International Workshop:
“Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations”
26 -29 March 2012
Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Long-Time *ab initio* Simulation of Sharply-Expanding Nonideal Plasmas

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ABSTRACT

We present a new *ab initio* method of numerical simulation of sharply-expanding nonideal plasmas. Its most important feature is introduction of a scalable coordinate frame, moving with plasma. As a result, the effect of plasma expansion is reduced to some effective viscous forces for the charged particles performing their motion in a formally fixed spatial domain. This approach enables us to integrate the equations of motion over extremely long time intervals, without an appreciable loss of accuracy.

The most interesting result of such simulations is a temperature variation in the strongly expanding ultracold plasmas, which was found to follow the law $t^{-1.2}$ instead of t^{-2}, as would be expected for a free adiabatic expansion of monatomic gas [Yu.V. Dumin, *Plas. Phys. Rep.*, v.37, p.858 (2011)]. This finding is in perfect agreement with recent experimental data on the dynamics of ultracold plasmas released from the magneto-optical traps [R.S. Fletcher, *et al.*, *Phys. Rev. Lett.*, v.99, p.145001 (2007)].

Yet another advantage of the proposed algorithm is its ability to resolve formation of the weakly-bound electron–ion pairs (*i.e.* highly-excited Rydberg atoms) from the "first principles". Each of such atoms is identified by a series of synchronous equidistant peaks in both kinetic and potential energies of the system.

Physical Background

A new branch of plasma physics, emerged in the last decade, is studying the clouds of ultracold ionized gases created in the magneto-optical traps.

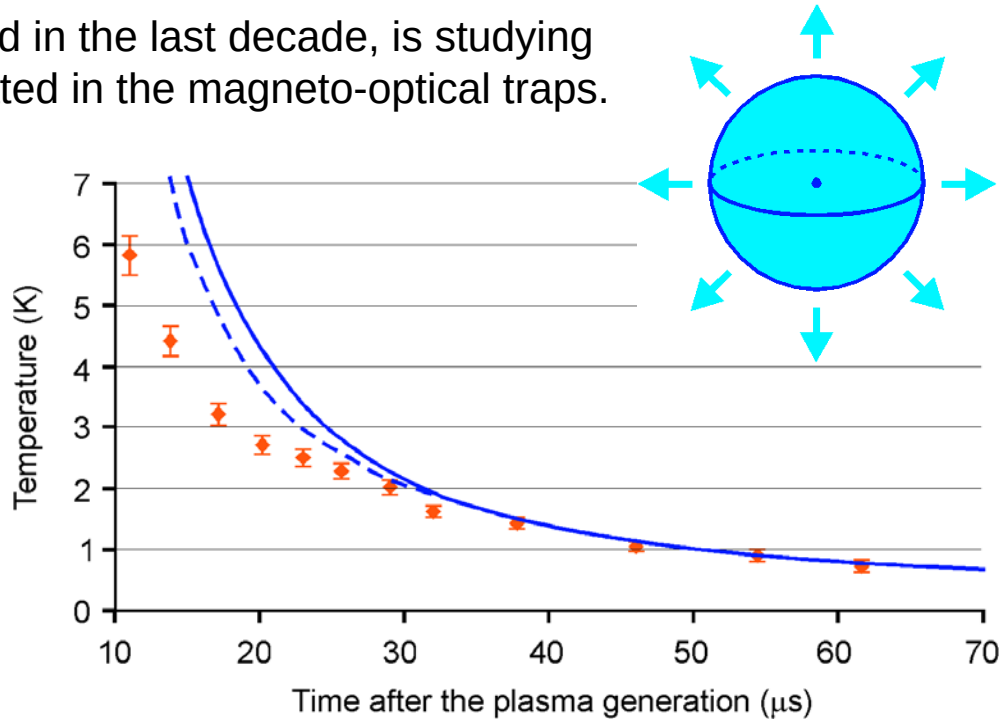
The most interesting findings are:

