CHAOS **24**, 013118 (2014)

Chaoticity threshold in magnetized plasmas: Numerical results in the weak coupling regime

A. Carati,[1,a)] F. Benfenati,[1] A. Maiocchi,[1] M. Zuin,[2,b)] and L. Galgani[1]
[1]*Università degli Studi di Milano, Milano, Italy*
[2]*Consorzio RFX, Associazione EURATOM-ENEA sulla Fusione, Padova, Italy*

(Received 11 July 2013; accepted 29 January 2014; published online 12 February 2014)

The present paper is a numerical counterpart to the theoretical work [Carati *et al.*, Chaos **22**, 033124 (2012)]. We are concerned with the transition from order to chaos in a one-component plasma (a system of point electrons with mutual Coulomb interactions, in a uniform neutralizing background), the plasma being immersed in a uniform stationary magnetic field. In the paper [Carati *et al.*, Chaos **22**, 033124 (2012)], it was predicted that a transition should take place when the electron density is increased or the field decreased in such a way that the ratio ω_p/ω_c between plasma and cyclotron frequencies becomes of order 1, irrespective of the value of the so-called Coulomb coupling parameter Γ. Here, we perform numerical computations for a first principles model of N point electrons in a periodic box, with mutual Coulomb interactions, using as a probe for chaoticity the time-autocorrelation function of magnetization. We consider two values of Γ (0.04 and 0.016) in the weak coupling regime $\Gamma \ll 1$, with N up to 512. A transition is found to occur for ω_p/ω_c in the range between 0.25 and 2, in fairly good agreement with the theoretical prediction. These results might be of interest for the problem of the breakdown of plasma confinement in fusion machines.
 [http://dx.doi.org/10.1063/1.4865255]

One of the most relevant open problems of plasma physics, particularly in connection with the operation of fusion machines, is the breakdown of magnetic confinement. Catastrophic events, called disruptions, occur when density exceeds a certain limit, and no general agreement seems to exist for an explanation.[2] It is even under discussion, at a phenomenological level, on which parameters should the density limit depend, whether on the plasma current or on the imposed magnetic field (see Ref. 3, Fig. 6). In the work,[1] the attention was restricted to the role of the imposed magnetic field B, and theoretical indications were given that a bold chaoticity involving all single electrons should take place for large enough electron density n_e or small enough field B. In fact, the chaoticity border was predicted to be given by the relation (in Gauss units)

$$n_e \simeq \frac{B^2}{4\pi mc^2}, \quad \text{or equivalently} \quad \frac{\omega_p}{\omega_c} \simeq 1, \tag{1}$$

where m is the electron and c the speed of light, while ω_p and ω_c are the familiar plasma and cyclotron frequencies, to be defined later. In Ref. 1, it was also shown that law (1) fits pretty well a large set of experimental data for disruptions in actual fusion machines.

The main idea leading to (1) as a chaoticity threshold for the motions of the electrons is as follows. Ordered gyrational motions induced by the field obviously prevail when the mutual interactions among the electrons are negligible, i.e., for small densities. On the other hand, perturbation increases with increasing density. Indeed the main perturbation is due to so-called microfield, namely, the sum of the Coulomb forces acting on each electron and due to all the other ones. This is a highly fluctuating quantity, whose typical intensity E was estimated long ago by Iglesias *et al.*[4] to be given, for a one–component plasma at temperature T and electron density n_e, by

$$E \simeq \sqrt{4\pi n_e k_B T}, \tag{2}$$

where k_B is the Boltzmann constant. Thus, a threshold should occur when the microfield and the Lorentz force balance, i.e., when one has

$$E_\perp \simeq Bv_\perp/c, \tag{3}$$

where $\perp$ denotes transverse part. Using $v_\perp \simeq \sqrt{2k_BT/m}$, with (2) and $E_\perp = \sqrt{2/3}\,E$, this leads for the threshold to the condition (1), apart from a numerical factor of order 1.

In the present paper, the results of numerical computations in the weak coupling regime are reported, which appear to confirm the theoretical prediction (1).

I. INTRODUCTION

The idea that a transition from order to chaos may occur in dynamical N particle systems and may play some physically relevant role is a familiar one since the year 1960s, and was much discussed also in the frame of plasma physics. Particular attention in plasma physics was given to situations in which it is the magnetic field itself that exhibits field lines presenting chaoticity properties, because this should induce some chaoticity in the motions of the electrons too.[5–7]

a)Electronic mail: andrea.carati@unimi.it
b)Electronic mail: matteo.zuin@igi.cnr.it

However, this fact does not explain the disruptions observed in fusion machines. For another recent attempt see Ref. 8.

