

Relaxation properties in classical diamagnetism

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It is an old result of Bohr that, according to classical statistical mechanics, at equilibrium a system of electrons in a static magnetic field presents no magnetization. Thus a magnetization can occur only in an out of equilibrium state, such as that produced through the Foucault currents when a magnetic field is switched on. It was suggested by Bohr that, after the establishment of such a nonequilibrium state, the system of electrons would quickly relax back to equilibrium. In the present paper we study numerically the relaxation to equilibrium in a modified Bohr model, which is mathematically equivalent to a billiard with obstacles in a magnetic field that is adiabatically switched on. We show that it is not guaranteed that equilibrium is attained within the typical time scales of microscopic dynamics. Depending on the values of the parameters, one has a relaxation either to equilibrium or to a diamagnetic (presumably metastable) state. The analogy with the relaxation properties in the FPU problem is also pointed out.

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It is well known since the time of the dissertation of Bohr (see ref. 1, page 380, or refs 2–3) that, according to classical statistical mechanics, at equilibrium a system of free electrons doesn't exhibit any diamagnetism. Indeed, the Maxwell–Boltzmann distribution of the electron velocities depends, at a fixed temperature, only on the system's energy. On the other hand, the value of energy does not depend on the magnetic field. So the electron velocity distribution, being unaffected by the magnetic field, is the same as for a vanishing field, and thus magnetization vanishes. The same line of reasoning is followed in the classical textbooks 4–5 of Feynman and Pauli.

On the other hand it is found experimentally that there exist systems of electrons which exhibit a diamagnetic behavior, so that the electron velocity distribution has to remain far from equilibrium for a long time. A paradigmatic example is that of plasmas (see for example ref. 6). Thus one meets with the dynamical problem of ascertaining whether in systems of such a type of a relaxation to equilibrium actually occurs, and which is the corresponding characteristic time.

In the present paper we study numerically a dynamical system which captures in the simplest possible way the main dynamical features of such a problem, namely, a billiard with obstacles in a magnetic field which is adiabatically switched-on. We find that, starting with the electrons at equilibrium, i.e. with a uniform spatial distribution and a Maxwell–Boltzmann velocity distribution, the switching on of the field produces an out-of-equilibrium state with a nonvanishing magne-

tization. This fact is well known, and was particularly emphasized for example by Bohr, who pointed out (see ref. 1, page 382) that a relaxation to equilibrium should later occur in a very short time (in his very words, “... *the induced collective motions of the electrons will disappear very rapidly after the magnetic field has become constant*”). We show, however, that the subsequent behavior depends on the density of obstacles (which may be considered to mimic the interaction of the electrons with a background of ions). For high enough densities the system indeed quickly relaxes to equilibrium (i.e., to a vanishing magnetization), whereas for small obstacles densities the system relaxes, within the available integration time, to an apparent stationary state, presenting a nonvanishing (negative) magnetization.

The existence of large relaxation times to equilibrium (or possibly to a kind of metaequilibrium state) in dynamical systems is known for systems which can be reduced to perturbations of integrable ones, such as the FPU model (see for example the reviews 7 and 8) or systems of diatomic molecules. The main result of the present paper is that large times to equilibrium can occur also for systems which are perturbations (due the magnetic field) of chaotic systems, such as billiards with obstacles.^{9,10}

I. INTRODUCTION

From a macroscopic point of view, the phenomenon of magnetization consists in the fact that a body, when immersed in a magnetic field \mathbf{B} , becomes a magnet with a certain magnetic moment \mathbf{M} . The corresponding magnetization (magnetic moment per unit volume \mathbf{M}/V) can be taken to be proportional to the external field, i.e., one can take $\mathbf{M}/V = \chi\mathbf{B}$, the magnetic susceptibility χ constituting the response function to the insertion of the field. From a microscopic point of view, if the contribution of the spins is neglected, the magnetic moment \mathbf{M} is due only to the amperian currents, and is proportional to the total angular momentum \mathbf{L} of the system of electrons. Indeed one has (see ref. 11 sec. 9–5, or ref. 6, page 16)

$$\mathbf{M} = \frac{q}{2c} \sum_i \mathbf{x}_i \wedge \mathbf{v}_i = \frac{q}{2mc} \mathbf{L}$$

where \mathbf{x}_i and \mathbf{v}_i denote the position and velocity of the i -th electron, while q and m are the electron charge and mass (we are using Gaussian units). So, the fact that the system possesses a magnetization after the insertion of the field corresponds to the dynamical fact that its angular momentum has acquired a nonvanishing value, starting from the vanishing one of equilibrium.

In the linear approximation, the response function χ might be computed in dynamical and statistical terms, making use of the Green–Kubo formula, according to which the magnetic susceptibility is proportional to the time autocorrelation of angular momentum. This fact is recalled here in an Appendix. As was previously mentioned, in classical mechanics the susceptibility vanishes when the system has relaxed to equilibrium, and this means that the time autocorrelation of magnetization did relax to zero. In terms of dynamical systems theory, this amounts to ascertaining that such a time decorrelation of angular momentum actually occurs, and to establish which is the corresponding relaxation time.

