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NEAR-COLLISIONS IN A COULOMB SYSTEM: NUMERICAL SIMULATIONS—A PRELUDE TO HYBRID FUSION

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In the microcanonical phase space of a classical Coulomb system with positive (D) and negative (e) particles, low-energy near-collisions of two positive particles are dominated by (DeD) configurations. Computed from the area of the energy hypersurface where these events take place, the probability for (DeD) near-collisions is many orders of magnitude above the probability for tunneling through the Coulomb barrier in a $(DeD)^+$ bound state, when e is a light particle.

If the Coulomb system is embedded in a metallic lattice, access to the near-collision regions in the phase space is hindered by the regularity of the lattice. One should then expect, at most, intermittent and irreproducible behavior associated to mechanisms like Arnold's diffusion. Mechanisms to restore ergodicity are proposed.

Numerical simulations are performed on a three-body system to compare the observed rate of near-collisions in actual orbits (with random initial conditions) with the phase-space estimates. It is found that local conservation of angular momentum causes large deviations from the phase-space estimates.

1. Introduction

In 1989 there was a lot of excitement centered around the cold fusion claims of Fleischmann–Pons[1] aand Jones.[2] Interest in this field has since subsided because the claims of excess heat production could not be confirmed and, if any positive results did exist, their unpredictable bursting nature made them basically irreproducible.[3,4] The cold fusion controversy had nevertheless the merit to call attention to the possibility that fusion effects might be obtained if on one side one profits from the large number of deuterons that can be packed inside certain types of solid matter[a] and, at the same time, some mechanism is found to help them overcome the Coulomb barrier. As the deuterons are already confined inside the solid, we would not have to worry about confinement, the main problem in hot plasma fusion. On the other hand, remember that deuterium nuclei when loaded into palladium are on the average 2–3 Å apart, i.e. further apart than in gaseous deuterium at room

[a]Palladium, titanium, iron under pressure, etc.

temperature. It would therefore take a strong act of faith to suppose that they would start fusing simply because they are in a metallic lattice. The emphasis therefore should not be on whether cold fusion was or was not spontaneously observed in the past experiments, but on the question of what to do to the confined deuterons to help them overcome the Coulomb barrier in a reproducible manner.

A local accelerating mechanism is for example proposed in fractofusion,[5] where the electrical fields provoked by fracture would accelerate the deuterons. This however does not seem to produce any useful rates and in any case is not the type of mechanism that could be used for steady state operation. Another mechanism for the "*hybrid fusion*" idea had its origin around May 1989 when there was still a lot of excitation concerning the Fleischmann–Pons' and Jones' claims. At the time I have discussed these matters with a colleague and a back of the envelop estimate (of the kind later published in a sophisticated form by Legget and Baym[6]) convinced us that the crystal fields could not, in any likely way, be sufficient to overcome the Coulomb barrier in the DD system. Looking for a sufficiently soft process that could be a candidate to mediate an eventual fusion process, we concluded that, if any, it could only be of the three-body deuteron–electron–deuteron type. It could not however be of the bound-state type because of the extremely small fusion rate (10^{-74} s^{-1}) in a $(DDe)^+$ molecule.[7] The only possibility to be checked was therefore an actual scattering process. Making a phase-space uniformity assumption, i.e. essentially assuming all configurations on the energy surface to be equally probable, we made a rough estimate of a bound for the rate of D–e–D near-collisions. We found a rate higher than in the bound-state calculations; however, even in this perfectly ergodic conditions, it is smaller than the one needed for the heat-producing rate claimed by Fleischmann and Pons. The question of whether such ergodicity conditions could ever be realized inside solid matter remained very much open. In fact we did not think of them very likely in a crystal at equilibrium, where deuterons tend to occupy more or less well-defined lattice positions. References 8 and 9 discussing the kind of nuclear physics to be expected if fusion was an effect of three-body processes were circulated as preprints but never formally published. Cold fusion ideas were falling in repute; there was an incident where the editor of a reputed magazine refused the papers on the ground that "... there is no point in speculating about nonexistent effects." In retrospect, this was probably a fortunate occurrence because it gave me time to work out these ideas carefully. Better estimates of the three-body near-collision rates were performed, which were later published,[10] being slightly disguised as a mathematical exercise in classical statistical mechanics. In that paper, some definite assumptions were made concerning an ergodic measure for the many-body electron–deuteron Coulomb gas and again, the question of how likely it is for an actual system to choose such a dynamical measure was left open. A hint that some type of nontrivial dynamical measure might indeed be at work in the few cold fusion events that were not explained away is the fact that they occurred in bursts, mostly infrequent and unsystematic bursts. This indeed seems

characteristic of the intermittence of a nonintegrable system with support on a dynamical measure close to a quasilaminar regime.