In Ref. 1, the idea was advanced that an explanation may be found in a more global chaoticity phenomenon that involves each electron, even in the presence of completely ordered field lines. Moreover, the phenomenon should concern a macroscopic quantity of a great physical relevance, namely, the system's magnetization. Indeed indications were given that, for high enough density or small enough field, the gyrational character of the electron motions should be lost, so that magnetization (with its confining feature) would be no more present. The threshold was estimated to be given by the law (1), which in particular is independent of the so–called Coulomb coupling parameter Γ. The latter is defined by

$$\Gamma \stackrel{\text{def}}{=} e^2/ak_BT, \tag{4}$$

namely, as the ratio between Coulomb potential energy at the mean interelectron distance a, and the energy k_BT. Here, e is the modulus of the electron charge.

In the present paper, a check of the theoretical prediction (1) is provided in the so-called weak coupling regime $\Gamma \ll 1$. This is obtained through a numerical study on a one-component plasma in which the time-autocorrelation function of magnetization is computed. The choice of looking at the time-autocorrelation function of some dynamical variable is made in the spirit of ergodic theory. Indeed, by definition a system is chaotic if the time-autocorrelation functions of all quantities tend to zero when the time t tends to infinity. Conversely, a system may be said to present regular or ordered features *up to a given observation time* τ, if there exists some physically significant quantity, the time-autocorrelation of which remains near to its initial value up to the observation time τ. In fact, the quantity we consider is a macroscopic one which is of paramount relevance in the problem of plasma confinement, namely, magnetization (which is just proportional to the system's orbital angular momentum). We will show that the numerical results allow one to give an estimate for a chaoticity threshold in the sense just mentioned. Moreover, the threshold turns out to be in fairly good agreement with the theoretical prediction (1).

In Sec. II, the model is described, and some details about its numerical implementation are given. The numerical results are reported in Sec. III. Some further discussions are given in the conclusive Sec. IV. Finally, an appendix is devoted to recalling the Ewald procedure for expressing through rapidly converging series the electric field due to a periodic configuration of point sources.

II. THE MODEL AND ITS NUMERICAL IMPLEMENTATION

Let us recall that a one-component plasma model is just a system of point electrons with mutual Coulomb interactions. Neutrality is guaranteed by the existence of a uniform positively charged background, which however has no influence on the motions of the electrons. So, denoting by $\mathbf{x}_i$ the position vector of the generic i–th electron, each electron is subject to the sum of the Coulomb forces due to all the other ones, and to the Lorentz force $(-e/c)\,\dot{\mathbf{x}}_i \wedge \mathbf{B}$ due to a uniform stationary external magnetic field $\mathbf{B}$ (which we take directed along the z axis). The electric force on the i–th electron, which depends on the positions of all the other ones, will be simply denoted by $e^2\mathbf{E}(\mathbf{x}_i)$.

In order to deal with an actually manageable model, we introduce periodicity conditions, taking as fundamental cell a cubic box of side L containing N electrons. In order to guarantee that the solutions of the equations of motion be spatially periodic, we proceed in the following way. Denote by $\mathbf{x}_j$, $j = 1,\ldots, N$, the position vectors of the electrons in the fundamental cell, and by $\mathbf{n}$ a vector with integer coordinates, i.e., $\mathbf{n} \stackrel{\text{def}}{=} (n_x\mathbf{e}_x + n_y\mathbf{e}_y + n_x\mathbf{e}_z)$, with n_x, n_y, and $n_z \in \mathbb{Z}$, while $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$, are unit vectors along the axes. Having fixed arbitrary initial data $\mathbf{x}_j^0$, $\dot{\mathbf{x}}_j^0$, $j = 1, \ldots, N$, for the electrons in the fundamental cell, we introduce for the other electrons the initial data $\mathbf{x}_{j+\mathbf{n}}^0 = \mathbf{x}_j^0 + L\mathbf{n}$ and $\dot{\mathbf{x}}_{j+\mathbf{n}}^0 = \dot{\mathbf{x}}_j^0$. Such initial configurations of the charges produce a spatially periodic force field, and thus the initial conditions guarantee spatial periodicity of the solutions for all times t, i.e.,

$$\mathbf{x}_{j+\mathbf{n}}(t) = \mathbf{x}_j(t) + L\mathbf{n}. \tag{5}$$

So the motion of the complete system is determined by the motions of the N electrons in the fundamental cell. In particular, if at a certain time an electron leaves the fundamental cell, then there is a corresponding one entering it. The spatial periodicity of the solutions allows for another great simplification, which concerns the expression of the electric field $\mathbf{E}(\mathbf{x}_j)$ acting on the j–th electron. Indeed, since the classical work of Ewald[9] on the microscopic foundations of crystal optics, it is well known that, due to the peroidicity of the configuration, the field $\mathbf{E}(\mathbf{x}_j)$ acting on the j–th electron can be expressed as the sum of two rapidly converging series in the form

