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Anomalous diffusion of fermions in superlattices

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Abstract

We study a diffusion of fermions in the periodic two-dimensional lattice of fermions. We show that effects connected with antisymmetrization of the wave function increase chaoticity of motion. Various types of anomalous diffusion, which we characterize by a power spectral analysis are found. The nonlocality of the Pauli potential destroys cantori in the phase space. Consequently, the diffusion process is dominated by long free paths and the power spectrum is logarithmic at small frequency limit.

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The transport properties of Hamiltonian systems depend on structure of the phase space. For typical fully chaotic systems the motion is random and the transport can be described in terms of the diffusion process, similarly to the Wiener or Ornstein-Uhlenbeck processes. In those cases the velocity autocorrelation function falls exponentially with time and the mean squared displacement $\sigma^2(t) = \langle (x(t) - x(0))^2 \rangle$ grows linearly with time. However, there are also other possibilities of diffusive behaviour connected with a faster or slower time dependence of σ^2. The former happens if, for instance, the phase space exhibits regular structures (KAM tori) and trajectories are trapped in a self-similar hierarchy of cantori [1]. The diffusion is enhanced also for fully chaotic systems possessing families of infinitely long free paths, like the periodic Lorentz gas (PLG) [2].

From the point of view of transport phenomena, many physical systems can be reduced to a simple lattice of periodic potentials. Anomalously enhanced diffusion connected with the existence of long free paths has been found for example in classical molecular dynamics describing peripheral collisions of α-cluster nuclei or atomic aggregates [3] . This model is a complicated dynamical system taking into account all α-particle degrees of freedom. Nevertheless, its transport properties and diffusion characteristics appear to be the *same* as for the two-dimensional ($2D$) PLG , independently of the details of interactions involved. The dynamics of electrons in crystals moving in a magnetic field or the ballistic-electron dynamics in lateral superlattices , are another examples which can be modelled in terms of periodic $2D$ lattices [4,5]. Semiclassical billiard model has also been applied for understanding of the low-field magnetoresistance phenomena in narrow-channel geometries [6] .

Both low energy heavy-ion collisions for α-cluster nuclei and electron dynamics in crystals for large lattice spacings, can be reasonably well described in a classical limit, i.e. when the width of wave packet corresponding to moving particle is approximately fixed [3,4] . However if we consider system of fermions (electrons, nucleons), the quantum mechanical symmetry related to the identity of particles and resulting in the antisymmetry of the wave function should be taken into account. How does a fermionic nature of the basic constituents influence both the structure of the corresponding classical phase space and the transport phenomena is then the fundamental question which we shall address in the present Letter.

The model which seems best suited for addressing such questions is the one based on the coherent state formalism [7] . This formalism allows to define a classical limit [7] and, at the same time, to accommodate the effects of quantum statistics [8,9] . The i-th single particle state is described by the Gaussian wave packet :

$$\phi_i(\boldsymbol{r}) \equiv \langle \boldsymbol{r} | \phi_{\boldsymbol{Z}_i} \rangle = \left(\frac{1}{\pi b^2}\right)^{3/4} \exp\left[-\frac{(\boldsymbol{r}-\boldsymbol{Z}_i)^2}{2b^2}\right] , \tag{1}$$

where $\boldsymbol{Z}_i$ denotes the mean position of the packet i . These single particle states are not mutually orthogonal and, thus, their overlaps $n_{ij} = \langle \phi_i | \phi_j \rangle = \exp[-(\boldsymbol{Z}_i{}^* - \boldsymbol{Z}_j)^2/4b^2]$ do not vanish. The A-fermion system is then described by a Slater determinant : $\Phi(\boldsymbol{Z}) = (A!)^{-1/2} \det[\phi_i(\boldsymbol{r}_j)]$ whose norm $N(\boldsymbol{Z})$ is equal to $\det[n_{ij}]$. In this way the state of the system is entirely specified by the parameters $\boldsymbol{Z} \equiv \{\boldsymbol{Z}_i : i = 1, \ldots, A\}$ which for a proper treatment of the dynamics have to be considered as complex ($\boldsymbol{Z} = \boldsymbol{R} + i\boldsymbol{P}$) variables [8]. The units are specified by setting $\hbar = b = m = \hbar\omega = 1$. The Gaussian form of the wave packet proves appropriate for semiclassical studies of the structure of the phase space [10]. Since we refer to the classical limit, the width of these Gaussians is kept fixed in time.