As shown in Ref. 10, there are low-energy configurations in the Coulomb system where two deuterons and an electron nearly collide and the area of the energy hypersurface where these events take place is small but not negligible. However, at least at low temperatures and under normal conditions, the deuteron nuclei in a metal are known to stay near more or less well-defined lattice positions (for example, the octahedral sites in palladium). This means that the whole palladium–electrons–deuterons many-body system explores only a tiny amount of its energy hypersurface in phase space. We know this to be the case also for nearly integrable systems where the KAM tori are the barriers blocking diffusion in phase space. Therefore, even if the energy surface contains (chaotic) regions with positive Lyapunov exponents, the system may be locked in the neighborhood of a regular motion and not explore the irregular components of phase space. We also know, however, that high-dimensional nonintegrable systems cannot be perfectly contained by KAM tori because mechanisms like Arnold's diffusion give them a small but nonvanishing probability of escaping to other regions of phase space. Therefore, even starting from an ordered lattice configuration, the three-body near-collisions would still be possible, although highly unprobable and certainly unpredictable and irreproducible. To rely on this intermittent behavior would not seem very appropriate for practical purposes. Therefore, the question is how to induce a fuller exploration of phase space by the Coulomb system. A few requirements may be easily stated:

i) First, we should insure that the deuteron nuclei are relatively free to move in the metal lattice and not tightly confined to interstitial positions. For palladium this implies that the concentration should be well above the β phase, because for one deuteron in each octahedral site the absorption energy is larger than in the free D_2 molecule and the deuterons are tightly bound.[11] Octahedral and tetrahedral sites should both be occupied. After the lattice is charged in this way, the working temperature may then be raised to a level where thermal excitation is above the hopping energy.

ii) Even with the deuterons loosely bound, the existence of the periodic potential of the lattice favors regularity in the motion which opposes our ergodicity requirements. A possible solution is the introduction of additional nonintegrable perturbations. Crossed electric and magnetic fields are known to induce chaotic motion in Coulomb systems. One might surround the sample with coils and electrodes along the three coordinate directions and choose at random the directions of electric and magnetic pulses.

iii) The procedures suggested above will naturally lead to a fuller exploration of the available phase space by the electron–deuteron many-body system. However, if the purpose is to increase the rate of D–e–D near-collisions, special attention must be paid to the role of local conservation laws, in particular the local angular momentum. This will be discussed in the context of the numerical simulations in Sec. 2.

The electron–deuteron system in the metallic lattice is a quantum mechanical system. However, the positive Lyapunov exponent (chaotic) regimen that is the most effective one to explore all regions of phase space is not adequately described by the usual quantum mechanical techniques and the quantum theory of nonintegrable systems is still in its infancy.[12] Fortunately, in the few cases that have been fully studied, the behavior of quantum systems seems to be closer to the classical behavior for the irregular motion components than for the regular ones. A study of the corresponding classical system may therefore provide a good approximation to the ergodic properties.

The rate of DD near-collisions being dominated by three-body events,[10] the numerical simulations concentrate on the three-body system of two likely charged particles and one of the opposite charge. Due to the special boundary conditions used in the numerical simulations (which are different from those implicit in the estimates of Ref. 10), the appropriate phase-space probability for three-body near-collisions is recomputed in Sec. 2. The phase-space rates are then compared with the rates observed in numerical simulations with random initial conditions. Random initial conditions are more favorable for collision processes than an ordered configuration (as in a metal lattice) and a certain amount of noise was allowed for in the simulations. Nevertheless, the observed rates are smaller than the phase-space estimates. The reason for this is that the near-collision events are concentrated in a narrow band near zero angular momentum, whereas random initial conditions explore a wide range of angular momenta. The simulation noise allows for some change in angular momentum, nevertheless, approximate conservation of this quantity makes near-collisions (for typical initial conditions) much less probable than a phase-space uniformity calculation would imply. One conclusion is that to be close to a full exploration of phase space, not only do the deuterons have to be free to move about (as they are in the numerical simulations) but also one must be sure to populate the *local* low-angular-momentum configurations. In principle, if a mechanism is devised for "*local angular-momentum cooling*" to emphasize low-angular-momentum states without hurting ergodicity, then near-collision rates above the phase estimates may be obtained. In simulation, this is relatively easy to achieve by detecting the induced field generated by the moving charges and then applying the appropriate counterfield externally. However, it is not so clear at this time of how to implement such an action in an actual experiment because what is important to cancel are the local angular momenta and not the global angular momentum of a sample with many deuterons and electrons.