Now, whereas in the case of monatomic gases it is well known that the relaxation times are very short, being of the order of the mean collision times, extremely long relaxation time are phenomenologically known to exist in many systems, typically in glasses, and analytically were proven to exist (even in the thermodynamic limit) in dynamical systems such as slightly coupled rotators¹³ or slightly coupled nonlinear oscillators¹⁴. On the other hand we know that in the case of a plasma (which is the paradigmatic physical system we have in mind here) the relaxation times can actually be macroscopically long, as is observed both in astrophysics and in the laboratory. So the problem we are discussing here is whether long relaxation times to equilibrium occur also for simple mathematical models of Bohr’s type describing a system of independent electrons in a magnetic field, colliding with a wall and with background ions. In particular, if it is found that the relaxation process presents for example two time scales, then in the intermediate range of times

one is in presence of some nonvanishing “effective magnetization”, notwithstanding the fact that at equilibrium the magnetization should vanish.

In the present paper we consider a model of noninteracting electrons moving in a circular billiard with obstacles, also subject to the action of a magnetic field which is adiabatically switched on, and then kept constant. The obstacles may be considered to mimic the interactions of the electrons with a positive ionic background, and are expected to play a relevant role in driving the system back to equilibrium. We integrate numerically the equations of motion, and estimate the response of the system in terms of the magnetization. This is at variance with the available literature concerned with numerical studies on billiards in an external magnetic field,^{15–18} which all, to our knowledge, deal with the case of a static field. Indeed our main interest is in providing an estimate of magnetization, and this can be obtained either directly by studying the response of the system to a variable field, as we are doing in the present paper, or by using the Green–Kubo relation in a static field. On the other hand, in the available literature dealing with a static field the attention is addressed to quantities, such as the Lyapunov exponents, which have no obvious relation to the quantities entering the Green–Kubo formula, and thus to magnetization, which is the observable of interest for us.

In our problem, there are two limit cases, namely: i) that without obstacles, that we call *the original Bohr model*, which is integrable, and ii) that with obstacles but no magnetic field, which is mixing. In the first case there is no relaxation, so that the system exhibits a permanent diamagnetic behavior. In the second case the time correlation of angular momentum quickly decays to zero, so that no diamagnetic behavior is expected. We are interested in the intermediate case, with obstacles and with a field which is adiabatically switched on, which we call *the modified Bohr model*. The results we found can be summarized as follows: for high obstacles densities the magnetization relaxes to zero within the available simulation time. Below a certain threshold density, it instead relaxes to a nonvanishing value, which appears to be stationary up to the available simulation time. So the time-scale for relaxation (if there is any relaxation at all) has to be much larger than the time scale over which the system was integrated. In the latter case, we also investigated the dependence of the asymptotic value of magnetization on the obstacles density, and found that it tends to zero as a stretched exponential of the density as the density increases.

In section 2 the model and the integration algorithm are described; in addition, some preliminary results for the simplified model with no obstacles (the original Bohr model) are illustrated, because in such an integrable case a check can be made of the reliability of our procedure. In section 3 the case of interest (presence of obstacles, with a field which is adiabatically switched on, i.e., the modified Bohr model) is studied, and the above mentioned results are illustrated. The conclusions follow. Appendix A is

devoted to an analytical study of the integrable original Bohr model (no obstacles), and to a microscopic deduction of the existence of a magnetic pressure. A formula of Green–Kubo type for the magnetization is deduced in Appendix B.

II. THE MODEL, AND PRELIMINARY NUMERICAL CHECKS

The model concerns a system of N identical point particles of mass m and charge q , moving in a plane. We denote by $\mathbf{x}_i = (x^{(i)}, y^{(i)})$, $i = 1, \dots, N$, the coordinates of the i -th particle and by $\mathbf{p}_i = (p_x^{(i)}, p_y^{(i)})$ their conjugate momenta. The magnetic field is taken perpendicular to the plane and homogeneous, i.e., we take $\mathbf{B}(t) = (0, 0, B(t))$, so that the vector potential \mathbf{A} at point \mathbf{r} is given by $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B} \wedge \mathbf{r}$, where \wedge denotes the vector product. The particles do not interact with each other, and so the Hamiltonian is simply given by

$$H(\mathbf{p}_i, \mathbf{x}_i, t) = \frac{1}{2m} \sum_{i=1}^N \left(\mathbf{p}_i - \frac{q}{2c} \mathbf{B}(t) \wedge \mathbf{x}_i \right)^2 + \sum_{i=1}^N V(\mathbf{x}_i), \quad (1)$$

where $V(\mathbf{r})$ is a confining potential, i.e. a function vanishing inside the allowed domain and diverging outside it (corresponding to a boundary condition of elastic reflection). We take for m and q the mass and the charge of the electron, and we use atomic units, in which the electron mass, the modulus of the electron charge and the reduced Planck constant \hbar are all set equal to 1. The number N of particles in most simulations is taken in the range $10^3 \div 10^4$, and in some cases is increased up to 10^5 .

