Normal and Anomalous Diffusion in Soft Lorentz Gases

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Motivated by electronic transport in graphenelike structures, we study the diffusion of a classical point particle in Fermi potentials situated on a triangular lattice. We call this system a soft Lorentz gas, as the hard disks in the conventional periodic Lorentz gas are replaced by soft repulsive scatterers. A thorough computational analysis yields both normal and anomalous (super)diffusion with an extreme sensitivity on model parameters. This is due to an intricate interplay between trapped and ballistic periodic orbits, whose existence is characterized by tonguelike structures in parameter space. These results hold even for small softness, showing that diffusion in the paradigmatic hard Lorentz gas is not robust for realistic potentials, where we find an entirely different type of diffusion.

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The rise of new micromanipulation techniques, molecular nanodevices, and nanotechnologies has fueled the scientific interest in *small systems* [1–4]. These are objects composed of small numbers of particles far from the thermodynamic limit, which exhibit only a few relevant degrees of freedom [4]. Their microscopic equations of motion are typically highly nonlinear, yielding fluctuations with macroscopic statistical properties reminiscent of interacting many-particle systems. Small systems can thus serve as a laboratory for understanding the emergence of irreversibility and complexity from chaotic dynamics [5,6]. They become especially interesting under nonequilibrium conditions, where they exhibit macroscopic transport phenomena like diffusion. By combining nonlinear dynamics with nonequilibrium statistical physics, the origin of macroscopic transport from microscopic chaos in small systems was explained by formulas expressing transport coefficients in terms of dynamical systems quantities [7–10]. Similarly irreversible entropy production was found to emerge from fractal measures [7,8] and fractal attractors [10–12]. These results paved the way for fundamental concepts like the chaotic hypothesis generalizing Boltzmann's ergodic hypothesis [13] and fluctuation theorems generalizing the second law of thermodynamics [4,8,9,14].

Classical transport in small systems has a quantum mechanical analog as electronic transport in solid-state nanodevices [15]. Recently growing interest has been attracted by periodic nanosystems such as *artificial graphene* [16] fabricated in semiconductor heterostructures [17–19] or on metallic surfaces [20,21]. In the latter case, the electrons are confined to a honeycomb geometry by CO molecules positioned with a scanning tunneling microscope in a triangular configuration. This system exhibits the properties of graphene, but in a setup that is tunable regarding, e.g., the electronic density, lattice constant, geometry, and the coupling with the environment.

Interestingly, the topology of "molecular graphene" as described above is exactly the same as one of the most paradigmatic models in dynamical systems theory, the periodic *Lorentz gas* [7–9,22–24]. They mimic the motion of classical electrons in metals. They consist of a point particle scattering elastically with fixed *hard* spheres distributed either randomly or periodically in space. Originally they were devised to reproduce Drude's theory from microscopic dynamics [22]. In ground-breaking mathematical works, Lorentz gases were shown to exhibit chaos and well-behaved transport properties [25,26], followed by understanding diffusion in computer simulations combined with stochastic theory [27–29]. Lorentz gases thus became standard models to explain the interplay between chaos and transport: highlights were a proof of Ohm's law from first principles [30], the analytical and numerical calculation of Lyapunov exponents [7,8,12] and fractal attractors [12], as well as developing a chaotic scattering theory of transport [7]. The growing interest in graphenelike systems now brings direct technological relevance to investigate classical diffusion in *soft* Lorentz gases equipped with more realistic potentials.

The conventional two-dimensional periodic Lorentz gas is a Hamiltonian particle billiard in which a point particle of mass m performs free flights with constant velocity v between elastic collisions at hard disks of radius r_0. The centers of these disks form the nodes of a triangular lattice with lattice spacing $2r_0 + w$, where w denotes the smallest distance between two nearby disks. Here, following previous studies on artificial graphene [31], we introduce a *soft*

Lorentz gas, where the hard disks are replaced by Fermi potentials,

$$V(\mathbf{r}) = \frac{1}{1+\exp((|\mathbf{r}|-r_o)/\sigma)}, \tag{1}$$

with σ determining the softness of the potential; see Fig. 1. Related models have been used to reproduce experimental results on the magnetoresistance of electrons in semiconductor antidot lattices [32–36]. In the following we set $m = r_0 = 1$ by keeping the total energy constant, $E = 1/2$. We thus have two control parameters, σ and the minimal gap size w between two nearby potentials for the given energy E. Making σ smaller, we approach the hard scatterer limit of the conventional Lorentz gas. A crucial question is to which extent chaotic diffusion in the hard Lorentz gas [7–9,22–24,30] is robust by softening the potential, i.e., for more realistic models. In this Letter we show that even a slight softening introduces substantial additional complexity leading to entirely new transport properties.