Another situation where ergodic near-collisions might play a role is the controversial cluster-impact fusion events,[13] which may not be significant after all.[14] However, I have not analyzed these experiments in any significant detail to have a definite opinion.

2. Phase Space Versus Dynamical Simulations

Consider a set $\{P_+\}$ of N_+ positively charged particles of mass m_+ and charge $+e$ and a set $\{P_-\}$ of N_- negatively charged particles of mass m_- and charge $-e$, in interaction by Coulomb forces. Their coordinates and velocities are denoted by (X_i, V_i) and (Y_i, W_i) respectively. Let a be a natural length scale. We define the scaled variables

$$x_i = a^{-1}X_i\,, \qquad \nu_i = \mu_\nu^{-1}V_i\,, \tag{2.1a}$$

$$y_i = a^{-1}Y_i\,, \qquad \omega_i = \mu_\nu^{-1}W_i\,, \tag{2.1b}$$

$$\tau = \mu_\tau^{-1}t\,, \tag{2.1c}$$

with

$$\mu_\nu = \frac{a}{\mu_\tau}\,, \qquad \mu_\tau = \frac{\sqrt{m+a^3}}{e}\,, \qquad \gamma = \frac{m_-}{m_+}\,. \tag{2.2}$$

Then the nonrelativistic equations of motion are

$$\frac{dx_i}{d\tau} = \nu_i\,, \qquad \frac{d\nu_i}{d\tau} = \sum_{j\neq i}\frac{\epsilon_{ij}}{\rho_{ij}^2}\frac{\rho_{ij}}{\|\rho_{ij}\|}\,, \tag{2.3a}$$

$$\frac{dy_i}{d\tau} = \omega_i\,, \qquad \frac{d\omega_i}{d\tau} = \frac{1}{\gamma}\sum_{j\neq i}\frac{\epsilon'_{ij}}{\rho_{ij}^2}\frac{\rho_{ij}}{\|\rho_{ij}\|}\,, \tag{2.3b}$$

where ρ_{ij} stands for $x_i - x_j$ or $y_i - y_j$ and ϵ_{ij}, ϵ'_{ij} have $-$ or $+$ signs according to whether the particles in the ij pair are of the same or opposite sign.

As in Ref. 10, the instances of close proximity of two charges of the same sign (which for definiteness one takes to be positive) are characterised by the notion of "ϵ-collision". There is an ϵ-collision when two positive particles reach a distance equal to or smaller than ϵ and move towards each other, that is there is a pair i, j such that $\|x_i - x_j\| < \epsilon$ and $(x_i - x_j)\cdot(\nu_j - \nu_i) > 0$. As shown in Ref. 10, in an ergodic component of the invariant measure of the system, the rate of ϵ-collisions is

$$n_\epsilon = \int d\mu \sum_{k<l}\delta(\|x_k - x_l\| - \epsilon)\|\nu_k - \nu_l\|\theta[(x_k - x_l)\cdot(\nu_l - \nu_k)]\,. \tag{2.4}$$

For the microcanonical ensemble in the center of mass, the invariant measure is

$$d\mu = N^{-1}\delta(E - E_0)\delta^3\left(\sum_i \nu_i + \gamma\sum_j \omega_j\right)\prod_{i\in\{P_+\}} d^3x_i d^3\nu_i \prod_{j\in\{P_-\}} d^3y_j d^3\omega_j\,, \tag{2.5}$$

where

$$E = E_k + V = \frac{1}{2}\sum_{i\in\{P_+\}}\|\nu_i\|^2 + \frac{\gamma}{2}\sum_{j\in\{P_-\}}\|\omega_j\|^2 + \sum_{\substack{i<j\\ i,j\in\{P_+\}}}\frac{1}{d(x_i, x_j)}$$

$$+ \sum_{\substack{i<j\\ i,j\in\{P_-\}}}\frac{1}{d(y_i, y_j)} - \sum_{\substack{i\in\{P_+\}\\ j\in\{P_-\}}}\frac{1}{d(x_i, y_j)}\,.$$