The time dependence of the magnetic field is taken as

$$B(t) = \frac{B_0}{2} \left(1 + \tanh \frac{t - t_i}{t_c} \right), \quad (2)$$

where t_c is the characteristic time over which the magnetic field varies, and t_i is, in a sense, the time at which the field is switched on. Indeed, for times $t - t_i < -5t_c$ the magnetic field essentially vanishes, while for $t - t_i > 5t_c$ the field is essentially constant, equal to B_0 . The values of the modulus of the magnetic field $|B_0|$ are taken in the range $10^{-3} \div 10^{-2}$ (in atomic units), while t_c is taken of order 10^6 (in our time unit) and t_i of the order $5 \cdot 10^7$.

Concerning the domain, the electrons are first of all enclosed in a circle, with elastic reflections at the border. Furthermore, in order to mimic at least qualitatively a more realistic situation in which the electrons interact with the ions of a background, we add inside the circular domain a square lattice of circular obstacles. The radius R of the circle is taken fixed equal to 5×10^4 (expressed in atomic units, i.e. the Bohr radius), while the radius r of each obstacle is taken equal to 10, and the lattice step in the range from 10^3 to 10^4 .

From Hamiltonian (1) one gets the equations of motion, which are all decoupled because the particles have

no mutual interaction. Such equations are numerically integrated using the “leap frog” algorithm¹² which we now briefly describe. The integration step of the “leap frog” method from the values $\mathbf{p}_i, \mathbf{x}_i$ at time t to the values $\mathbf{p}'_i, \mathbf{x}'_i$ at time $t + \tau$ is performed by a canonical transformation with generating function

$$S = \sum_{i=1}^N \mathbf{p}_i \cdot \mathbf{x}'_i - \tau H(\mathbf{p}_i, \mathbf{x}'_i, t + \tau). \quad (3)$$

This gives an implicit integration scheme, which can be easily made explicit for the particular form of our Hamiltonian (1).

The collision with the boundary is dealt with as follows: one performs an integration step and then checks whether the particle remains inside the allowed domain. If this is not the case, the evolution is made not according to the leap frog algorithm, but with a different procedure: the position \mathbf{x}_i and the component of \mathbf{p}_i tangent to the boundary are left unchanged, while the normal component of the momentum \mathbf{p}_i changes its sign. One checks that this approximation is sufficient to keep constant the energy of the system (in the case of a time independent field).

Concerning the initial data, they are taken at random in the following way: the initial positions of the particles are uniformly distributed inside the allowed domain, while the initial velocities are distributed according to a Maxwell–Boltzmann distribution at a certain temperature T . We take a temperature T such that $k_B T = 1/250$ in our units (k_B being the Boltzmann constant). This corresponds to about 10^3 K, or to a mean electron velocity approximately $1/3000$ the speed of light.

Finally, we explain how the magnetic moment $\mathbf{M} = (0, 0, M)$ is computed. The instantaneous value of the magnetic moment, which we denote by $(0, 0, \mathfrak{M})$, is given by

$$\mathfrak{M} = \frac{q}{2mc} L, \quad (4)$$

where L is the component of the total angular momentum normal to the plane. Such a quantity is found to exhibit, in our numerical computations, some fluctuations. So, in order to smooth them out, we perform a moving average, i.e., we report, in place of its instantaneous values, the corresponding time averages over a small time interval (of the order of one hundredth of the total integration time).

This ends the description of the model and of the numerical procedure we dealt with it. Now, up to the end of the present section, we illustrate the results of some preliminary computations that were performed as a check of the reliability of our procedure. All such results refer to the original Bohr model, in which the internal obstacles are absent and the magnetic field is time-independent (with $|B| = 0.001$). Such results are shown in Figure 1, in which the magnetic moment per electron M/N is reported versus time for three different samples

of $N = 1000$ electrons each, extracted in the way described above with $k_B T = 1/250$. One sees that for each sample the magnetization fluctuates about an apparently constant nonvanishing value, which varies from sample to sample.

These facts can be explained analytically by remarking that, in the case of a circular domain without obstacles, just in virtue of the symmetry under rotations about the center of the domain, there exists (even in the case of a time dependent field) an integral of motion P_θ , which is easily seen (see Appendix A) to be

$$P_\theta = L + \frac{q}{2c} B \sum_i |\mathbf{x}_i|^2. \quad (5)$$

So, what remains constant is P_θ and not the angular momentum, i.e. the magnetic moment. Thus the latter fluctuates, and moreover depends on the initial datum (i.e. on the sample). On the other hand, in the limit of large N two facts occur, namely: i) the initial value of the total angular momentum tends, by the law of large numbers, to zero; and ii) the quantity $\sum_i |\mathbf{x}_i|^2$, multiplied by m , just equals the moment of inertia of the disk (of radius R , with a uniform distribution of the electrons) and thus tends to a constant; consequently the angular momentum becomes an integral of motion. In conclusion, the fact exhibited in Figure 1, i.e., that the magnetic moment has an approximately constant value which depends on the sample, is just a statistical feature due to the finiteness of the samples ($N = 1000$).