Our key quantity is the diffusion coefficient

$$D = \lim_{t\to\infty} \frac{\langle[\mathbf{r}(t)-\mathbf{r}(0)]^2\rangle}{4t}, \tag{2}$$

where the numerator denotes the mean square displacement (MSD) for the position $\mathbf{r}(t)$ of a particle at time t. The angular brackets hold for an ensemble average over initial conditions. If the MSD grows linearly in time, the above limit exists and the system exhibits normal diffusion. If the MSD grows faster than linear in time this limit diverges, and the system displays superdiffusion [37]. Technical details of the simulations carried out with the Bill2D software package [38] are explained in Sec. I of our Supplemental Material [39], which includes Ref. [40].

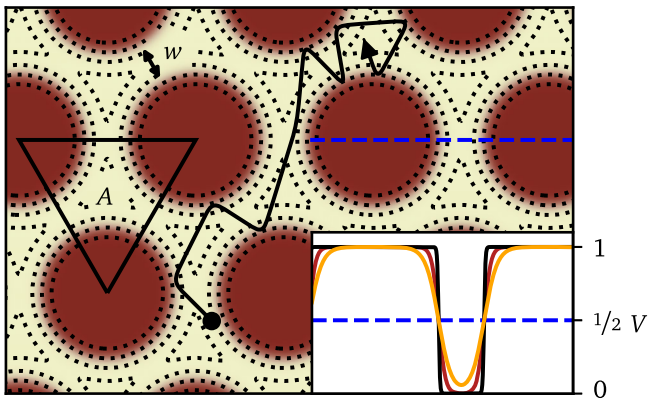

FIG. 1. The soft Lorentz gas: A point particle moves in a plane of partially overlapping Fermi potentials (inset) whose centers are situated on a triangular lattice (main figure). The dotted lines are contour lines, w denotes the minimal distance between adjacent potentials for total energy $E = 1/2$, and A defines a triangular unit cell. The inset shows Fermi potentials along the dashed (blue) line in the main part for different values of the softness parameter σ defined in Eq. (1).

Figure 2 depicts the diffusion coefficient D as a function of the gap size w between the scattering centers for a slightly softened (main part) and the hard (inset) Lorentz gas. While for the hard scatterers $D(w)$ is monotonically increasing and looks rather smooth, in the soft model D is a nonmonotonic, highly complicated function of w. This suggests that the diffusive properties must have changed profoundly. The diffusion coefficient for the hard Lorentz gas has been analyzed in detail in previous literature (cf. Sec. III A in the Supplemental Material [39], which includes Refs. [41–48]). Here we first explore whether there is any simple diffusion law for the soft model revealing an at least on average monotonic increase of $D(w)$ by ignoring any fine structure. We find that a Boltzmann-type random walk approximation works well to understand the coarse functional form of $D(w)$ [49]. For this we assume that diffusion is governed by "flights" of length ℓ_c during time intervals τ_c after which a particle experiences a "collision." We define a collision as an event where a particle hits the contour line of a scatterer at $E = 1/2$ in the triangular unit cell A displayed in Fig. 1. By assuming in the spirit of Boltzmann's molecular chaos hypothesis that all collisions are uncorrelated, the diffusion coefficient can be approximated as $D_B(w) = \ell_c^2(w)/[4\tau_c(w)]$. In Sec. II of the Supplemental Material [39] we derive an analytical formula for D_B as well as an improved numerical version $D_{\mathrm{B,num}}$. The results are shown as a pair of lines in Fig. 2: both yield an approximately linear increase of D for larger w, which matches well to the coarse functional form of the simulation results. For smaller w our analytical approximation does not reproduce the

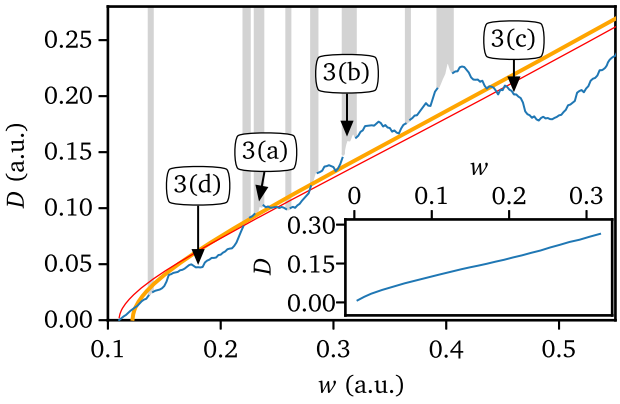

FIG. 2. Diffusion coefficient D as a function of the gap size w. The (blue) wiggled line shows simulation results for $D(w)$ Eq. (2) in a slightly softened potential [$\sigma = 0.05$ in Eq. (1)]. The thick (orange) line represents the corresponding analytical random walk approximation D_B, the thin (red) line the numerical $D_{\mathrm{B,num}}$ as explained in the text. The labeled numbers 3(a) to 3(d) refer to the periodic orbits depicted in Fig. 3. Gray columns indicate parameter intervals in which $D(w)$ does not exist. The inset displays $D(w)$ obtained from simulations for the conventional hard Lorentz gas [49].

onset of diffusion correctly while our improved numerical version captures it at least qualitatively well.