The time development of the dynamical variables can be determined from the time-dependent variational principle:

$$\delta \int_{t_1}^{t_2} dt \langle \Phi(\boldsymbol{Z}) | \left(i\frac{d}{dt} - \hat{H}\right) | \Phi(\boldsymbol{Z}) \rangle \, (N(\boldsymbol{Z}))^{-1} = 0. \tag{2}$$

The resulting equations of motion take the form:

$$i \sum_{j\beta} S_{i\alpha,j\beta} \dot{Z}_{j\beta} = \frac{\partial H}{\partial Z^*_{i\alpha}} \tag{3}$$

where $\alpha, \beta \equiv x, y, z$. H is the expectation value of the many body Hamiltonian $H(\boldsymbol{Z}^*, \boldsymbol{Z}) = \langle \Phi(\boldsymbol{Z}) | \hat{H} | \Phi(\boldsymbol{Z}) \rangle N(\boldsymbol{Z}^*, \boldsymbol{Z})^{-1}$ and the Hermitian matrix : $S_{i\alpha,j\beta} = (\partial^2/\partial Z^*_{i\alpha} \partial Z_{j\beta}) \log N$ is positive definite. Such a scheme constitutes a formal basis for various molecular dynamics approaches respecting the quantum statistics for fermions [9,11] .

In general, the matrix $S_{i\alpha,j\beta}$ is non-diagonal due to the antisymmetrization. Therefore, neither $\boldsymbol{Z}_i$ and $\boldsymbol{Z}^*_i$ nor their real $\boldsymbol{R}_i$ and imaginary $\boldsymbol{P}_i$ parts form the canonically conjugate variables. For the two particle system, an exact transformation can be performed to the canonically conjugate variables $\boldsymbol{W}_i$ $(i = 1, 2)$ [12] , which cannot get closer than $\sqrt{2}$ independently of the difference between $\boldsymbol{Z}_1$ and $\boldsymbol{Z}_2$. This topological hole in the phase-space, existing also for $A \geq 3$, corresponds to the Pauli forbidden region [12,13]. An explicit expression for the canonical variables is not known for $A \geq 3$ and, in the following discussion, Eq. (3) will be solved in variables $\boldsymbol{Z}, \boldsymbol{Z}^*$.

We consider the motion of a single fermion inside an infinite $2D$ lattice of periodically distributed centers which are fermions themselves. In order to study effects caused by the antisymmetrization of the wave function, we discard entirely the two-particle interaction term in the Hamiltonian. Since the effective Pauli potential is short range we take into account only the influence of the neighbour lattice sites. We checked that it is enough to consider at most 16 of them ($A = 17$). The Pauli forbidden regions manifest themselves by the strong increase of $H(\boldsymbol{Z}_1^*, \boldsymbol{Z}_1)$ generated by the kinetic energy operator ($\boldsymbol{Z}_1 = \boldsymbol{R}_1 + i\boldsymbol{P}_1$ is the coordinate of the wandering fermion). Equivalently, the form of energy surfaces in $\boldsymbol{R}_1$ depends on momentum like variables $\boldsymbol{P}_1$ and the hilly structures in this effective Pauli potential become smaller with increasing $\boldsymbol{P}_1$. Thus the antisymmetrization produces a nonlocal time-dependent effective potential when the particle approaches the lattice site occupied by a fermion. The nonlocality of the Pauli potential is a quantum effect, which is neglected in purely classical models. In the following, we will analyze its role in the diffusion process. For this purpose, we compare two cases. The first one refers to the full, nonlocal Hamiltonian (the "nonlocal case"). The second one (the "local case") is specified as follows. We construct a local potential $V_l(\boldsymbol{R}_1)$ putting all momenta in the Hamiltonian H to zero and define a new Hamiltonian $H_l = \boldsymbol{P}_1^2/2 + V_l$. Then we solve the classical equations of motion with H_l, i.e. Eq. (3) where $S_{i\alpha,j\beta}$ is now simplectic.

The particle dynamics depends on the distance d between centers. If d is large, the particle can move freely like in the PLG with the open horizon. Small d corresponds to the closed horizon, i.e. the particle is captured among neighbouring centers. For intermediate distances, the particle can wander through the lattice but is subjected to the interaction with neighbouring centers for all times. We study these three cases for $d = 16, 4$ and 8 respectively, at the energy $E = 0.2$.