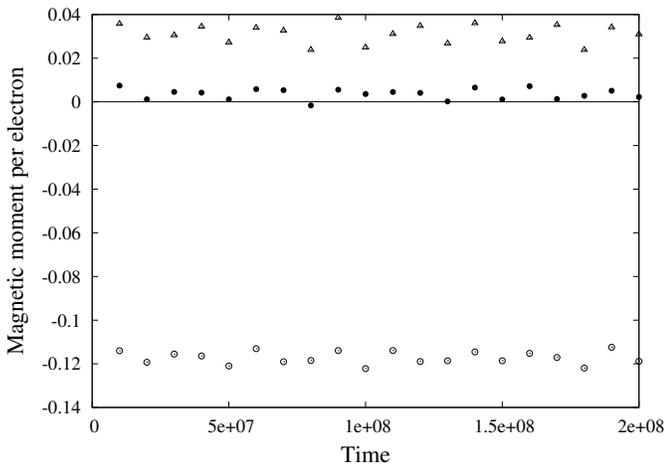


FIG. 1. Magnetic moment per electron M/N versus time in the original Bohr model, for three different samples of 10^3 electrons. The magnetic field is equal to 0.001.

In order to check the correctness of this interpretation, we performed (still for the case of a time independent field) ten runs with larger samples ($N = 10^5$), considering two different types of boundary conditions. Namely, five cases with elastic collisions at the circular boundary as before, and five cases in which the boundary was

eliminated at all (i.e., the initial data were still taken uniformly distributed in the disk as before, but the electrons were allowed to subsequently move freely in the whole plane). The results are summarized in Table I, in which the mean and the standard deviation over the five runs are reported for the case of presence of boundary (top) and of absence of boundary (bottom) respectively. One sees that in the presence of the boundary the val-

TABLE I. Magnetic Moment per electron in the case of a constant field (without obstacles), in the presence (top) or in the absence (bottom) of the boundary. The magnetic field is taken equal to 0.01, the radius of the circle is taken equal to 5000, the number of electrons is taken equal to 10^5 .

	mean	standard deviation
with boundary	-0.0007	0.0024
without boundary	-0.3994	0.0022

ues of the magnetic moment per electron are statistically consistent with a vanishing value, the mean being much smaller than the standard deviation. Instead, in the absence of the boundary the moment of inertia of the system is not guaranteed to remain equal to its initial value (i.e., to the moment of inertia of the disk), and correspondingly a nonvanishing value of the mean magnetic moment per electron is found. Notice that, in the absence of the boundary, the motion of each electron is known to be just the classical one of Larmor, namely, with constant speed $v_i = v_i^0$ on a circle of radius $r_i^0 = mc v_i^0 / qB$. In such a case the magnetic moment is thus easily computed to be given by

$$M = \frac{q}{2c} \sum_i v_i^0 r_i^0 = \frac{K}{B}$$

where K is the kinetic energy. This is in very good agreement with the value reported in Table I, because the formula gives for M/N the value $k_B T / B = 1/2.5 = 0.4$ against the numerical value 0.3994. By the way, the fact that magnetization should not vanish in the absence of boundary was already pointed out in a recent paper^{19,20}

So we have explained why, for finite samples, in the presence of the boundary nonvanishing values of the magnetization are found, notwithstanding the fact that, according to the Maxwell-Boltzmann statistics, a vanishing value is to be expected for an infinite sample. However, it is worth mentioning that the vanishing of magnetization was explained by Bohr himself by a different argument of a dynamical type (see also⁶, page 58). This is of interest for us, because we will see in the next section that such an argument may also explain the existence of a nonvanishing magnetization when the field, instead of being constant, is adiabatically switched on.

The well known Bohr argument is that the value of magnetization turns out to be due to the contributions of two populations. The first one is the population of the bulk electrons, which stay deep inside the domain

without hitting the boundary. They move in circles, producing a magnetic field which is directed against the external one. The second population is made of electrons which repeatedly hit the boundary and produce a current directed opposite to that of the first population. The two contributions would exactly cancel each other (in the limit of an infinite number of electrons). This was the conclusion of Bohr.

Things are however different if one considers a time-dependent magnetic field, as occurs when the field is adiabatically switched on. This is discussed in the next Section.

III. RESULTS

We eventually come to the case of interest, in which the magnetic field is adiabatically switched on, so that it should drive the system, from the initial equilibrium state, to an out of equilibrium state. We will first show what happens in the absence of obstacles, and will later show the role the latter play in possibly driving the system back to equilibrium.