$$\begin{aligned}\mathbf{E}(\mathbf{x}_j) = &\sum_{\mathbf{n}} \sum_{l\neq j} \frac{\mathbf{r}_{l,\mathbf{n}}}{|r_{l,\mathbf{n}}|^3}\left[\operatorname{erfc}(\alpha r_{l,\mathbf{n}}) + \frac{\alpha r_{l,\mathbf{n}}}{\sqrt{\pi}}\exp(-\alpha^2 r_{l,\mathbf{n}}^2)\right] \\ &+ \frac{4\pi}{L^3}\sum_{\mathbf{k}\neq 0}\sum_{l}\frac{\mathbf{k}}{|\mathbf{k}|^2}\exp(-\mathbf{k}^2/4\alpha^2)\sin(\mathbf{k}\cdot\mathbf{r}_l),\end{aligned} \tag{6}$$

where $\operatorname{erfc}(x)$ is the usual complementary error function, while we have denoted $\mathbf{r}_l \stackrel{\text{def}}{=} \mathbf{x}_j - \mathbf{x}_l$ and $\mathbf{r}_{l,\mathbf{n}} \stackrel{\text{def}}{=} \mathbf{x}_j - \mathbf{x}_l + L\mathbf{n}$. Furthermore, α is the Ewald convergence parameter which is arbitrary, and may be chosen in such a way as to guarantee a rapid convergence of both series. This formula is by now a common tool in molecular dynamics simulations (see for example Ref. 10), and its derivation is here sketched in the Appendix. For a new application to the original problem for which the formula was conceived, namely, the microscopic foundations of crystal optics, see Ref. 11.

In dealing concretely with the problem at hand, it is expedient to introduce suitable rescaled variables, in terms of the mean interelectron distance a and of the natural time unit related to the electron cyclotron frequency ω_c.

The distance a is defined by $a = n_e^{-1/3}$, where n_e is the electron density n_e given by $n_e = N/L^3$. Let us now recall

the standard definitions of the cyclotron and the plasma frequencies ω_c, ω_c, namely,

$$\omega_c \stackrel{\text{def}}{=} eB/mc\,, \quad \omega_p \stackrel{\text{def}}{=} \sqrt{4\pi e^2 n_e/m}. \tag{7}$$

We will also refer to the Debye length λ_D and the Larmor radius r_L, which are defined by

$$\lambda_D \stackrel{\text{def}}{=} \sqrt{k_B T/n_e e^2}\,, \quad r_L \stackrel{\text{def}}{=} v_\perp/\omega_c. \tag{8}$$

Rescaling time by the electron cyclotron frequency ω_c, and position vectors by the mean interparticle distance a, i.e., introducing $\tau \stackrel{\text{def}}{=} \omega_{ct}$ and $\mathbf{y}_j \stackrel{\text{def}}{=} \mathbf{x}_j/a$, the Newton equations of motion for each of the N electrons take the form

$$\ddot{\mathbf{y}}_j = \mathbf{e}_z \wedge \dot{\mathbf{y}}_j + \left(\frac{\omega_p}{\omega_c}\right)^2 \mathbf{E}(\mathbf{y}_j) \tag{9}$$

(the dots denoting derivatives with respect to τ). Thus, the rescaled equations contain only one (dimensionless) parameter, the ratio ω_p/ω_c, and in particular do not depend on the Coulomb coupling parameter Γ (the latter, however, due to its dependence on T and on n_e, will enter the problem through the choice of the initial data). Obviously the rescaled density is equal to 1, and time turns out to be expressed in units of $1/\omega_c$.

In the rescaled units, the electric field acting on the j–th electron takes the form

$$\mathbf{E}(\mathbf{y}_j) = \sum_{\mathbf{n}} \sum_{l \neq j} \frac{\mathbf{r}_{l,\mathbf{n}}}{|r_{l,\mathbf{n}}|^3} \left[\operatorname{erfc}(\alpha r_{l,\mathbf{n}}) + \frac{\alpha r_{l,\mathbf{n}}}{\sqrt{\pi}} \exp(-\alpha^2 r_{l,\mathbf{n}}^2)\right] + \frac{4\pi}{N} \sum_{\mathbf{k}\neq 0} \sum_l \frac{\mathbf{k}}{|\mathbf{k}|^2} \exp(-\mathbf{k}^2/4\alpha^2) \sin(\mathbf{k}\cdot\mathbf{r}_l), \tag{10}$$

where $\mathbf{r}_l \stackrel{\text{def}}{=} \mathbf{y}_j - \mathbf{y}_l$, while $\mathbf{r}_{l,\mathbf{n}} \stackrel{\text{def}}{=} \mathbf{y}_j - \mathbf{y}_l + L\mathbf{n}/a$. For the Ewald convergence parameter, we chose[10] $\alpha = \pi^{1/2} N^{1/6} L^{-1}$.