N is a normalisation factor, and E_k and V are the kinetic and potential energies respectively. For the numerical simulations, the particles are considered to be inside a unit cube with periodic boundary conditions. The distance function $d(x_i, x_j)$ is the length of the smallest line segment connecting the two particles, taking into account the periodic boundary conditions.

As shown in Ref. 10, for sufficiently small ϵ, the rate n_ϵ of ϵ-collisions is dominated by three-body near-collisions with two particles of opposite charges. I will therefore concentrate on such a system with $N_+ = 2$ and $N_- = 1$. Integrating over the velocities in (2.4), one obtains in this case

$$n_\epsilon = \frac{112}{15\pi} \frac{\int d^3x_1 d^3x_2 d^3y \delta(\|x_1 - x_2\| - \epsilon)[E - V(x_1, x_2, y)]^{5/2}}{\int d^3x_1 d^3x_2 d^3y [E - V(x_1, x_2, y)]^2} . \tag{2.7}$$

For two positive and one negative particles in the unit cube, with interactions as defined in (2.6), we obtain by the numerical integration of (2.7) the upper points (labelled by $\times$) in Fig. 1, for $E = 0$. To have an idea of the physical significance of the phase-space estimates, notice that if n_ϵ is the number of ϵ-collisions per unit scaled time τ in a cube of scaled unit volume, then the rate $n_\epsilon^{(\text{phys})}$ of ϵ-collisions per unit physical volume and unit physical time is

$$n_\epsilon^{(\text{phys})} = \frac{n_\epsilon}{a^3 \mu_\tau} , \tag{2.8}$$

where n_ϵ is a function of the scaled $\epsilon = \epsilon_{\text{phys}}/a$.

From the phase-space points in Fig. 1, it is seen that n_ϵ may be fitted by

$$n_\epsilon = C\epsilon^\alpha , \tag{2.9}$$

with $C \simeq 154$ and $\alpha \simeq 2.7$. The power dependence is between the nonrelativistic and the relativistic analytical estimates (at small ϵ) of Ref. 10. Notice, however, that because of the choice of periodic boundary conditions and the definition of the distance between particles as the length of the smallest segment (including those across the cube walls), the dynamics is somewhat different from the one in Ref. 10. The order of magnitude of the rates for the physically relevant distances is, however, similar.

From (2.8) and (2.9), one writes

$$n_\epsilon^{(\text{phys})} = \frac{C\left(\frac{\epsilon_{\text{phys}}}{a}\right)^\alpha e}{a^3\sqrt{m_+ a^3}} . \tag{2.10}$$

An interesting quantity is $\Gamma_\epsilon = a^3 n_\epsilon^{(\text{phys})}$ which gives in physical units the number of ϵ-collisions per second. For $a = 2 \cdot 10^{-8}$ cm, $m_+ = m_D$, and using the phase-space values, one obtains, for example,

$$\Gamma_\epsilon \simeq 2 \cdot 10^4 \text{ s}^{-1} \quad \text{for} \quad \epsilon = 10^{-12} \text{ cm} , \tag{2.11a}$$

$$\Gamma_\epsilon \simeq 3 \cdot 10^3 \text{ s}^{-1} \quad \text{for} \quad \epsilon = 5 \cdot 10^{-13} \text{ cm} . \tag{2.11b}$$