The first result for a field which is adiabatically switched on is summarized in Figure 2, which refers, as in the original Bohr model, to a circular domain with no obstacles. The figure shows that the magnetic moment,

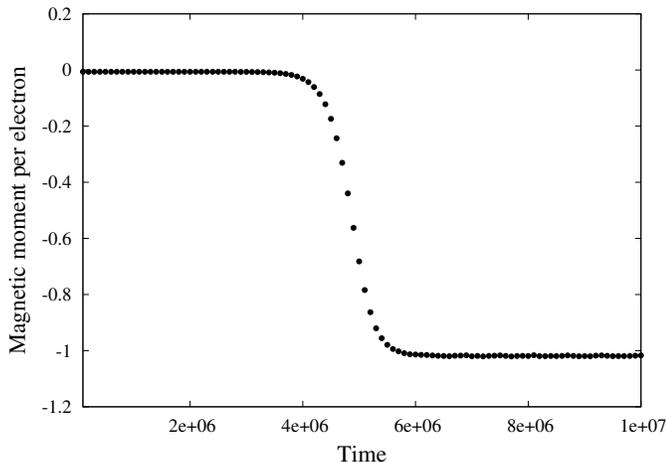


FIG. 2. Magnetic moment per electron M/N versus time, for a circular domain of radius 5000 and no obstacles, with a magnetic field adiabatically switched on with a characteristic time equal to 5×10^5 . The number of electrons is 5000, and the final field strength is 0.01.

starting from a value near to zero, becomes negative when the field is switched on, and seems to keep a constant value at later times. Thus there is no relaxation to a vanishing magnetization at all, and the model exhibits a fully diamagnetic behavior. The reason is apparent from inspection of Figure 3, in which the positions of the electrons at the end of the same simulation considered in

Figure 2, are shown. Indeed, one sees that the electrons

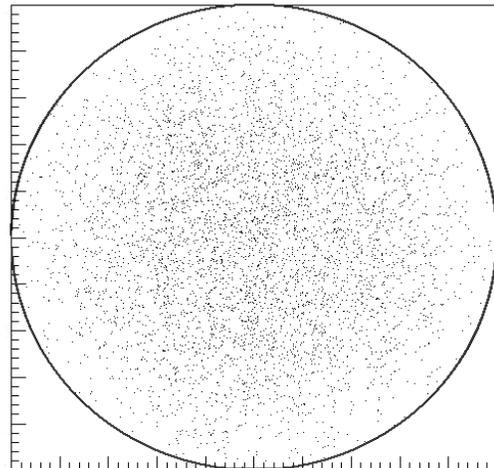


FIG. 3. Plot of the positions of the electrons at the end of the simulation considered in Figure 2.

are no more uniformly distributed, as they were initially, in the whole available domain, but are instead concentrated away from the boundary. This corresponds macroscopically to the appearing of a magnetic pressure which confines the electrons away from the boundary (just as occurs in the magnetic confinement in Tokamaks). A microscopic explanation of the existence of such a magnetic pressure is recalled in Appendix A. Thus, the contribution to magnetization due to the “bulk” electrons and that due to those hitting the boundary become different, the Bohr compensation no more occurs, and the magnetization turns out to be different from zero. This, by the way, shows that, in order to obtain a classical diamagnetism, it is not necessary to physically eliminate the boundary from the model (as was done in Ref. 19 for a case of a constant field), because a diamagnetism already manifests itself even in the presence of the boundary, just as a consequence of the adiabatic switching on of the field.

From a mathematical point of view, the appearing of a magnetization for the circular domain with no internal obstacles is due to the existence of the integral of motion P_θ (5) previously mentioned. Indeed one has $P_\theta = 0$ for all times, because P_θ vanishes initially, since initially one has $L = 0$ and $B = 0$. So one has $L = -\frac{q}{2c} B \sum_i |\mathbf{x}_i|^2$. Knowing the final value B_0 of B , and remarking that the value of $m \sum_i |\mathbf{x}_i|^2$ attains a positive value near to the moment of inertia of the disk, one sees that L (and so also M) keeps a fixed nonvanishing value after the field has been switched on. Thus the magnetization presents no relaxation to equilibrium at all.

However, P_θ is no more an integral of motion when the internal obstacles are inserted.²⁰ Thus, the total angular

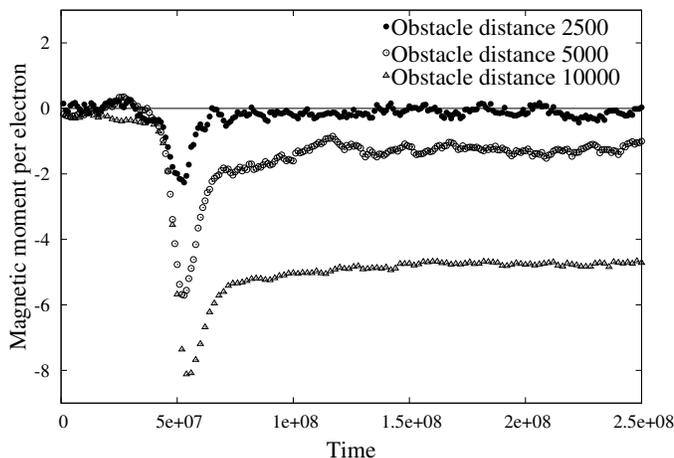


FIG. 4. Magnetic moment per electron M/N versus time in the case of a circular domains and a lattice of obstacles, for three different obstacle distances. The field strength is equal to 0.001, the switching time t_c is equal to 5×10^6 and the number of electrons is $N = 2500$.