The equations of motion (9), with the electric field in the Ewald form (10), were integrated numerically, using a symplectic splitting method. Conservation of energy in every run was better than a part over 10^3. The integration time was chosen proportional to ω_c in order that all different cases be integrated for the same "physical time." In any case, the time was always some hundreds cyclotron periods.

The initial data were chosen in the following way: the electron positions $\mathbf{y}_j$ were taken uniformly distributed in the fundamental cell (of side $N^{1/3}$), while the velocities were extracted from a Maxwellian with a given temperature T. This is the point where the Coulomb coupling parameter Γ enters the problem.

For what concerns the number N of electrons in the fundamental cell, our computational power allows us to work with a maximal value of $N = 512$. This induces a lower bound on Γ, namely, $\Gamma \geq N^{-2/3}$. Indeed, in order to correctly simulate the Coulomb cumulative force acting on an electron, the side of the fundamental cell has to be at least equal to the Debye length, which, in our rescaled units, takes the value $\lambda_D = \Gamma^{-1/2}$. We took $\Gamma = N^{-2/3}$. Computations were performed both for $N = 128$ and $N = 512$, which correspond to $\Gamma = 128^{-2/3} \simeq 0.04$ and $\Gamma = 512^{-2/3} = 1/64 \simeq 0.016$, respectively.

III. THE NUMERICAL RESULTS

We now come to the main issue, i.e., whether the motions are ordered or chaotic, in the sense previously explained. Obviously what plays the role of the unperturbed system with completely ordered motions is the limit case with $\omega_p/\omega_c = 0$, for which the Coulomb interactions disappear and one has pure Larmor gyrations. The problem then is to determine whether a transition to chaoticity takes place as the parameter ω_p/ω_c is increased and Γ is varied. To this end, we considered the magnetization (along the field) of a cell, namely,

$$\mathcal{M} \stackrel{\text{def}}{=} (e/2mc) \sum \left(\mathbf{y}_j \wedge \dot{\mathbf{y}}_j\right)_z, \tag{11}$$

looking at its time-autocorrelation function (normalized by Nk_BT)

$$\mathcal{C}_{\mathcal{M}}(t) \stackrel{\text{def}}{=} \frac{\langle \mathcal{M}(t)\mathcal{M}(0)\rangle}{Nk_BT}, \tag{12}$$

and at its Fourier transform $\hat{\mathcal{C}}_{\mathcal{M}}(\omega)$. The latter is a physically very relevant quantity because, according to linear response theory (see Refs. 12 and 13, or Appendix B of Ref. 14), $i\omega\hat{\mathcal{C}}_{\mathcal{M}}(\omega)$ gives the susceptibility $\chi(\omega)$ at frequency ω.

In the formula defining the time-autocorrelation $\mathcal{C}_{\mathcal{M}}(t)$, the average $\langle\cdot\rangle$ should in principle be a phase–average with respect to Gibbs measure; in our computations, however, we estimated it by the time-average along a single orbit (with "generic" initial data extracted as previously explained), as often done in numerical works. We did not investigate the relations between the two averages. Moreover, the Fourier transform $\hat{\mathcal{C}}_{\mathcal{M}}(\omega)$ was estimated by the amplitude of the discrete Fourier transform of $\mathcal{C}_{\mathcal{M}}(t)$, which will be simply called the *spectrum*. So we computed both the time-autocorrelation $\mathcal{C}_{\mathcal{M}}$ as a function of t, and the corresponding spectrum as a function of angular frequency ω/ω_c.

Having fixed $\Gamma = 1/64$, by increasing ω_p/ω_c we found that a threshold occurs for ω_p/ω_c between 0.25 and 2. This is exhibited in Fig. 1, where the results are reported for $\omega_p/\omega_c = 0.25$ on the left and for $\omega_p/\omega_c = 2$ on the right. The time-autocorrelations are reported in the upper part of the figure, and the spectra in the lower part.

For $\omega_p/\omega_c = 0.25$, the time-autocorrelation is seen to display regular oscillations with a decreasing amplitude: we were unable to follow this relaxation process up to the end. The oscillations are apparently peaked about the cyclotron frequency and its low harmonics (as should be, due to the nonlinearities in the equations of motions). This is clearly exhibited by the spectrum, with its large peak at $\omega/\omega_c = 1$, and the smaller ones about the low harmonics $\omega/\omega_c = 2$, 3,…. Of special relevance is the peak at $\omega = 0$, which corresponds to the existence of a nonvanishing static susceptibility, i.e., to the existence of diamagnetism. There also appears a continuous component, which accounts for the extremely slow drift towards equilibrium. This case clearly corresponds to prevalently ordered motions with a corresponding nonvanishing diamagnetism, and should be interpreted as an indication that the perturbation due to the Coulomb interactions is not yet sufficiently large to produce prevalent chaotic motions.

