated field.

A steady-state wake profile, induced by impurities under gas flow scattering, can be considered as a residual perturbation of gas density established after its evolution over a long time. However, the properties and behavior of the system during its transit to the steady regime can significantly differ from those at steady state. For example, under abrupt activation of gas or liquid flow (or sudden impurity displacement), formation of a wake around impurities can be accompanied by propagation of a shock wave and sign change of correlation function or dissipative force between impurities [18, 30, 31].

In this paper, we consider the properties of nonequilibrium formations resulting from scattering of gas stream by a cloud of impurities and examine the role of collective effects, with particular attention to the formation dynamics of common impurity wake (density perturbation “coat”) in case when the stream-inducing driving field is applied suddenly (nonadiabatically). Specifically, we analyze the properties of spatiotemporal evolution of shock waves generated collectively by a system of scatterers. We examine the effects of inner structure of impurity clusters, total drag (friction) force, and possible shock wave enhancement due to collective scattering accompanied by the nonlinear blockade effect in a gas.

We focus on purely dissipative (diffusive) system and make use of the minimal classical two-component lattice gas model with hard-core repulsion. Despite the short range of inter-particle interaction it was shown to give rise to peculiar nonlinear effects essentially manifested at high gas concentrations. These are the dissipative pairing effects [6, 7], the wake inversion and switching of wake-mediated interaction [7, 16], formation of nonequilibrium structures [4, 45, 47] etc. As will be shown, the nonlinear effects considerably affect collective scattering.

Kinetics of a two-component lattice gas is described by the standard continuity equation (see, e.g., [19, 20]),

\[ \dot{n}_i^\alpha = \sum_j (J_{ij}^\alpha - J_{ji}^\alpha) + \delta J_{i}^\alpha, \]

where \( \alpha = 1, 2 \) labels the particle species and \( n_i^\alpha = 0 \) are the local occupation numbers of particles at the \( i \)th site. \( J_{ij}^\alpha = \nu_{ij}^\alpha n_i^\alpha \left( 1 - \sum_j n_j^\beta \right) \) gives the average number of jumps from site \( i \) to a neighboring site \( j \) per time interval, \( \nu_{ij}^\alpha \) is the mean frequency of these jumps\(^3\). To describe the scattering of particle stream by an impurity cloud we assume, see Refs. [7, 16, 17], that one of the two components \( n_1 \equiv u(r) \) describes the distribution of impurities and is static \( (\nu_{ij}^1 \equiv 0) \), while another one \( n_2 \equiv n(r, t) \) is mobile. The presence of a weak driving field (force) \( \mathbf{G}, \quad |\mathbf{g}| = |\mathbf{G}|/(2kT) < 1 \) \((\ell \) is the lattice constant\), leads to asymmetry of particle jumps for mobile component: \( \nu_{ji}^2 \approx \nu[1 + g \cdot (r_i - r_j)/\ell] \). As in [7, 16], we use the

\[ \nu_{ji}^2 \approx \nu[1 + g \cdot (r_i - r_j)/\ell]. \]

\( ^1 \) That is each lattice site can be occupied by only one particle.

\( ^2 \) Particularly, the nonlinear effects of gas flow screening and common wake formation for a pair of impurities were addressed in [7], where consideration was restricted to the steady-state situation.

\( ^3 \) The term \( \delta J_{i}^\alpha \) stands for Langevin source: fluctuations of the number of jumps between adjacent sites [20]. For simplicity, it will be neglected along with fluctuation-induced forces.
mean-field approximation; in this case \( n(r,t) \) describes the mean occupation numbers\(^4\) or the density distribution of flowing gas particles, \( n_0 \equiv n(|r| \to \infty) \) being the equilibrium gas concentration (bath fraction). In what follows, we consider the two-dimensional (2D) case.

Collective scattering effects. We start by outlining the two basic effects readily seen from Figs 1(a)–(e). Panels (a) to (c) represent the nonequilibrium steady-state density distribution\(^5\) \( n(r) \) produced under scattering of streaming gas particles on the collection of point impurities arranged into the compact impermeable obstacle, dense impurity cluster (fractured obstacle) and sparse cluster, all of which consist of the same number of impurities \( N \). The qualitative differences in scattered field \( \delta n(r) = n(r) - n_0 \) constitute the essence of the first effect: Fragmentation\(^6\) of a solid obstacle into a cluster of

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\(^4\) Equations for the average local occupation numbers or mean concentration \( n(r,t) \), can be obtained within the local equilibrium approximation (the Zubarev approach) \([20, 21]\) which coincides, in our case, with the mean-field approximation \([22]\). By using this approximation we neglect short-range correlations and memory effects \([19]\).

\(^5\) In the numerical calculations we deem the steady state as established if the changes of mean concentration distribution \( n(r,t) \) per time step become negligibly weak at \( t \to \infty \).