momentum of the electrons is no more conserved. We first checked numerically that this occurs, as it should, even in the absence of a magnetic field: indeed, starting from a positive value, the total angular momentum was found to steadily decrease towards zero. The speed of convergence, however, was found to depend on the parameters of the model (number of electrons, distance between the obstacles, and so on).

Then, we considered the case of interest, with the presence of the obstacles and the field adiabatically switched on. The results are summarized in Figure 4, in which the magnetic moment per electron versus time is reported for three different values of the obstacles distance (with $B_0 = 0.001$, $t_c = 5 \times 10^6$ and $N = 2500$). When the distance is equal to 2.5×10^3 , the system relaxes to a non diamagnetic state in a time of order 10^7 . The same happens for smaller distances. Instead, if one increases the obstacles distance up to 5×10^3 (i.e., by just a factor of two), the relaxation occurs with at least two time scales: after a fast relaxation to a nonvanishing value (with a time scale of the same order of magnitude for the full relaxation to equilibrium in the previous case), there follows a much slower relaxation, which we actually were unable to follow up to the end within the available time. So we actually meet with a kind of “effective” or “apparent” magnetization, the absolute value of which increases as the distance is increased, as illustrated by the third curve in the figure, corresponding to a distance 10^4 .

So, one has a sort of threshold in the obstacles distance. Above it the system attains, after a short relaxation time, a kind of “effective” equilibrium state. This is a phenomenon analogous to the familiar one of FPU systems at low energies (see for example the reviews 7 8).

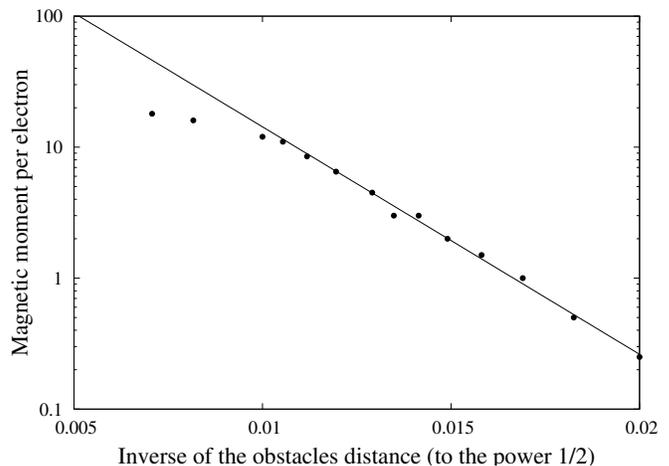


FIG. 5. Absolute value $|M|/N$ of the asymptotic magnetic moment per electron versus inverse obstacles distance a to the power $\frac{1}{2}$, in semilogarithmic scale. The straight line is the fit with $\exp[-(a^*/a)^{1/2}]$ for a suitable a^* . The field strength is equal to 0.001, the switching time t_c is equal to 5×10^6 and the number of electrons is $N = 2500$.

There naturally arises the problem of estimating the time required to attain the true equilibrium with a vanishing magnetization, or the time of persistence of the apparent equilibrium. This problem is at present beyond our possibilities, both analytical and numerical. A related, much simpler, problem is to estimate how the apparent magnetization depends on the obstacles distance. The apparent magnetic moment was determined numerically for the distance in the range from 2.5×10^3 up to 2.5×10^4 , and the magnetic moment was found to decrease as the distance is decreased. The results, reported in Figure 5, show that apparently it decreases as a stretched exponential of the density (or of inverse distance). Instead, for large distances a kind of a plateau is observed, which should correspond to the value of the permanent magnetization occurring in the absence of obstacles.

IV. CONCLUSIONS

In the present paper we pointed out the role of chaoticity of the dynamics in driving the magnetization back to equilibrium (i.e., to a vanishing value). Indeed, if the dynamics is not chaotic, as in the original Bohr model corresponding to a circular billiard without obstacles, there is no relaxation at all. Instead, if the system is sufficiently chaotic, as is the modified Bohr model corresponding to a circular billiard with obstacles, then the magnetization should decay to zero, as required at equilibrium. Actually, this was found to occur for suitable values of the physical parameters (we typically considered the obstacles distance) of the model, whereas for other values of

the parameters the magnetization was found not to decay to zero within the available time. In the latter case an effective diamagnetism shows up, in the vein of the metastability phenomena which are familiar for example in the frame of glasses and also in the FPU problem. This possibly is the main result of the present paper.