We now focus on the pronounced irregular fine structure of $D(w)$ in the soft system, which is in sharp contrast to the diffusion coefficient of the hard disk model. Irregular diffusion coefficients have been reported for parameter-dependent deterministic diffusion in much simpler chaotic dynamical systems, such as one-dimensional maps [50–53], the standard map [54,55], and particle billiards [49,56–58]. To our knowledge this is the first time that a diffusive fine structure has been unambiguously revealed in quite a realistic soft Hamiltonian system. For the hard Lorentz gas irregularities in $D(w)$ also exist but are extremely tiny [49,59], hence barely visibly in Fig. 2. A second crucial difference is that our softened model generates an intricate set of superdiffusive parameter regions in which $D(w)$ does not exist. The hard Lorentz gas displays only superdiffusion for all parameters $w > w_\infty$ after a specific geometric transition at $w_\infty \simeq 0.3094$ [60,61] by exhibiting superdiffusion that is different from the soft model as discussed in Sec. III A of the Supplemental Material [39].

The origin of the anomalous diffusion as well as of the irregularities in $D(w)$ of the soft Lorentz gas can be understood in terms of periodic orbits [52,53,59,62,63], as is explained by Fig. 3. It shows orbits both in position space and insets of corresponding Poincaré surfaces of section at four specific parameter values of w: Figs. 3(a) and 3(b) refer to quasiballistically propagating periodic orbits while 3(c) and 3(d) represent localized ones. These periodic orbits exhibit different structures due to different types of scattering, as is reflected in the corresponding Poincaré surfaces of section. The variables $(x, \sin\theta)$ for the latter are defined on the boundary where a particle leaves the unit cell A in Fig. 1. Here x represents the position of the particle in a gap, $\sin\theta$ is the angle between its velocity vector and the normal to the boundary. These islands of periodicity are typically extremely small and very difficult to detect in the whole phase space. By matching the parameter values of w for these periodic orbits to the structure of $D(w)$ in Fig. 2, we see that the two propagating orbits correspond to two superdiffusive regions while the two localized orbits identify (approximately) two local minima in the curve. While localized orbits only slightly suppress normal diffusion without making it anomalous [50,59,64], islands of periodicity in phase space, also called *accelerator modes* [54,55], generate superdiffusion [37,65–67]. A more detailed analysis yields that all these periodic orbits are topologically extremely unstable under parameter variation: they exhibit complicated bifurcation scenarios that eventually destroy any superdiffusive window leading to parameter regions of normal diffusion before new bifurcations create new superdiffusive windows [68].

Periodic orbits thus form the backbone to understand the complicated structure of the parameter-dependent diffusion coefficient in Fig. 2. We now explore them in the full

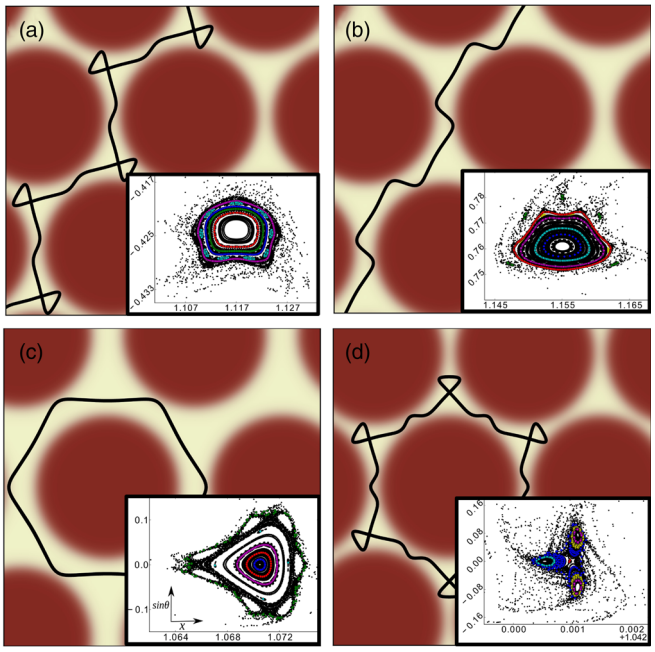

FIG. 3. Periodic orbits and islands of periodicity in phase space at different parameter values w corresponding to Fig. 2. Shown in position space are characteristic periodic orbits for (a) $w = 0.234$, (b) $w = 0.31$, (c) $w = 0.46$, (d) $w = 0.18$. (a) and (b) feature quasiballistically propagating orbits yielding superdiffusive parameter regions in Fig. 2 while (c) and (d) generate local minima in $D(w)$. The insets display associated islands of periodicity in the Poincaré surface of section phase space $(x, \sin\theta)$ as defined in the text.