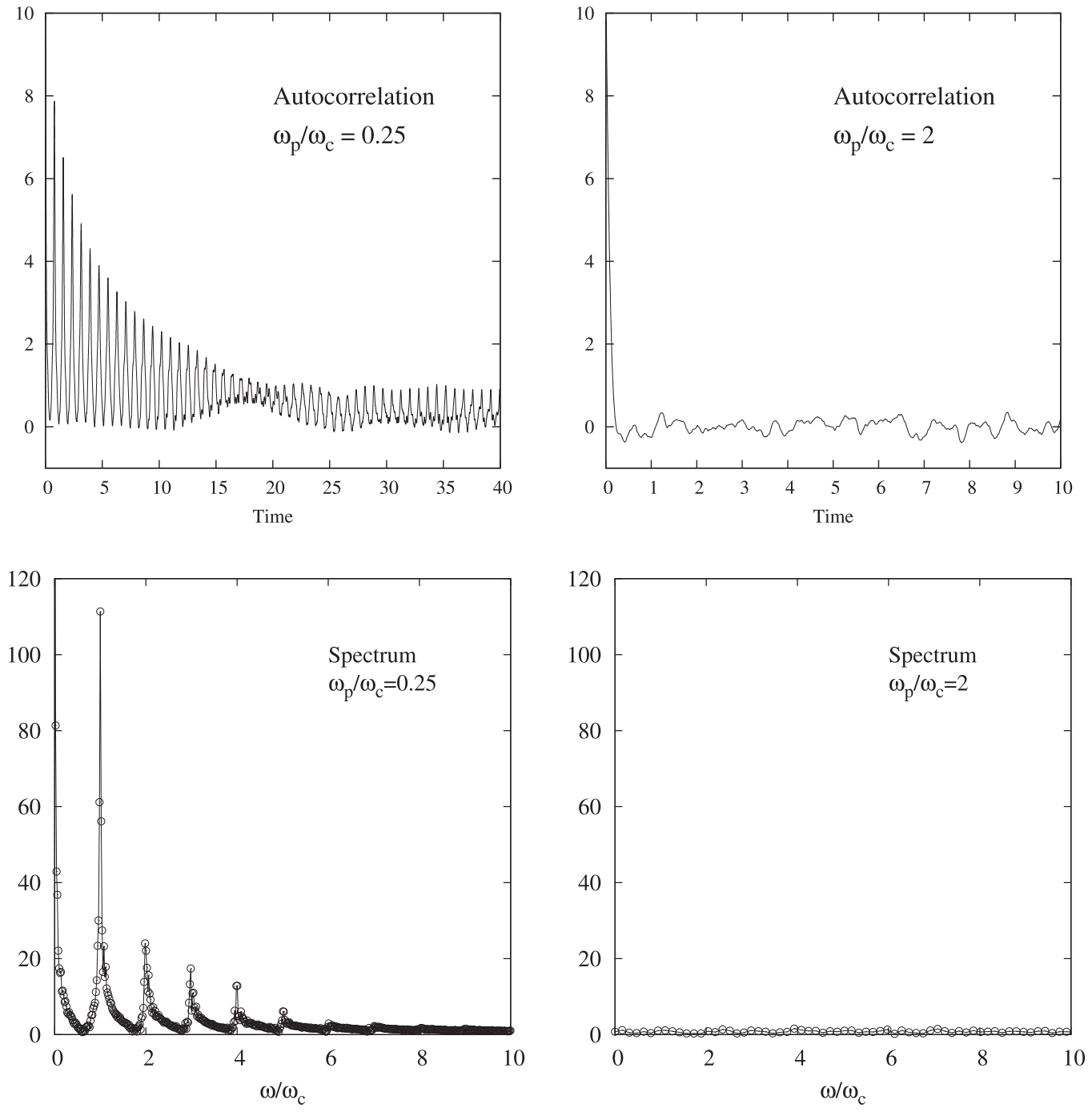

FIG. 1. Top: Autocorrelation $\mathcal{C}_{\mathcal{M}}(t)$ of magnetization versus time for $\omega_p/\omega_c = 0.25$ (left) and for $\omega_p/\omega_c = 2$ (right). The time units in the two cases were chosen in such a way that the "physical" time scale is the same in both figures (actually, we chose $\omega_c = 1$ at the right, and $\omega_c = 8$ at the left). Notice the fast decay to zero at the right. Bottom: Discrete Fourier transform (absolute value) of $\mathcal{C}_{\mathcal{M}}(t)$ versus ω/ω_c for $\omega_p/\omega_c = 0.25$ (left), and for $\omega_p/\omega_c = 2$ (right). Peaks (and thus also magnetization) have disappeared at the right. Here, $\Gamma = 1/64$.