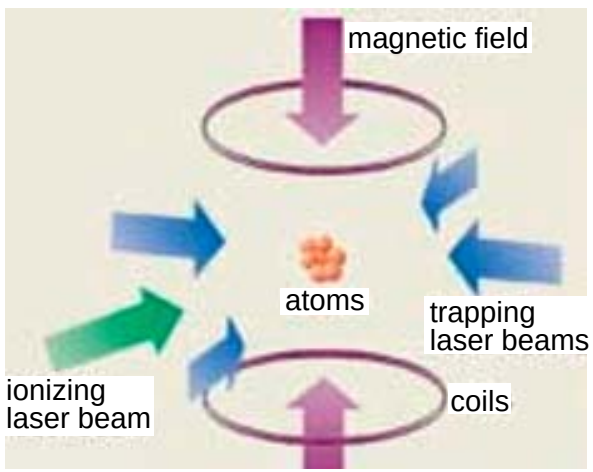
- Temperature of monatomic plasma during its free expansion decays as

$$T_e \propto t^{-(1.2 \pm 0.1)}$$

instead of $T \propto V^{1-\gamma} = V^{-2/3} \propto R^{-2} \propto t^{-2}$, as should be expected for an ideal gas ($\gamma = 5/3$) moving by inertia ($R(t) \propto t$);

- The plasma expansion and cooling is accompanied by the formation of a considerable number of Rydberg atoms.





<u>Characteristic plasma parameters</u>:

initial temperature $T_e \sim 0.1 \div 10$ K

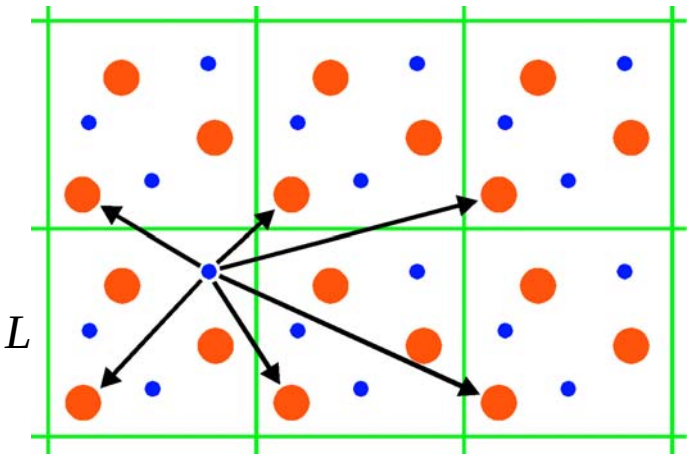
initial density $n \sim 10^9$ cm^{-3}

size of the cloud $R \sim 0.3 \div 15$ mm

coupling parameter $\Gamma_e \sim 0.01 \div 1$
(most typical, 0.1)

Numerical Model: Formulation

The aim of our study is to simulate the "infinite" (unbounded) plasma. Therefore, we integrate the equations of motion for a relatively small number of charged particles in the "basic" cell, taking into account all Coulomb's interactions as accurately as possible (including the particles in the infinite number of "mirror" cells):



$$m\,\frac{d^2}{dt^2}\,\mathbf{r}_i = \sum_{j=1}^{N} Ze^2\,\frac{\mathbf{R}_j-\mathbf{r}_i}{|\mathbf{R}_j-\mathbf{r}_i|^3} + \sum_{j=1,\,j\neq i}^{ZN} e^2\,\frac{\mathbf{r}_i-\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|^3}$$

$$+\sum_{k=1}^{3}\sum_{n_k=-\infty,\,n_k\neq 0}^{+\infty}\left\{\sum_{j=1}^{N} Ze^2\,\frac{[\,\mathbf{R}_j+L\sum_{l=1}^{3}n_l\mathbf{e}_l\,]-\mathbf{r}_i}{|[\,\mathbf{R}_j+L\sum_{l=1}^{3}n_l\mathbf{e}_l\,]-\mathbf{r}_i|^3}\right.$$

$$\left.+\sum_{j=1}^{ZN} e^2\,\frac{\mathbf{r}_i-[\,\mathbf{r}_j+L\sum_{l=1}^{3}n_l\mathbf{e}_l\,]}{|\mathbf{r}_i-[\,\mathbf{r}_j+L\sum_{l=1}^{3}n_l\mathbf{e}_l\,]|^3}\right\}$$

An important feature of our approach is introduction of the scalable coordinate frame, where the size of the basic cell increases linearly with time:

$$L = L_0 + u_0\,t$$

(which corresponds physically just to the inertial expansion of the plasma cloud).