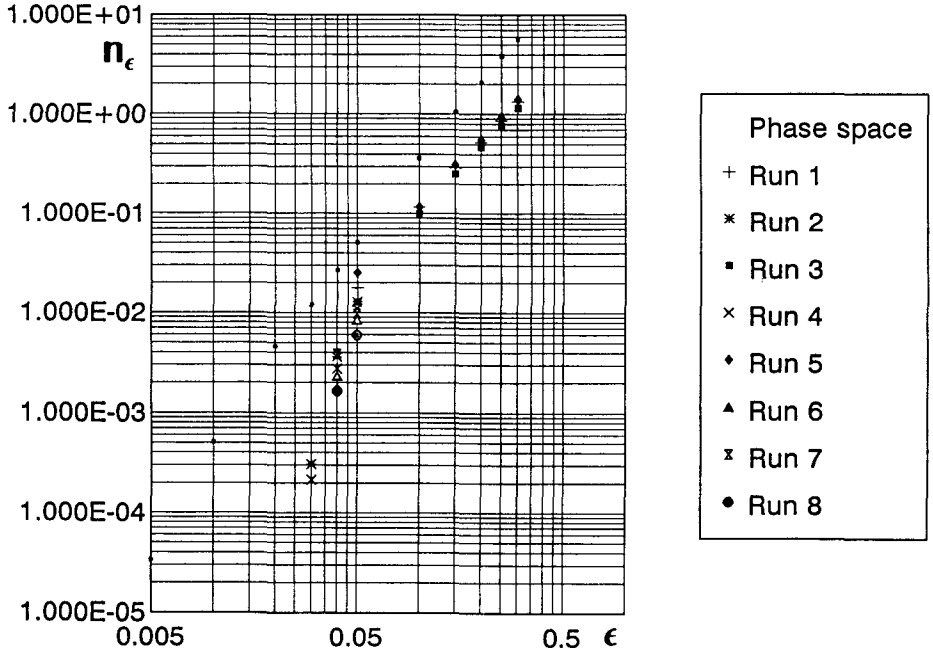
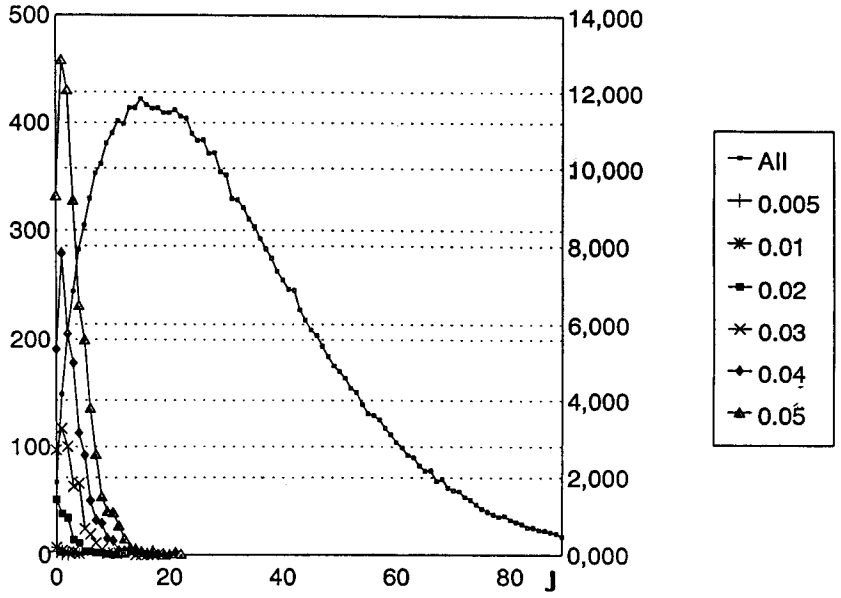


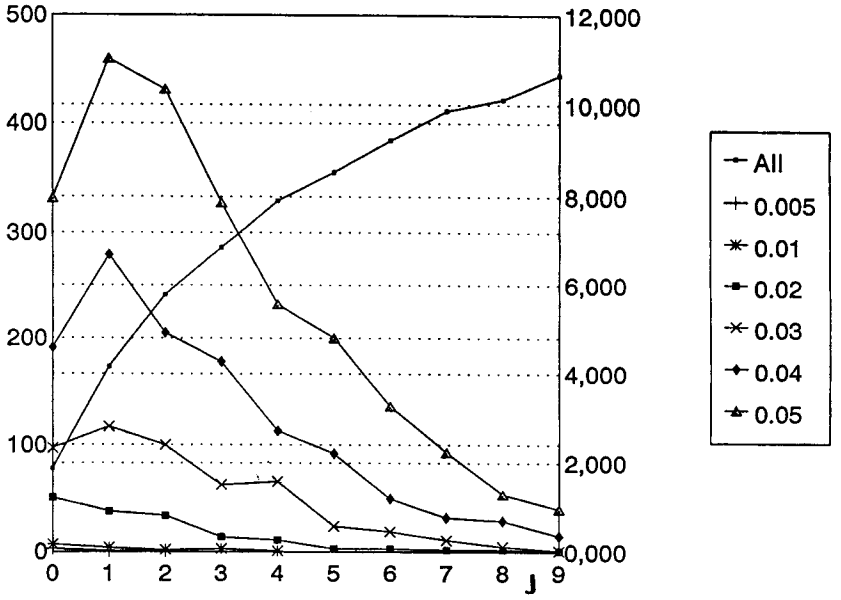
Fig. 1. Rate of ϵ-collisions in scaled variations. Phase space vs dynamical simulations.