The transition to chaos, however, already occurred at $\omega_p/\omega_c = 2$. Indeed in this case the autocorrelation is seen to go to zero in an extremely short lapse of time (even shorter than one cyclotron period $2\pi/\omega_c$), so that the peaks disappear from the spectrum and only the continuous part remains. This means that for $\Gamma = 1/64$ the threshold in ω_p/ω_c lies between 0.25 and 2.

For $\Gamma = 128^{-2/3}$, the corresponding figures (at the same two values ω_p/ω_c) are qualitatively similar to those for $\Gamma = 1/64$ and are not reported here.

IV. CONCLUSIONS

So, we have performed a numerical investigation on the onset of chaoticity in a one-component plasma immersed in a uniform stationary external magnetic field. To this end, we solved numerically the Newton equations of motion for the corresponding first principles N–particle model in a cell, with periodic boundary conditions, looking at the behaviour of the time-autocorrelation function of magnetization and at the corresponding spectrum.

The results show that, even in the so-called "weak coupling" regime $\Gamma \ll 1$ (precisely, at $\Gamma = 128^{-2/3} \simeq 0.04$ and $\Gamma = 1/64 \simeq 0.016$), as ω_p/ω_c is increased up to a value of about 1, the mutual Coulomb interactions among the electrons are already so strong that the motions become chaotic, losing the prevalent gyrational character, so that magnetization disappears within just one cyclotron period.

These numerical results are in rather good agreement with the theoretical prediction (1) that an onset of chaoticity should show up at about $\omega_p/\omega_c = 1$. In fact, the theoretical prediction even says that such a threshold should be independent of the value of the Coulomb coupling parameter Γ. Notice that this is not at all obvious, notwithstanding the fact that the only parameter entering the equations of motion (9) is ω_p/ω_c, because the parameter Γ enters in the choice of the initial data.

Computations relative to the "strong coupling" regime $\Gamma \gg 1$ for exactly the same model of a one–component plasma discussed here, were performed in the paper.[15] In such a paper, quantities of a different type were observed, namely, the diffusion coefficients. From the figures reported, one may surmize that some transition is taking place at about $\omega_p/\omega_c = 1$. Some preliminary results of ours seem to confirm this fact. We plan to come back to this point, in the future.

A remark is in order. The idea that the onset of chaoticity should take place when a balance occurs between the two forces acting on each electron, namely, the confining Lorentz magnetic force and the microscopic Coulomb field due to all the other charges (the so called microfield), is a quite natural one. On the other hand the microfield is in practice a highly fluctuating random variable. Thus, the really relevant feature leading to the theoretical prediction (1), which in particular makes the threshold independent of the coupling parameter Γ, is the estimate (2) for the *typical value* of the microfield, which is much larger than one might naively guess. So one might say that our numerical results are actually providing, at least for a one component plasma in the weak–coupling regime, a check for the estimate on the size of the microfield, that was given long ago by Iglesias, Lebowitz and MacGowan.

As a final remark, one may point out that law (1) has the same formal aspect as the so-called Brillouin density limit, which is usually discussed in connection with nonneutral plasmas[16] (i.e., plasmas composed of electrons only). However, the Brillouin density limit for nonneutral plasmas has apparently little to do with the chaoticity threshold discussed here. Indeed, in the frame of nonneutral plasmas the Brillouin density limit just gives a constraint for the existence of particular solutions, in which the whole nonneutral plasma, dealt with in the continuum approximation, performs rigid rotations about a symmetry axis. Here, instead, the discrete nature of matter plays an essential role. So, when the mutual interactions are neglected, each electron is performing a peculiar gyration about its own Larmor center. Furthermore, in order to take into account the perturbation due to the Coulomb forces one has to take into consideration a microscopic force such as the microfield. On the other hand, such a force, being a highly fluctuating quantity, cannot be calculated through elementary macroscopic arguments, and has to be estimated by statistical methods, as was done in Ref. 4.

ACKNOWLEDGMENTS

The present paper is dedicated to Francesco Guerra (La Sapienza University at Rome) on the occasion of his seventieth birthday.

APPENDIX: DEDUCTION OF THE EWALD FORMULA

In this appendix, we sketch the deduction of the Ewald summation formula without any pretension of mathematical rigour, taking it almost literally, apart from notations, from the lectures given by Born at MIT in the winter 1925–1926 (see Ref. 17, pp. 158–161).