Fig.1 presents the Poincaré sections for $d = 8$ (open horizon) and $d = 4$ (closed horizon). For the open horizon (Figs. 1a, 1b) a point on the (x, p_x) plane has been marked as soon as the particle crossed the edge of the cell, whereas for the closed horizon (Figs. 1c, 1d) the condition $y = 0$ has been applied. In the latter case, the Poincaré sections clearly show what happens when the nonlocality is switched on: the completely integrable system turns into a predominantly chaotic one with only isolated islands of tori. The chaoticity increases also for the open horizon. Fig. 1a reveals intricate winding lines between the solid structures which indicate the presence of cantori in the local case. The transport in this region is inhibited, i.e. chaotic trajectory may penetrate into this hierarchy of barriers and remain trapped for an arbitrary long time. All those cantori are destroyed due to the nonlocality (Fig. 1b).

The most interesting feature, however, is the occurrence of variety of deterministic diffusive motions, which we have analyzed by means of the velocity power spectrum defined in terms of the time series for the velocity component v_x:

$$S(\omega) = S_x(\omega) \sim \left| \int_{-\infty}^{+\infty} v_x(t) \exp(i\omega t) dt \right|^2. \tag{4}$$

Final values of $S(\omega)$ have been obtained by averaging over 10^3 time series (for various initial conditions) of length $6.5 \cdot 10^4$. Having the power spectrum calculated we can obtain the velocity autocorrelation function $C(t)$ taking the inverse Fourier transform. Using the Green-Kubo formula (see e.g. [1]), we can then find the mean squared displacement of the particle σ^2, directly determining the diffusion coefficient. For the largest lattice spacing ($d = 16$) both local and nonlocal cases are identical and give $S(\omega) \sim \ln \omega$ at small ω (Fig. 2a). Therefore $C(t) \sim 1/t$ and $\sigma^2 \sim t \ln t$. It means that the diffusion process is accelerated and the diffusion coefficient diverges logarithmically, like for the PLG. Long free paths of the particle are responsible for this kind of behaviour. The presence of cantori in the phase space for the local case at $d = 8$ makes the diffusion even faster, changing the shape of $S(\omega)$ into the algebraic one: $S(\omega) \sim \omega^{-\alpha}$ with $\alpha = 0.58$ (Fig. 2b), associated with $1/f$ noise and well known from earlier studies of similar systems [1,5]. For the nonlocal case the cantori vanish and the free paths determine the dynamics. The power spectrum becomes logarithmic again. Finally, Fig. 3 presents results for the closed horizon. The local case which is integrable [14] , involves a number of isolated frequencies, whereas the nonlocality generates chaos with a continuous spectrum of frequencies. Its low frequency limit is again algebraic ($S(\omega) \sim \omega^{-\alpha}$ with $\alpha = 0.61$) because of trapping of orbits in the network of cantori still existing in the phase space (Fig. 1d).

We have shown that the nonlocality of the effective potential connected with the incorporation of the Pauli exclusion principle into the molecular dynamics causes the increase of chaoticity. This nonlocality is able to destroy most of the KAM tori modifying diffusion properties of the system. The trapping of orbits in cantori becomes less important due to the nonlocality and effects associated with the infinitely long free paths take over. However, the role of nonlocality depends on the lattice spacing. For small lattice parameters the classical description is not applicable. The diffusion motions in closed horizon limit are different in the classical PLG and in the superlattice of fermions. In the latter case, the velocity autocorrelation function of fermions is never decreasing exponentially or faster and the diffusion process is *always* anomalously enhanced. On the other hand, if lattice parameter is large enough then nonlocal and local cases coincide making the purely classical description more reliable. Due to the presence of long free paths the system possesses specific fluctuation properties, e.g. the diffusion coefficient grows logarithmically with time. Physically, this situation is important. For example, motion of electrons in strong magnetic fields has been modelled by $2D$ lattices with much larger lattice parameters than in natural crystals [4,5]. In the nuclear molecular dynamics, long free paths correspond to the deep-inelastic reactions [3]. In all those different cases, the diffusion properties are *universal* and insensitive to the details of short-range interactions. Such universality allows to describe phenomena involving long free paths in a framework of the Langevin equation with algebraically correlated noise [15]. The results presented in this Letter show that it is also true if one considers fermions, i.e. take into account the Pauli exclusion principle.

Our results have been obtained neglecting the two-particle interaction and are relevant for modelling transport properties of fermions in e.g. Boltzmann-Langevin formalism if in medium two-particle cross-section is small with respect to the size of the topological hole due to the antisymmetrization. In this limiting case, two-particle collisions in the collision integral of the Boltzmann-Langevin equation would generate, even for large densities, the anomalously enhanced diffusion process with $D \sim t^{\alpha}$ $(\alpha \simeq 0.6)$ and not the normal diffusion as it is usually assumed [16,17]. The consequences of this finding for transport properties in realistic situations of nuclear heavy-ion collisions or metallic cluster collisions should be further studied.

