Chaos induced by Pauli blocking

S. Drożdż, J. Okołowicz, M. Ploszajczak, E. Caurier and T. Srokowski

1 Institute of Nuclear Physics, PL – 31-342 Kraków, Poland
2 GANIL, BP 5027, F-14021 Caen Cedex, France
3 Centre de Recherches Nucléaires, F-67037 Strasbourg Cedex, France

ABSTRACT

Dynamics of classical scattering in the system of fermions is studied. The model is based on the coherent state representation and the equations of motion for fermions are derived from the time-dependent variational principle. It is found that the antisymmetrization due to the Pauli exclusion principle, may lead to hyperbolic chaotic scattering even in the absence of interaction between particles. At low bombarding energies, the same effect leads to the screening of the hard, short-ranged component in the two particle interaction and thus regularizes the dynamics.

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One of the central issues in the theory of complex dynamical systems is the classical-quantum correspondence for classically chaotic motion. Classically, chaos is a well defined concept but a way it manifests itself on the quantum level still remains a matter of controversy. One of the reasons of this controversy is the quantum mechanical symmetry related to the identity of particles. Of particular interest and importance in this context are the effects resulting from antisymmetry of an underlying wave function for fermionic systems. Most of the physical objects, like atoms or atomic nuclei, providing empirical input for the above studies, are collections of fermions. The fundamental question then is in which sense does a fermionic nature of the basic constituents influence the structure of the corresponding classical phase space. And, in particular, does it increase or reduce the amount of instabilities leading to chaotic behavior?

The model which seems best suited to incorporate the elements needed and thus for addressing such questions is the one based on the coherent state formalism. This formalism allows to define a classical limit and, at the same time, to accommodate the effects of antisymmetrization. Consistently, the i-th single particle state is described by the Gaussian wave packet:

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

where \( Z_i \) is the location of the center of gravity of the packet. These single particle states are not mutually orthogonal and, thus, their overlaps \( n_{ij} = \langle \phi_i | \phi_j \rangle = \exp \left[ -\frac{(Z_i^* - Z_j)^2}{4b^2} \right] \) do not vanish. The A-fermion system is then described by a Slater determinant \( \Phi(Z) = (A!)^{-1/2} \det[\phi_i(r_j)] \) whose norm \( N(Z) \) is equal to \( \det[n_{ij}] \). In this way the state of the system is entirely specified by the parameters \( Z \equiv \{ Z_i : i = 1, \ldots, A \} \) which for a proper treatment of the dynamics have to be considered as complex \( (Z = R + iP) \). The units are specified by setting \( \hbar = b = m = \hbar \omega = 1 \). The time development of the dynamical variables can be
determined by the time-dependent variational principle:

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

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 $\alpha, \beta = x, y, z$. $H$ is the expectation value of the many body Hamiltonian $H(Z^*, Z) = \langle \Phi(Z)| \hat{H} |\Phi(Z) \rangle N(Z^*, Z)^{-1}$ and the Hermitian matrix:

$$S_{i\alpha,j\beta} = \frac{\partial^2}{\partial Z^*_{i\alpha} \partial Z_{j\beta}} \log N. \tag{4}$$

is positive definite. Such a scheme constitutes a formal basis for various molecular dynamics approaches [3, 4, 5] and the Gaussian form of the wave packet proves appropriate for semiclassical studies of the structure of the phase space [6].

In general, due to the antisymmetrization, the off diagonal terms in $S_{i\alpha,j\beta}$ do not disappear. Therefore, neither $Z_i$ and $Z^*_i$ nor their real $R_i$ and imaginary $P_i$ parts form the canonically conjugate variables. For the two particle system, an exact transformation can be performed to the new, canonically conjugate variables $W_i \ (i = 1, 2)$ [7]. These $W_i$ cannot get closer than $\sqrt{2}$ independently of the difference between $Z_1$ and $Z_2$. Thus a topological hole, existing also for $A \geq 3$, corresponds to the Pauli forbidden region [7, 8]. However, an explicit expression for the canonical variables is not known for $A \geq 3$ and, therefore, the equations (3) will be solved in original variables $Z$.