For simplicity, consider a lattice of identical charges located at points $\mathbf{x_n} = L\mathbf{n}$ ($\mathbf{n}$ being a vector with integer components), and the (formal) potential $V(\mathbf{x})$ of the field they produce

$$V(\mathbf{x}) = \sum_{\mathbf{n}} \frac{1}{|\mathbf{x} - \mathbf{x_n}|}.$$

First, using the identity

$$1/|\mathbf{x}| = \frac{1}{2\pi^2} \int \mathrm{d}\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}/\mathbf{k}^2,$$

one reduces such a series to a series over the reciprocal lattice as follows:

$$V(\mathbf{x}) = \sum_{\mathbf{n}} \frac{1}{|\mathbf{x} - \mathbf{x_n}|} = \sum_{\mathbf{n}} \frac{1}{2\pi^2} \int \mathrm{d}\mathbf{k}\, \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x_n})}}{\mathbf{k}^2}$$
$$= \frac{1}{2\pi^2} \int \mathrm{d}\mathbf{k}\, \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\mathbf{k}^2} \sum_{\mathbf{n}} e^{-i\mathbf{k}\cdot\mathbf{x_n}} = \frac{4\pi}{V_c} \sum_{\mathbf{h}} \frac{e^{i\mathbf{k_h}\cdot\mathbf{x}}}{\mathbf{k_h}^2},$$

where in the last line use was made of the identity

$$\sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{x_n}} = \frac{(2\pi)^3}{V_c} \sum_{\mathbf{h}} \delta(\mathbf{k} - \mathbf{k_h}),$$

V_c being the cell volume, while $\mathbf{k_h}$ are the vectors of the reciprocal lattice. We recall that, given a lattice of points $\mathbf{x_n}$ in a vector space, the reciprocal lattice $\mathbf{k_h}$ is the set in the dual space such that $\langle \mathbf{x_n}, \mathbf{k_h} \rangle$ is an integer multiple of 2π. In $\mathbb{R}^3$, if $\mathbf{a}_i$, $i = 1, 2, 3$, is a basis for the direct lattice, the vectors $\mathbf{b}_k = (2\pi/V_c)/(\mathbf{a}_i \wedge \mathbf{a}_j)$ constitute a basis for the reciprocal lattice. In our case, being the lattice cubic, the reciprocal vectors are again in the form $\mathbf{k_h} = 2\pi\mathbf{h}/L$, with $\mathbf{h}$ a vector with integer components.

The series over the reciprocal lattice, when the divergence corresponding to the term $\mathbf{h} = 0$ is removed, is only conditionally convergent, but it can be conveniently split as follows (α being an arbitrary real parameter):

$$V(\mathbf{x}) = \frac{4\pi}{V_c} \sum_{\mathbf{h}\neq 0} e^{i\mathbf{k_h}\cdot\mathbf{x}} \frac{e^{-\mathbf{k_h}^2/4\alpha^2}}{\mathbf{k_h}^2} + \frac{4\pi}{V_c} \sum_{\mathbf{h}} e^{i\mathbf{k_h}\cdot\mathbf{x}} \frac{1 - e^{-\mathbf{k_h}^2/4\alpha^2}}{\mathbf{k_h}^2},$$

where now the first series converges absolutely, while the second one can be expressed as an absolutely convergent series by going back to the direct lattice.

In fact, using

$$\frac{1-e^{-\mathbf{k}_\mathbf{h}^2/4\alpha^2}}{\mathbf{k}_\mathbf{h}^2}=\int_0^{1/4\alpha^2} \mathrm{d}\xi\, e^{-\xi\mathbf{k}_\mathbf{h}^2}$$

together with (see below)

$$\frac{4\pi}{V_c}\sum_{\mathbf{h}} e^{i\mathbf{k}_\mathbf{h}\cdot\mathbf{x}}\, e^{-\xi\mathbf{k}_\mathbf{h}^2}=\frac{1}{\sqrt{4\pi\xi^3}}\sum_{\mathbf{n}} e^{-\frac{1}{4\xi}|\mathbf{x}-\mathbf{x}_\mathbf{n}|^2}, \tag{A1}$$

one obtains

$$\frac{4\pi}{V_c}\sum_{\mathbf{h}} e^{i\mathbf{k}_\mathbf{h}\cdot\mathbf{x}}\frac{1-e^{-\mathbf{k}_\mathbf{h}^2/4\alpha^2}}{\mathbf{k}_\mathbf{h}^2}=\frac{1}{\sqrt{4\pi}}\sum_{\mathbf{n}}\int_0^{1/4\alpha^2}\frac{\mathrm{d}\xi}{\xi^{3/2}}\, e^{-\frac{1}{4\xi}|\mathbf{x}-\mathbf{x}_\mathbf{n}|^2}.$$

Relation A1 can be rather easily proved by noting that the series at the rhs. is periodic as a function of $\mathbf{x}$, so that the series at the lhs. is just its Fourier expansion. One only has to check that the suitable Fourier coefficients, say $c_\mathbf{h}$, turn out to be exactly given by

$$c_\mathbf{h}=e^{-\xi\mathbf{h}^2}.$$

This requires the evaluation of an elementary Gaussian integral, which is not performed here.