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FIGURES

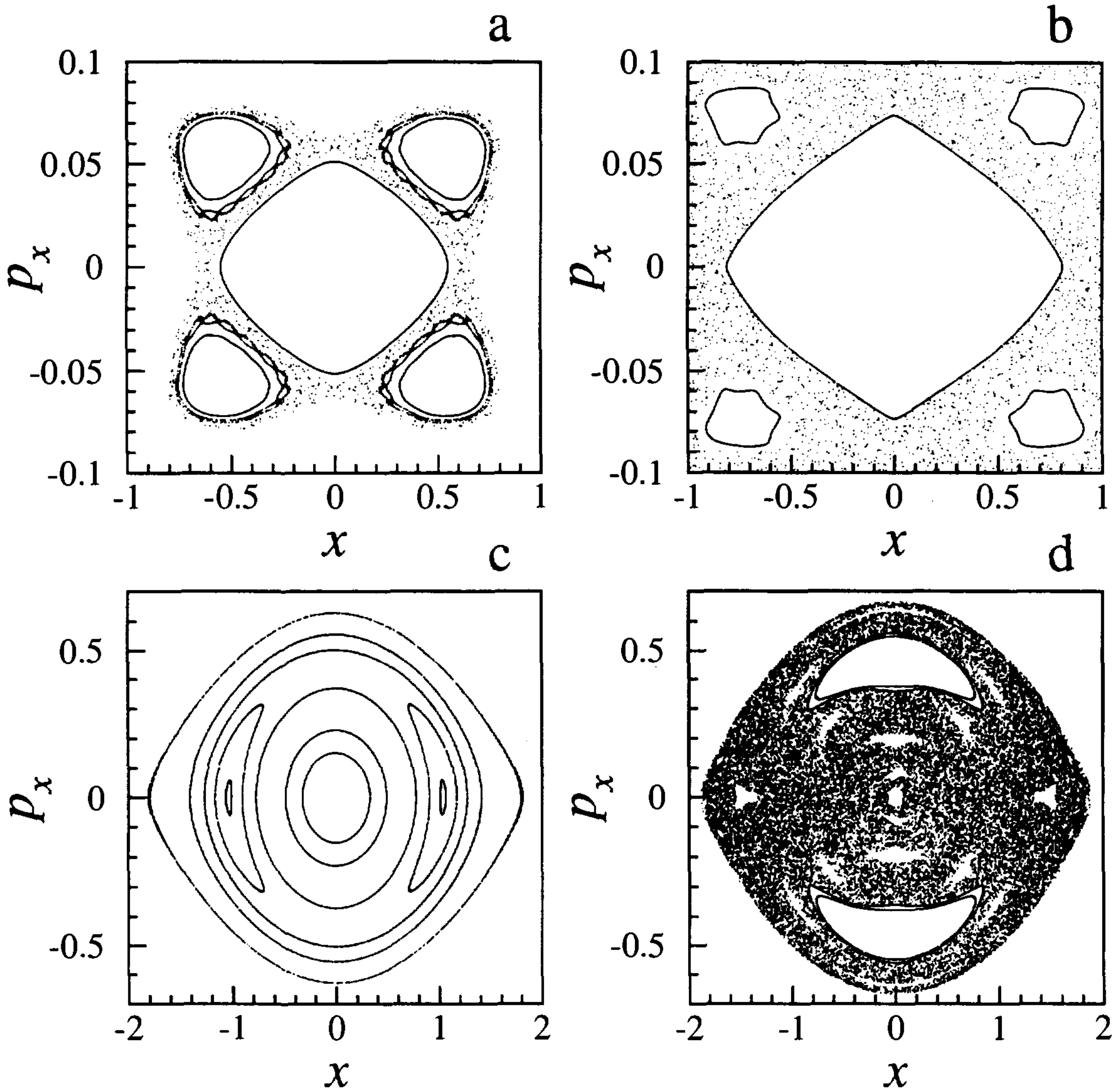

FIG. 1. The Poincaré sections for the lattice parameters $d = 8$ (upper part) and $d = 4$ (lower part). Both local (left part) and nonlocal (right part) cases are shown. The energy is $E = 0.2$. In (a), for the sake of clarity, only one chaotic trajectory is shown; the rest of the phase space (only its fragment is presented in the figure) is filled with chaotic trajectories. White areas inside regular structures are filled with tori.