\(^6\) The dynamic fragmentation process is not addressed here for the simplicity of consideration; a sample (predefined) impurity clusters mimicking the decomposed obstacles are considered instead.
separate impurities can enhance the gas stream scattering. This effect results from the collective blockade effect [7, 16] which leads to screening of gas stream between impurities. For impurity cluster density \( \phi = N/\pi R^2 < 1 \), as Fig. 1(b) suggests, the blockade region is considerably larger than for compact (solid) cluster \( \phi = 1 \), Fig. 1(a),(f)] as well as diluted one, \( \phi \ll 1 \).

The second effect consists in enhancement of scattering that is provoked by inhomogeneity of impurity distribution within a cluster, Figs 1(c)–(e) and (f). This effect is analogous to that of light scattering on inhomogeneities in distribution of atoms (dipole moments) that is determined by the fluctuation of their number density in a definite volume or by the two-point correlation function [23–27]. As is seen from Figs 1(c)–(e), the scattering is less efficient for regularly ordered cluster. Note that disordered cluster can provoke strong local fluctuations of scattered field \( \delta n(x) \) inside a cluster, see Fig. 2, i.e., \( \delta n^2(x) > n_0^2 \). This means that the problem of gas stream scattering on such a structure cannot be adequately described by introducing the effective diffusion coefficient for a cluster or its penetration index [16], Figs 1(e)–(f). In addition, this can lead to high-magnitude local fluctuations of induced dissipative interaction between impurities.\(^7\)

The magnitude of scattered field \( \delta n(x) \) can be characterized by a quantity like total density dispersion \( \varepsilon \equiv \delta n^2 \propto \int \delta n^2(x) \, dx \). For the cluster of \( N \) infinitely distant (independent) impurities, i.e., when their mean separation length \( \bar{s} \to \infty \), the dispersion is simply \( \varepsilon \propto \sum_{i=1}^{N} \delta n_i^2 \approx N \delta n_0^2 \propto N \), where \( \delta n_0^2 \) is dispersion for a single impurity. Figure 1(i) shows that dependence \( \varepsilon(N) \) for impurity cluster can become power-law and, in particular, for random cluster is \( \propto N^2 \) that signifies the intrinsically collective behavior.

The total drag force acting on impurity cluster also turns out to be quite sensitive to its density and cluster inner structure. As Fig. 1(g) suggests, the behavior is qualitatively different for random and regular clusters. At early stages of confluence, \( \phi \ll 1 \), when collective wake-mediated interactions come into play, the regular cluster tends to reduce the total drag force exerted by the gas particles, Fig. 1(g). Conversely, the random cluster tends to increase the drag force until the common blockade region ahead of impurities is formed. The latter screens the impurity cluster as a whole from streaming gas particles thereby reducing the drag force. This transformation of common perturbation “coat” is reflected in the enhancement peak where the total drag force exerted on extended \( \phi \approx 0.1 \) inhomogeneous cluster is stronger than for close-packed (solid) one, see Fig. 1(g). Upon further increase of cluster density the blockade region takes more advantageous streamlined shape as, e.g., shown in Figs 1(c) or (b), that also contributes towards drag force decrease. At the same time, the dependence of \( \sqrt{\varepsilon} \) on random-cluster density \( \phi \) has a characteristic enhancement peak which is absent for regular cluster, as shown in Fig. 1(h). Thus, collective gas scattering compounded by nonlinear effects can exhibit a qualitatively different behavior that depends strongly on the spatial arrangement of impurities in the cluster.

Dynamics. We now consider the time-dependent properties of wake profile formation under sudden application of stream-inducing driving field. The underlying feature, common for random, regular, and solid clusters, consists in propagation and stopping of two oppositely directed (downstream and upstream) shock waves. We give a
The approximate kink half-height $n(x_f)$ is now determined as shown in Fig. 3(a). Approximately, $n_f$ behaves in time as $n_f \propto n_0 + (1/2)\delta n(-R) - A\tau^5$; for sparse clusters, Figs. 1(c)–(e), $\gamma$ is close to 1 and $A < 1$.

**Shock-wave stopping effect.** It follows from Eq. (3) that at $n_f = 0.5$ the shock front motion vanishes, $v = 0$. In 2D case, as shown in Fig. 3(a), this is manifested as the shock front stopping: as the upstream shock wave advances, its height decreases and the concentration value at front position\(^{12}\) $n(x_f)$ descends until it approaches the value $n(x_f) = 0.5$. At this stage, the shock front velocity undergoes a slowdown and the shock wave ultimately comes to a halt forming a stable step-like structure resembling a “frozen” Bloch wall. During this process the growth of dense region becomes weaker due to stronger lateral diffusion outflow so that dense phase tends to form a streamline, nearly conical, shape.

In the case of half filling ($n_0 = 0.5$), the shock front does not undergo stopping, but advances through quiescent gas until merging into the final steady distribution with nearly power-law profile, Fig. 3(b). This is also the case for the downstream shock wave at $n_0 = 0.37$, Fig. 3(a), since in both cases the quantity $n(x_f)$ does not reach the value of 0.5. In other words, the stationary distribution is formed as a residual perturbation left after the shock front passage\(^{13}\).