These are fantastically high rates of instances of close proximity for two low-energy positively charged particles if compared, for example, with the tunneling rates for $(DDe)^+$ molecules ($\sim 10^{-74}$ s^{-1}). It shows how motion under ergodic conditions with a full exploration of phase space may be quite different from the regular components. If the classical mechanics results (2.11) give an order of magnitude estimate of the corresponding ergodic quantum system, we might say that the fusion rates under perfect ergodic conditions would be similar to what might be achieved with a bound $(DDE)^+$ molecule if E has a mass around 150 times that of the electron. Even in this ideal situation the rate would be smaller than what is obtained in $DD\mu$ systems (10^{11} s^{-1}).

To check how realistic the phase-space estimates are, I have performed a direct simulation of the dynamics in (2.3) for the same interaction, counting the number of ϵ-collisions per unit time. The lower points in Fig. 1 are obtained. Figure 1 shows the results of several runs with random initial conditions. The dynamical simulations are carried out at a constant total energy $E = 0$. At each time step the new total energy is recomputed, and to compensate for the numerical errors, the velocities of the particles are scaled up or down to readjust the energy E to zero. If, however, the error E is large (larger than 10% of the kinetic energy of the negatively charged particle), the time step is decreased and the dynamics recomputed until the error in E becomes small. This is particularly important to obtain good accuracy



(a)



(b)

Fig. 2. (a) Angular momentum distribution for randomly chosen configurations. (b) Same as (a) expanded near $J = 0$.

because when the particles are close to one another, the numerical errors are much larger than when they are far away from one another. Due to the readjustment of the total energy, the simulation remains rigorously in one energy hypersurface. Each numerical run represents a dynamical orbit with a small amount of noise. The noise originates from the round-off errors and from the readjustment of the velocities to maintain the total energy.

Random initial conditions are more favorable for ϵ-collision processes than an ordered configuration (as in a metal lattice). Nevertheless, we find that the observed rates are systematically smaller than the phase-space estimates. The deviation is more pronounced for very small ϵ. The reason for this is that the near-collision events are concentrated in a narrow band near zero angular momentum, whereas random initial conditions explore a wide range of angular momenta. The simulation noise allows for some change in angular momentum; nevertheless, approximate conservation of this quantity makes near-collisions (for typical initial conditions) much less probable than in a phase-space calculation. In Figs. 2(a) and (b), we have plotted the center-of-mass angular momentum distribution for random initial conditions and the same distribution for the configurations that correspond to ϵ-collisions of the indicated values. As expected, the instances of ϵ-collisions at small ϵ are concentrated in a very narrow angular momentum band near zero. The deviations of the numerical simulations from the phase-space estimates appear therefore as a typical large deviation effect. As is well known in a system with pronounced large deviation effects, the most probable value (for finite samples) may be very different from the asymptotic probability distribution.[15]

One conclusion is that to be close to a full exploration of phase space, not only do deuterons have to be free to move about (as they are in the numerical simulations) but also a mechanism has to be devised to populate the *local* low-angular-momentum configurations. The application of random electro-magnetic pulses which is suggested in Sec. 1 as a means to avoid regular configurations will also enable the exploration of a wider range of angular momenta. It would be even better, however, to devise a mechanism of "local angular-momentum cooling" to emphasize low-angular-momentum states. In simulation, this is relatively easy to achieve by detecting the induced field generated by the moving charges and then applying the appropriate counterfield externally. However, it is not so clear at this time of how to implement such an action in an actual experiment because what is important to detect and cancel are the local angular momenta and not the global fields of a sample with many deuterons and electrons.