This fact may have some physical significance. Indeed, in the literature there are reported evidences of empirical metastability phenomena for the magnetic susceptibility. See for example Ref. 22 (and Ref. 23), in which a hysteresis curve is shown for the diamagnetic constant of water. See also Ref. 24 for a diamagnetic hysteresis in beryllium, and Ref. 25 for constricted diamagnetic hysteresis loops in high critical temperature superconductors.

As a final comment concerning a possible continuation of the present work, we come back to the remark made in the introduction, concerning the Linear Response Theory approach to magnetic susceptibility. There, it was recalled that the relaxation of magnetization to equilibrium can also be discussed, through the Fluctuation–Dissipation theorem, in terms of the decaying to zero of the time–autocorrelations of magnetization itself. Indeed, one has

$$\langle \mathbf{M}(t) \rangle = \beta \int_{t_0}^t ds \dot{\mathbf{B}}(s) \cdot \langle \mathbf{M}(s) \mathbf{M}(t) \rangle, \quad (6)$$

as is briefly recalled in Appendix B. So, in that approach one essentially has to study the time–autocorrelation of angular momentum in a billiard with obstacles in a magnetic field which is adiabatically switched on. Alternatively, one can also consider the case of a constant magnetic field, with a suitable initial out of equilibrium state of magnetization. For the time–correlation of suitable observables in billiard flows in the absence of a magnetic field, see Ref. 26.

Appendix A: Analytical discussion of the integrable Bohr model

We first give here the elementary deduction of the form of the integral of motion P_θ mentioned in the text. Moreover, as we were unable to find a microscopic deduction of the existence of a magnetic pressure when a magnetization is present, we give here a sketch of such a proof, along the lines of the familiar deduction of the state equation of a gas through the virial theorem.

For what concerns the integral of motion, it suffices to write down the Lagrangian for our system, namely,

$$\mathcal{L} = \sum_i \frac{m}{2} \dot{\mathbf{x}}_i^2 + \frac{q}{c} \sum_i \mathbf{A}_i \cdot \dot{\mathbf{x}}_i - \sum_i V^{ext}(|\mathbf{x}_i|),$$

where V^{ext} is the confining potential at the wall, while the vector potential is given by $\mathbf{A}_i = \frac{1}{2} \mathbf{B} \wedge \mathbf{x}_i$. The particles are assumed to lie all on the same plane orthogonal to \mathbf{B} , and in polar coordinates the Lagrangian becomes

$$\mathcal{L} = \frac{m}{2} \sum_i (\dot{r}_i^2 + r_i^2 \dot{\theta}_i^2) + \frac{q}{2c} \sum_i B(t) r_i^2 \dot{\theta}_i - \sum_i V^{ext}(r_i).$$

Now, the coordinates θ_i are cyclic, and thus the corresponding momenta are conserved. Adding all them up one finds the integral of motion

$$P_\theta = \sum_i \partial_{\dot{\theta}_i} \mathcal{L} = m \sum_i r_i^2 \dot{\theta}_i + \frac{q}{2c} \sum_i B(t) r_i^2,$$

which is equivalent to the expression given in the text.

We come now to the magnetic pressure, for a system of electrons in space. We have the equations of motion

$$m \ddot{\mathbf{x}}_i = -\frac{q}{c} \mathbf{B} \wedge \dot{\mathbf{x}}_i + \mathbf{F}_i^{ext},$$

where \mathbf{F}_i^{ext} is the force exerted by the wall when the i -th particle collides with it. Then, as usual, multiplying each equation by \mathbf{x}_i , adding all the equations and taking the time average, one finds

$$2\overline{K} = -\frac{q}{mc} \mathbf{B} \cdot \overline{\mathbf{L}} + 3\overline{\mathfrak{V}^{ext}}$$

where overline denotes time average, K is the kinetic energy and $\mathfrak{V}^{ext} = \sum_i \mathbf{F}_i^{ext} \cdot \mathbf{x}_i$ is the virial of the external forces due to the wall. Again, as usual, one has that the mean kinetic energy is equal to the temperature times the number of particles, whereas the virial of the external force due to the wall just equals the mechanical pressure p times the volume V . Now, by definition, the mean of the angular momentum is proportional to the magnetic moment \mathbf{M} , and so one gets the state equation

$$Nk_B T = V(p + p_B),$$

where the magnetic pressure p_B is defined by

$$p_B = -\frac{1}{V} \mathbf{B} \cdot \mathbf{M}.$$

Thus, when the magnetization is different from zero, the mechanical pressure p at the wall has to diminish, and this means that the number of collisions with the wall is diminished too, i.e., that the electrons are concentrated away from the wall.