Upon obstacle decomposition, a qualitatively different behavior arises due to collective effects. The first specific property is that fragmentation of solid obstacle into impurity cluster can result in the enhancement of shock wave—its front speed acceleration and amplitude increasing, see Fig. 3(c) and corresponding steady-state profiles

\[ n_f = [n(\mp R, y = 0) + n_0]/2 \text{ with “−” for the frontal shock wave and “+” for the rarefaction-like (cavity) shock wave.} \]

\(^{12}\) The position of the shock front $x_f$ was roughly determined by the point where second derivative of the density profile $n(x; y = 0)$ changes its sign.

\(^{13}\) For the case $n_0 > 0.5$, the consideration is straightforward because of “hole-particle” symmetry of the system and is reduced to wake inversion \(^{16}\).
Figure 4. Momentary gas distributions $|\delta n(x, y)|$ at $\nu t = 3.9 \times 10^3$ illustrating the precursor propagation: bunch of gas particles (b) or holes (a) separating from the impurity cluster. The time evolution of density profile $\delta n(x, t; y = 0)$ of the hump-shaped solitary wave advancing upstream is shown on (c), the profile marked by an asterisk corresponds to the distribution on panel (b). Random cluster density $\phi = 0.0461$, gas bath fraction $n_0 = 0.2$ for (a), $n_0 = 0.8$ for (b) and (c), the external driving field $g$ is directed along the $x$-axis, $|g| = 0.5$.

in Fig. 1. The other one is what can be referred to as precursor effect.

At the initial stage, just after abrupt application of the external drive, an impurity cluster is capable to generate larger density perturbation, both “stored” within a cluster and around it, than that hold in a steady state. For this reason, the system tends to subsequently get rid of the excess density perturbation that can be realized by two mechanisms:

(i) The excessive portion of density perturbation “leaves” the cluster in form of solitary wave traveling downstream\(^{14}\) at $n_0 < 0.5$, Fig. 4(a), or upstream at $n_0 > 0.5$, Figs 4(b) or (c), that is in accordance with wake

inversion effect [16]. The “ejected” bunch of gas particles (or vacancies) and associated hump-shaped wave (or the inverse hump) have a characteristic length-scale (its half-width) commensurate with the cluster size $2R$. This precursor-like mechanism takes place for sparse clusters, $\phi \ll 1$, for which the common blockade region ahead of scatterers is either weak or not formed.

(ii) A different mechanism comes into play for modestly dense clusters, when the excessive perturbation is relaxed via temporal acceleration of the shock front at the initial times. It can be explained by considering the dynamic behavior for several realizations of random cluster with an intermediate value of fraction $\phi \approx 10^{-1}$, see Fig. 5. As Fig. 5(a) suggests, shock front speed acceleration is sensitive to the realizations of random cluster. This temporal acceleration is always preceded with or accompanied by the enhancement peak of total drag force, Fig. 5(b), while for the cluster realization without acceleration effect the drag force exhibit monotonic saturation. The temporal force enhancement signifies the presence of excess perturbation (within a cluster) that subsequently transfers into shock wave acceleration. Under sudden stream activation, the nonlinear blockade effect leads to local saturation of scalar density field, so that gas compressibility limit $n(r, t) \rightarrow 1$ is attained faster than the overall perturbation is redistributed to minimize the total drag force. This leads to the accelerated growth of blockade

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\(^{14}\) Note, that this situation recalls the cascade avalanche problem for a pile of sand where the effect of self-organized criticality occurs, see [46]. In our case, we observe only a single avalanche-like event, that can be due to the use of mean-field approximation and neglect of fluctuations in gas.
region at the initial times.

Concluding remarks. Our results show that scattering of gas flow on impurity cloud and shock-wave generation can be enhanced by decomposition of solid obstacle into fragments or sparse cluster of impurities. This enhancement is more efficient for disordered sparse cluster as compared with regular one. In addition, a disordered cluster of scatterers can provoke high local fluctuations of scattered field inside the cluster and lead to the so-called precursor effect at sudden application of the external driving field. These effects occur due to collective scattering accompanied by nonlinear blockade effect in a gas and reveal a close formal analogy to classical problem of light scattering in gases, liquids, and nanoparticle ensembles. An important point is that mentioned effects are, generally, determined by the values of set of parameters—bath fraction $n_0$, size and mutual alignment of impurities [7], magnitude of driving force—and may vanish, e.g., in the case of weak driving. Note that possible instabilities of shock front due to gas density fluctuations were not addressed in our consideration.

Obtained results can be related to hopping transport on crystalline surfaces under external forces (surface diffusion of adsorbed monolayers [20], biased growth of a layer under surface electromigration, or superionic conductors [47]), granular flows [41–43], colloidal dispersions, and traffic flow. Also, considered effects can be of interest for processes of sedimentation [37] or swarmings [38] of colloidal particles, and filtration processes in porous media [39, 40]. Note that the shock wave amplification effect correlates, to a certain extent, with the well known problem of air shock wave interaction with a porous screen where the effect of temporal enhancement of reflected shock wave was observed [34, 35].

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