3. Conclusions and Remarks

1. All more or less contrived mechanisms[17,18] that have been proposed to reduce the static Coulomb barrier between deuterons inside the metallic lattice fail to explain the bursting and irreproducible nature of those few cold fusion events that apparently cannot be explained away.

When the full microcanonical phase space of the deuteron–electron system is considered, one finds a probability for D–e–D near-collisions which are many orders of magnitude above the tunneling rate through the Coulomb barrier in the $(DDe)^+$ molecule.

Access to the D–e–D near-collision regions in phase space is hindered by the regularity imposed by the metallic lattice. In an actual physical system, one should at most expect intermittent and irreproducible behavior, associated to mechanisms like Arnold's diffusion.

2. Rather than expecting miracles or devising even more contrived theories, the sensible approach seems to be to simply accept the high dissolution rate of the deuterons in the metallic lattices as a marvelous confining mechanism and nothing else. If one wants then to use the deuterons absorbed in the lattice for fusion reactions (with practical applications), it seems inevitable that some other mechanism must be devised for this purpose. This two-way approach is the essence of what I have been calling the "*hybrid fusion*" concept.

Fractofusion is a hybrid fusion technique. *Ergodicity inducing* mechanism as explained in Sec. 1 is another approach that seems to deserve experimental exploration. Ergodicity inducing plus *local angular-momentum cooling* (for which I have no good ideas so far) would be another promising path.

3. The low-energy component of fusion events through D–e–D near-collisions has a preferred $T + p$ channel,[9] through the formation of the $^4He^*(20.1)$ excited compound nucleus.

References

1. M. Fleischmann, S. Pons, and M. Hawkins, *J. Electroanal. Chem.* **261**, 301 (1989); **263**, 187 (1989).
2. S. E. Jones *et al.*, *Nature* **338**, 737 (1989).
3. J. O'M. Bockris and D. Hodko, *Chemistry and Industry* **21**, 688 (1990).
4. J. O'M. Bockris, G. H. Lin, and N. J. C. Packham, *Fusion Technology* **18**, 11 (1990).
5. V. A. Kluyev *et al.*, *Pis'ma Zh. Tekh. Fiz.* [*Sov. Tech. Phys. Lett.*] **12**, 1333 (1986).
6. A. J. Legget and G. Baym, *Phys. Rev. Lett.* **63**, 191 (1989).
7. C. D. Van Siclen and S. E. Jones, *J. Phys.* **G12**, 213 (1986).
8. S. M. Eleutério and R. Vilela Mendes, "Three-body effects in cold fusion", preprint IFM 9/89, May 1989.
9. R. Vilela Mendes, "Three-body effects and neutron suppression in cold fusion", preprint IFM 10/89, May 1989.
10. R. Vilela Mendes, *Mod. Phys. Lett.* **B5**, 1179 (1991).
11. X. W. Wang, S. G. Louie, and M. L. Cohen, *Phys. Rev.* **B40**, 5822 (1989).
12. See, for example, R. Vilela Mendes, "Topics in the quantum theory of nonintegrable systems", in *Nonlinear Fields: Classical, Random, Semiclassical*, eds. P. Garbaczewski and Z. Popowicz (World Scientific, Singapore, 1991).
13. R. J. Beuhler, G. Friedlander, and L. Friedman, *Phys. Rev. Lett.* **63**, 1292 (1989); R. J. Beuhler *et al.*, *Phys. Rev. Lett.* **67**, 473 (1991); M. Fallavier *et al.*, *Phys. Rev. Lett.* **65**, 621 (1990).
14. R. J. Beuhler, G. Friedlander, and L. Friedman, *Phys. Rev. Lett.* **68**, 2108 (1992).

15. For an introduction to large deviation theory and a discussion of some applications, see J. Seixas and R. Vilela Mendes, *Nucl. Phys.* **B383**, 622 (1992).
16. B. J. B. Crowley, *Nucl. Fusion* **29**, 2199 (1989).
17. For a review up to middle 1990, see Ref. 4.
18. G. Preparata, "Towards a theory of cold fusion", Milano preprint MITH 93/7, and references therein.