Schematic models [9, 10, 11], based on the scattering of a particle on the target composed of three particles at the corners of equilateral triangle located in the reaction plane, proved very instructive in studying various aspects of the collision processes. In this case, the scattering problem reduces to two degrees of freedom. At the present exploratory stage we perform an analogous study. The target is given
by a three fermion (Gaussian wave packets (1)) configuration forming equilateral
triangle of side equal to 4. We begin by entirely discarding the interaction term
in the Hamiltonian in order to elucidate on the role of antisymmetrization itself.
The Pauli forbidden regions manifest themselves by the strong increase of $H(Z^*, Z)$
generated by the kinetic energy operator. Equivalently, the form of the energy
surfaces in $R$ depends on the momentum like variables $P$, as demonstrated in Fig. 1.
Here the $R$ dependence of the energy, as ‘seen’ by the fourth fermion located in the
reaction plane $(x, y)$, is plotted at two fixed values of $P$. With increasing $P$, the
hilly structures in this effective Pauli potential become relatively smaller and the
dynamics approach a free motion. Notice that a $P$ dependence of the Pauli potential
is an analog of the nonlocality for ordinary potentials.

In a real dynamical process $P$ changes in time and so does $H$. Nevertheless,
the appearance of the three center structures suggests [9, 10, 11] that for certain $P$
values one may expect a strong sensitivity on the initial conditions. That this really
happens is documented in Fig. 2 which shows, for the three different energies, the
impact parameter dependence of the deflection angle $\theta$ of the particle scattered off
the target. The motion is initialized by setting the appropriate initial value of $P_x$
with $P_y = 0$ and the impact parameter $R_y$. The presentation of the results is based
on the asymptotic values of the variables in the region where antisymmetrization
is no longer effective and, thus, $R, P$ are canonical conjugate. For energies either
small ($E = 0.2$) or large ($E = 0.6$), compared to the height of the effective Pauli
potential $V_{\max}(P = 0) \equiv \max H(R, P = 0) \simeq 1/2$ (see Fig. 1a), $\theta$ depends on the
impact parameter but this dependence is essentially continuous. At $E = 0.4$ and for
$R_y$ between 0 and 1, one observes behavior characteristic of the chaotic scattering.

Very interestingly, this scattering process carries all characteristics of the hyper-
bolic chaotic scattering [12]. For this type of scattering, theory predicts [12, 13, 11]
that the survival probability, \textit{i.e.} number \( N(t) \) of trajectories remaining in the interaction region up to time \( t \), follows:

\[
N(t) = N_0 \exp[-\lambda (1 - D) t],
\]

where \( \lambda \) is the Lyapunov exponent and \( D \) is the fractal dimension. The Lyapunov exponent \( \lambda \), calculated from the growth rate of separation ratio \( \delta / \delta_0 \) between the two neighboring (and long enough) trajectories \cite{14}, is independent on what pair of scattering trajectories is used and, thus, \( \lambda = 0.22 \) is well determined (Fig. 3a). Furthermore, the set of singularities seen in Fig. 2 for \( E = 0.4 \) possesses a well defined fractal dimension \( D \). This one can conclude from calculation based on the uncertainty exponent technique \cite{15} which gives \( D = 0.591 \) (Fig. 3b). Finally, following the concepts of the transport theory \cite{16}, by uniform random sampling of the whole interval of impact parameters one determines the survival probability \( N(t) \). In our case one observes (Fig. 3c) asymptotically exact exponential dependence, characteristic of the hyperbolic chaotic scattering, perfectly described by the above values of \( \lambda \) and \( D \).

These investigations provide convincing evidence that the chaotic scattering we deal with is of the hyperbolic type where the set of singularities is connected to the existence of only unstable periodic orbits. In the present case, however, these structures take place for a system of noninteracting fermions and are entirely due to the antisymmetrization. Independently, it is interesting to notice the appearance of such uniform fractal set of singularities for a nonlocal problem.