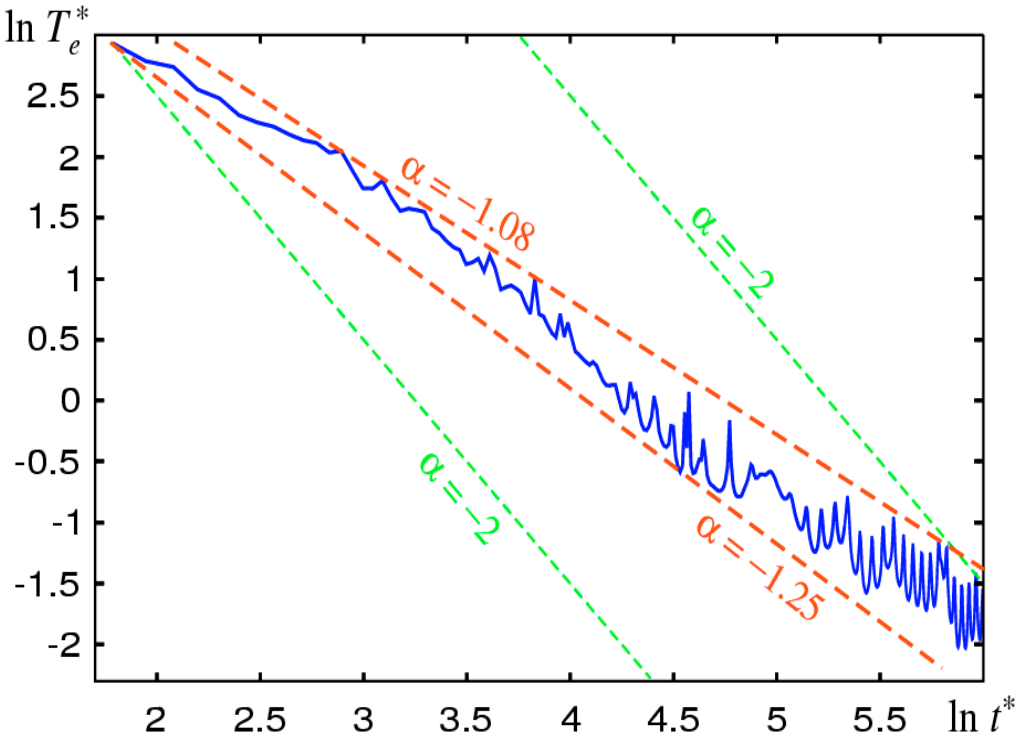
As a result, **the equations of motion in the renormalized variables** will take the form:

$$\ddot{\mathbf{r}}_i^{\,*} + \underbrace{2\,u_0^*\,(1+u_0^*\,t^*)^{-1}\,\dot{\mathbf{r}}_i^{\,*}}_{\text{effective dissipative force, resulting from the plasma expansion}} = (1+u_0^*\,t^*)^{-3}\,\mathbf{F}_i^*$$

Results of Numerical Simulation: **Plasma Temperature**

The value of temperature in the expanding cloud is established due to the interplay between a plasma heating by the electron–ion interactions and plasma cooling by the effective dissipative forces.

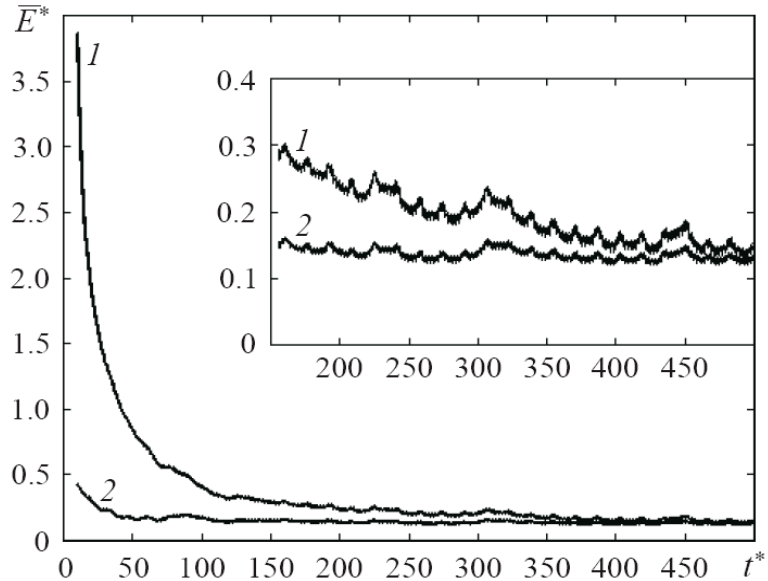
Temporal evolution of the electron temperature:



This is in perfect agreement with the experimental measurements, which give the value of exponent