Appendix B: Diamagnetism by the Green–Kubo relations

We deduce here the expression, given in the Conclusions, for the magnetization of a body according to the Fluctuation–Dissipation theorem. Consider the Hamiltonian (1) which we rewrite here, slightly changing the notation, as

$$H = \sum_{j=1}^n \left[\frac{1}{2m} \left(\mathbf{p}_j - \frac{e}{2c} \mathbf{B} \wedge \mathbf{q}_j \right)^2 + V(\mathbf{q}_j) \right]. \quad (\text{B1})$$

where the magnetic field $\mathbf{B}(t)$ depends on time explicitly, being switched on adiabatically from zero up to its final value. Notice that now, at variance with the main

text, the electron charge is denoted by e , while \mathbf{q}_j denotes the position of the j -th electron. Then, the Gibbs distribution

$$\rho_0 = \frac{e^{-\beta H_0}}{Z_0(\beta)}, \quad (\text{B2})$$

where H_0 is the Hamiltonian evaluated at zero field, will only be a zero-th order approximation of the true distribution ρ . This, we recall, has to satisfy the Liouville equation

$$\dot{\rho} + [H, \rho] = 0, \quad (\text{B3})$$

(where $[,]$ denotes Poisson bracket), together with the asymptotic condition $\rho \rightarrow \rho_0$ for $t \rightarrow -\infty$ (because the distribution should coincide with the Gibbs one before the magnetic field is turned on). Suppose now that the magnetic field can be treated as a small parameter, and expand the distribution ρ in powers of it. Setting²¹ $\rho = e^{-\beta H}(1 + \rho_1 + \dots)$, and substituting it into the Liouville equation, one gets for ρ_1 the equation

$$\dot{\rho}_1 + [H, \rho_1] = -\beta \dot{\mathbf{B}} \cdot \mathbf{M}, \quad (\text{B4})$$

where the magnetization \mathbf{M} is given by

$$\mathbf{M} \stackrel{\text{def}}{=} \frac{e}{2c} \sum \mathbf{q}_j \wedge \dot{\mathbf{q}}_j = \frac{e}{2mc} \sum \mathbf{q}_j \wedge \left(\mathbf{p}_j - \frac{e}{2c} \mathbf{B} \wedge \mathbf{q}_j \right). \quad (\text{B5})$$

We note that the magnetization, as a dynamical variable, depends explicitly on time besides on the point \mathbf{x} of phase space, so that we will write sometimes $\mathbf{M} = \mathbf{M}(\mathbf{x}, t)$ in order to emphasize this fact. Denoting by $\Phi_{t_0}^t$ the flow associated with Hamilton's equations at time t with initial data taken at time t_0 (remember that Hamilton's equations are not autonomous, so that it is mandatory to specify the time at which initial data are taken), if one looks for a solution of (B4) in the form $\rho_1(\mathbf{x}, t) = \chi(\Phi_{t_0}^t \mathbf{y}, t)$, then χ has to satisfy

$$\partial_t \chi(\Phi_{t_0}^t \mathbf{y}, t) = -\beta \dot{\mathbf{B}} \cdot \mathbf{M}(\Phi_{t_0}^t \mathbf{y}, t) \quad (\text{B6})$$

The function χ is thus simply obtained by integration, so that, putting $\mathbf{x} = \Phi_{t_0}^t \mathbf{y}$ in the resulting expression, one finds

$$\rho_1(\mathbf{x}, t) = -\beta \int_{t_0}^t ds \dot{\mathbf{B}}(s) \cdot \mathbf{M}(\Phi_{t_0}^s \mathbf{x}, s). \quad (\text{B7})$$

Here we used the group property $\Phi_{t_0}^s \Phi_{t_0}^{t_0} = \Phi_{t_0}^s$ of the flow; furthermore, the lower integration limit t_0 is intended to be a time before the magnetic field is switched on.

Recall now that the normalization constant, being time independent, is nothing but the partition function $Z_0(\beta)$ computed for a vanishing field, because it can be computed at time t_0 , i.e. when the magnetic field vanishes. Thus, to first order in the magnetic field, the magnetization at time t is given by

$$\langle \mathbf{M}(t) \rangle = \beta \int_{t_0}^t ds \dot{\mathbf{B}}(s) \cdot \int_{\mathcal{M}} d\mathbf{x} \frac{e^{-\beta H(\mathbf{x}, t)}}{Z_0(\beta)} \mathbf{M}(\Phi_{t_0}^s \mathbf{x}, s) \mathbf{M}(\mathbf{x}, t) \quad (\text{B8})$$

i.e. by

$$\langle \mathbf{M}(t) \rangle = \beta \int_{t_0}^t ds \dot{\mathbf{B}}(s) \cdot \langle \mathbf{M}(s) \mathbf{M}(t) \rangle, \quad (\text{B9})$$

where $\mathbf{M}(s)$ is the magnetization evolved backwards in time up to time s , starting from data at time t , and the averages are performed with respect to the Gibbs distribution at time t . This is the formula given in the Conclusions. In this expression the average is performed with respect to the *final data*. An analogous expression could also be given with the average performed with respect to the *initial data*, but we do not insist here on this point.

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