The most important result of the above analysis is that for a sufficiently dense system, the correlations resulting from Pauli blocking may lead to a significant modification of the particle dynamics. In certain situations, they may even convert free motion in the gas of non-interacting particles into the strongly chaotic one. In general, this is more likely to occur when the mean kinetic energy of particles in the gas
is comparable with the height of the effective Pauli potential. At very low energies, the range of Pauli blocking for sufficiently dense system extends to such a size that different topological holes start overlapping and the dynamics becomes regular again (see upper panel of Fig. 2). In more realistic case of interacting fermions, this effect may thus screen out the short range components of the two-body interaction. This dynamical screening may be especially important for the hard, short-range interactions like the one between the nucleons. Classically, such an interaction generates strongly chaotic behavior. However, its appearance inside the Pauli forbidden region may restructure and even eliminate the corresponding irregularities.

For a somewhat more quantitative illustration of this point, we present in Fig. 4 the energy surface plots in the similar configuration as in Fig. 1. This time, however, the constituents interact with the spherically symmetric, repulsive two-body interaction \( V(r) = V_0 \exp\left[-(r/r_0)^2\right] \), with \( V_0 = 10^{5/2} \) and \( r_0 = 10^{-1/2} \). For these parameters the interaction is comparatively hard and short-ranged. Upper panel of Fig. 4 corresponds to the situation with no antisymmetrization included. In (a) the side of the triangle equals 3 and in (d) it equals 4. In both cases the three hill structure shows up and, consequently, the scattering will be chaotic in the corresponding energy intervals. Including antisymmetrization changes the picture completely (see Fig. 4b). Here, not only the energy is reduced by almost two orders of magnitude but also the three hill structure, previously responsible for chaotic behavior, disappears. Increasing momentum, slowly recovers the original shape of the energy surfaces, as is shown in Fig. 4 (c) and (f) for \( P_x = 2\sqrt{10} \), but they still remain about one order of magnitude lower.

Returning to our introductory question we thus conclude that the fermionic nature of particles may drastically change the structure of the corresponding classical phase space. As the two extreme possibilities we identify the chaotic behavior in
absence of any interaction and the regularization of motion for strongly interacting particles. The first of them is very intriguing in view, for instance, of the fact that the hyperbolic chaotic scattering is considered as a classical manifestation of Ericson fluctuations \cite{17}. Equally interesting from the physical point of view is the second effect. The dynamical screening of the short-range components of the two-body interaction, is consistent with the success of the mean field concept in the region close to the Fermi surface for such a strongly interacting system as an atomic nucleus. In this connection, the space nonlocalities are identified \cite{18} as a crucial element enhancing the nucleon mean free path. Many related questions remain a subject for further investigations.

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Figure captions

**Fig. 1** Energy surface plots for noninteracting configuration generated by the three fermions located at the corners of equilateral triangle as seen by the fourth fermion at momentum $P_x = 0$ (a) and $P_x = \sqrt{10}$ (b). Triangle side length equals 4 and $P_y = 0$.

**Fig. 2** Deflection angle $\theta$ as a function of the impact parameter for three different energies under geometrical conditions corresponding to Fig. 1.

**Fig. 3** (a) Separation ratio between the neighboring trajectories for the scattering process at $E = 0.4$. Dots denote the dynamically determined values and the straight solid line represents a fit whose slope corresponds to the Lyapunov exponent $\lambda = 0.22$.

(b) Dependence of the fraction $f(\epsilon)$ of uncertain pairs of trajectories (differing in $\theta$ by more than $\pi/2$) as a function of the difference $\epsilon$ in initial values of the impact parameters. According to the uncertainty exponent technique the corresponding fractal dimension is $D = 0.591$.

(c) Survival probability expressed as a number of the scattering trajectories remaining in the interaction region up to time $t$. The straight line represents the theoretically determined dependence.

**Fig. 4** Energy surface plots for the three fermion configurations forming equilateral triangle of side equal to 3 (a, b, c) and 4 (d, e, f) respectively: (a) and (d) represent the potential energy without antisymmetrization for the two-body interaction defined in the text, (b) and (e) the total energy with antisymmetrization, (c) and (f) the total energy with $P = 2\sqrt{10}$.