parameter space (w, σ). For each point in (w, σ), the numerical discovery of a localized periodic orbit or a quasiballistic trajectory is marked in Fig. 4 as a blue or a red dot, respectively. Interestingly, our chart reveals a very

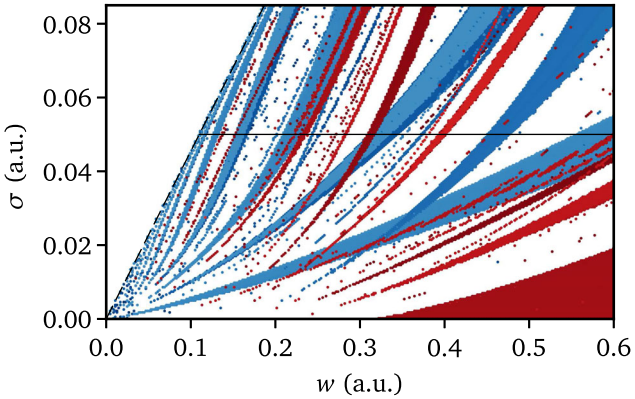

FIG. 4. Regions of periodic orbits in the parameter space of gap size w and potential softness parameter σ. Blue dots represent localized periodic orbits like (c) and (d) in Fig. 3, while red dots correspond to quasiballistic orbits like 3(a) and 3(b) therein. The black horizontal line at $\sigma = 0.05$ yields a cut through the parameter space corresponding to the diffusion coefficient $D(w)$ in Fig. 2.

regular topological structure underlying the seemingly totally irregular curve of $D(w)$ in Fig. 2, which lives on the horizontal black line at $\sigma = 0.05$ in Fig. 4. We see that all periodic orbits form regular "tongues" in parameter space which, however, we could not fit with simple functional forms like exponential, stretched exponential, or power laws. Whenever a tongue crosses the horizontal black line at $\sigma = 0.05$ we have a local extremum in the $D(w)$ curve of Fig. 2. Further details of this connection are described in Ref. [68]. In Sec. III B of [39] we explore the impact of these tongues on the diffusion coefficient under variation of σ. Therein we see that on a coarse scale $D(w)$ of the hard Lorentz gas is approached continuously by decreasing σ, interrupted by superdiffusive regions due to quasiballistic tongues. This scenario is in line with a mathematical theory on the existence of elliptic islands in the phase space of closed, nondiffusive billiards that are softened [69,70]. In these references the authors conjecture that islands are dense with respect to Lebesgue measure in parameter space for small σ. If this holds true, one expects $D(w)$ to be an irregular curve on arbitrarily fine scales with fractal properties [9,50,51,59,64].

In summary, we have studied diffusion under parameter variation in a soft Lorentz gas, which we put forward as a model for electronic transport in artificial graphene. We have found that the normal diffusion observed in the paradigmatic Lorentz gas with hard scatterers is not robust when softening them: instead, the type of diffusion immediately changes dramatically, generating an entirely different diffusion coefficient. This raises doubts about a universal applicability of the standard Lorentz gas for describing transport in realistic systems. In the soft Lorentz gas the diffusion coefficient turns out to be a highly irregular function under the variation of control parameters with regions exhibiting superdiffusion. This is explained in terms of periodic orbits that are topologically unstable under parameter variation while exhibiting very regular structures in parameter space. Analogous results hold for varying the energy E as a parameter [68], which experimentally corresponds to changing the temperature of the system. Note that, in superdiffusive parameter regions, ergodicity is broken; hence, for single particle experiments there will be a dependence on initial conditions [54,55]. In real systems with thermal noise we expect these superdiffusive regions, ergodicity breaking and irregularities on fine scales to disappear; however, larger irregularities should persist under noise [56,71]. Our results suggest to construct a more rigorous theory for calculating the diffusion coefficient curve in Fig. 2 from first principles, possibly based on generating partitions [72], which will be an extremely difficult task [9,63]. A second crucial challenge is to test for the diffusion coefficient of Fig. 2 in experiments.

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