$\alpha = -(1.2 \pm 0.1)$

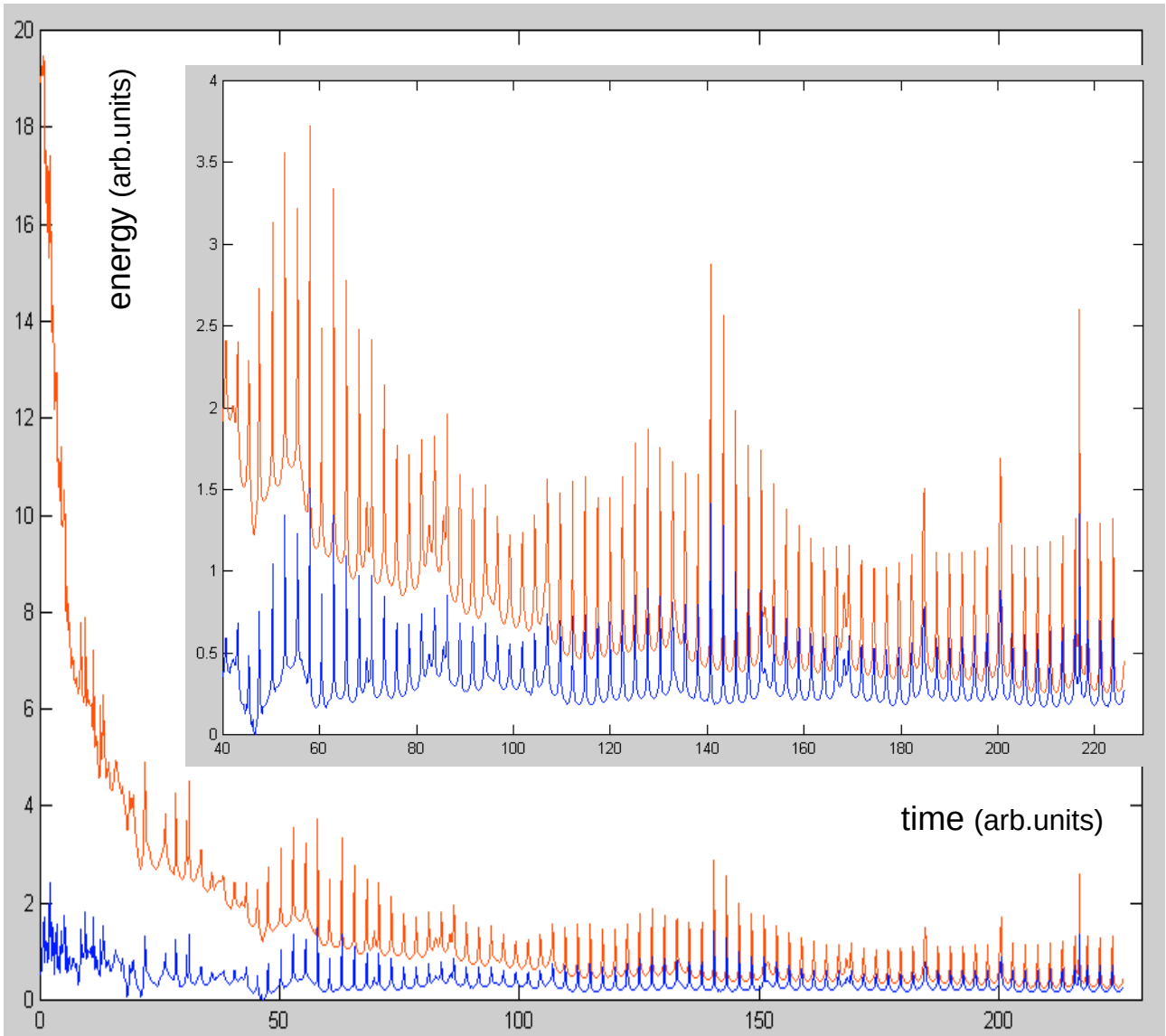
Is the simulated exponent caused by the effect of "virialization" between the kinetic and potential energies?



Temporal evolution of average kinetic energy $\overline{E}^*_{\text{kin}}$ (curve *1*) and one-half the absolute value of the potential (Coulomb) energy $|\overline{E}^*_{\text{cul}}|/2$ (curve *2*).

Therefore, the virialization really takes place but quite slowly, as compared to the establishment of α.

Results of Numerical Simulation: **Formation of Rydberg Atoms**



In this figure,

red curve corresponds to the kinetic energy of the system; and

blue curve, to the absolute value of the potential (Coulomb) energy.

The presence of Rydberg atoms is identified by the series of equidistant synchronous jumps in both energies. These jumps correspond to the instants when a weakly-bound electron passes through a pericenter of its elliptical orbit around the ion.

The amplitudes and separations of the peaks can be used to derive characteristics of the Rydberg atoms formed.