Then, the change of variable $(1/(4\xi))\,|\mathbf{x}-\mathbf{x}_\mathbf{n}|^2=z^2$ in the integrals at the rhs. gives

$$\frac{4\pi}{V_c}\sum_{\mathbf{h}} e^{i\mathbf{k}_\mathbf{h}\cdot\mathbf{x}}\frac{1-e^{-\mathbf{k}_\mathbf{h}^2/4\alpha^2}}{\mathbf{k}_\mathbf{h}^2}=\sum_{\mathbf{n}}\frac{\mathrm{erfc}(\alpha|\mathbf{x}-\mathbf{x}_\mathbf{n}|)}{|\mathbf{x}-\mathbf{x}_\mathbf{n}|},$$

so that in conclusion we arrive at the splitting

$$V(\mathbf{x})=\frac{4\pi}{V_c}\sum_{\mathbf{h}\neq 0}\frac{\exp(-\mathbf{k}_\mathbf{h}^2/4\alpha^2)}{\mathbf{k}_\mathbf{h}^2}e^{i\mathbf{k}_\mathbf{h}\cdot\mathbf{x}}+\sum_{\mathbf{n}}\frac{\mathrm{erfc}(\alpha|\mathbf{x}-\mathbf{x}_\mathbf{n}|)}{|\mathbf{x}-\mathbf{x}_\mathbf{n}|},$$

which is the Ewald summation formula.

Notice that, while the starting expression for the potential $V(\mathbf{x})$ was just formal (the series was everywhere divergent), the final expression is mathematically meaningful. It can be checked that the function defined by the final expression is analytic and harmonic for $\mathbf{x}\neq\mathbf{x}_\mathbf{n}$, while it diverges as $1/|\mathbf{x}-\mathbf{x}_\mathbf{n}|$ for $\mathbf{x}\to\mathbf{x}_\mathbf{n}$. Thus, the potential defined by the Ewald formula is a solution of

$$\Delta V=4\pi\sum_{\mathbf{n}}\delta(\mathbf{x}-\mathbf{x}_\mathbf{n}),$$

in strict mathematical sense.

The expression for the electric field given in (6) is obtained simply by summing over the different charges located in the fundamental cell, and then taking term by term the gradient of the resulting expression.

[1] A. Carati, M. Zuin, A. Maiocchi, M. Marino, E. Martines, and L. Galgani, Chaos **22**, 033124 (2012).
[2] M. Greenwald, Plasma Phys. Controlled Fusion **44**, R27 (2002).
[3] G. Pucella *et al.*, Nucl. Fusion **53**, 023007 (2013).
[4] C. A. Iglesias, J. L. Lebowitz, and D. MacGowan, Phys. Rev. A **28**, 1667 (1983).
[5] M. N. Rosenbluth, R. Z. Sagdeev, J. B. Taylor, and G. M. Zaslavsky, Nucl. Fusion **6**, 297 (1966).
[6] N. N. Filonenko, R. Z. Sagdeev, and G. M. Zaslavsky, Nucl. Fusion **7**, 253 (1967).
[7] A. Vasiliev, A. Neishtadt, and A. Artemyev, Phys. Lett. A **375**, 3075 (2011).
[8] D. A. Gates and L. Delgado–Aparicio, Phys. Rev. Lett. **108**, 165004 (2012).
[9] P. P. Ewald, Ann. Phys. **359**, 519 (1917); **369**, 253 (1921).
[10] P. Gibbon and G. Sutmann, *in Quantum Simulation of Complex Many–Body Systems: from Theory to Algorithms*, edited by J. Grotendorst, D. Marx, and A. Muramatsu (NIC Series, 2002), Vol. 10, pp. 467–506.
[11] A. Lerose, A. Sanzeni, A. Carati, and L. Galgani, "Classical microscopic theory of polaritons in ionic crystals," Eur. Phys. J. D (in press).
[12] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957).
[13] Yu. L. Klimontovich, *Statistical Physics* (Harwood Academic, Chur, 1982).
[14] F. Benfenati, A. Carati, and L. Galgani, Chaos **21**, 023134 (2011).
[15] T. Ott and M. Bonitz, Phys. Rev. Lett. **107**, 135003 (2011).
[16] R. C. Davidson, *Physics of Nonneutral Plasmas* (Addison Wesley, Redwood City, 1990).
[17] M. Born, *Problems of Atomic Dynamics* (Dover, New York, 2004).