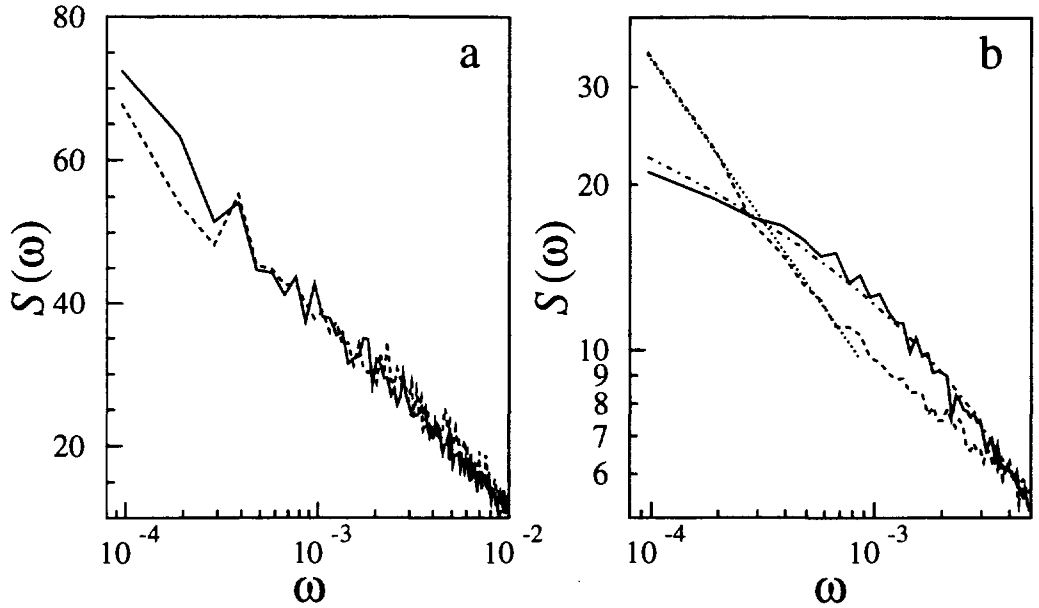

FIG. 2. The averaged power spectrum for the open horizon. The nonlocal and local cases are shown as solid and dashed lines, respectively. The lattice parameters are : (a) d = 16, and (b) d = 8. The dotted and dashed-dotted lines in part (b) exhibit powerlaw are logarithmic fits respectively. Note different scales on abscissae.

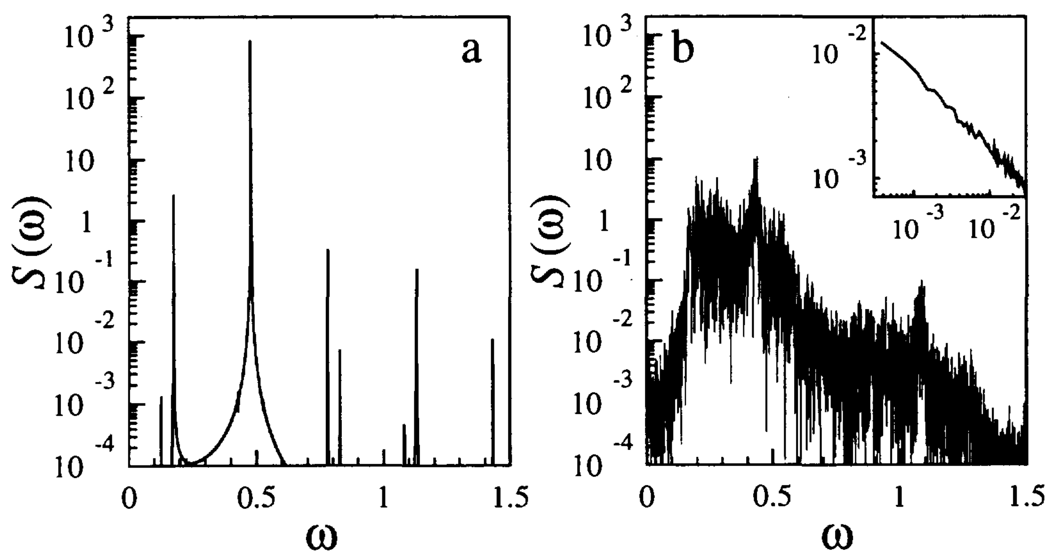

FIG. 3. The power spectrum for the closed horizon obtained from a single time series. (a) The local case. (b) The nonlocal case for a chaotic trajectory. The inset shows the average $S(\omega)$ in the low ω limit.