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CLASSICAL DENSE MATTER PHYSICS: SOME BASIC METHODS AND RESULTS

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Abstract. This is an introduction to the basic notions, some methods and open problems of dense matter physics and their applications in astrophysics. Experimental topics cover the range from the work of P. W. Bridgman to the discovery and basic results of use of the diamond anvil cell. On the theoretical side, the semiclassical method of P. Savić and R. Kašanin is described. The choice of these topics is conditioned by their applicability in astrophysics and the author's research experience. At the end of the paper is presented a list of some unsolved problems in dense matter physics and astrophysics, some (or all) of which could form a basis of future collaborations.

1. Introduction

The aim of this paper is to review some of the basic methods and results of classical dense matter physics. The term "classical" here has a loose meaning of " not so dense to require taking into account general relativistic effects". In practical terms, this corresponds to densities in the range $10^3 - 10^5 kg/m^3$. The text is divided into several sections. The first one is devoted to the main instrument of modern static high pressure experiments-the diamond anvil cell (DAC). In the follow-up, a short review is given of the theoretical method developed by P. Savić and R. Kašanin in Belgrade, and the paper ends with a list of selected open problems in dense matter physics and astrophysics.

This paper has been written with the astronomically oriented readers in mind. That is, people who are "at ease" in physics, but whose main interest is the application of dense matter physics to different kinds of celestial objects and not various technical details of pure physics.

In mentioning astronomy as a science, one is inclined to think about vast regions of nearly empty interstellar or interplanetary space, scarcely populated by stars and other celestial objects. Apart from this aspect of astronomy, there exists another "side of the story". Namely, in the interiors of stars, planets, and various other kinds of astronomical objects, materials are subdued to extremely high values of temperature and pressure. Although this has been known "in principle" for centuries, experimental studies of materials under high pressure have became possible only in the last 5-6 decades.

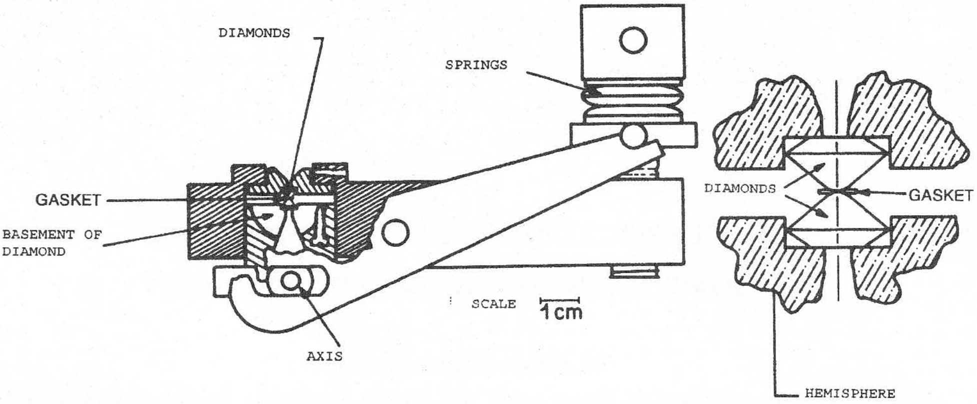

Fig. 1: the DAC of the NBS type

2. Static experiments

First attempts at studies of the behaviour of materials under high pressure have been made in the *XVIII* century (Block et. al., 1980). It has been noted at the time that a wealthy English "gentleman" named Mr. Canton, compressed water at room temperature to a pressure of about $0.1GPa$. To his astonishment, as a result of this compression, water was transformed into ice. This was an isolated attempt of experiments under high pressure. The start of systematic work had to wait for more than a century. For comparison, note a recent example of a modern study of ice in Putrino and Parinello (2002).

Systematic high pressure experiments were initiated by P. W. Bridgman at Harvard (Bridgman, 1964). For his monumental achievements Bridgman was awarded the Nobel prize for physics in 1946.

Bridgman used large volume presses which had the advantage that the they contained large samples, and that the $P-T$ gradients in them were small. At the same time, they had the drawback that the accessible region of $P-T$ space was limited, and (which was perhaps worse) were expensive to build and maintain in operational conditions.

A real breakthrough in high pressure experimental work occurred around the middle of the *XX* century, with the invention of the DAC. Details about this instrument are already available in the literature, and some have been discussed by the present author (Čelebonović, 1993 and references given there).

A cross section of a DAC (of the so-called NBS type) is shown in the following figure, taken from (Jayaraman, 1983).

The term DAC comes from the fact that the most important part of this instrument is a couple of diamonds and a thin metal plate (called the gasket) between them.Diamonds are important because they are hard and transparent;this implies that a specimen can be compressed to high pressure and remain visible. The optical accessibility of a specimen is a big advantage compared to Bridgman's experimental cells.A hole is drilled in the gasket, and in this way one gets a "working volume" in which the experiment is performed. Experiments in DACs are complicated by the miniaturized scale of the xpecimen and the working volume. The gasket is thin (usually, around 250 μm), and the diameter of the hole in it is about 200 μm. The typical size of the specimen is around 40μm. Note, as an additional difficulty, that the "working" volume contains the pressure sensor and the pressure transmitting medium. In the working volume pressure is transmitted hydrostatically. The chemical composition of the hydrostatic fluid depends on the pressure and temperature at which the experiment is preformed. For example, for $P \leq 11GPa$ a mixture of methyl and ethyl alcohol in the ratio 4 : 1 is universally used (Jayaraman, 1983).

The pressure is measured in the so-called "'ruby scale". It has been shown several decades ago (for example Jayaraman, 1983 and references given there) that the spectrum of ruby ($Al_2O_3 : Cr^{3+}$) excited with a laser beam or spectral lamp consists of two spectral lines with pressure dependent wavelengths. The physical process in which these two lines are created is the transition $^4A_2 \rightarrow ^2E$ in the ion Cr^{3+} (Eggert et al., 1989). The pressure dependence is linear up to at least $30GPa$, while in its no-linear form the ruby scale can be applied up to $250GPa$.The intensity of the ruby lines diminishes with increasing pressure, and this scale becomes inapplicable for pressure higher than $250GPa$. Above that treshold, measurements can be performed only by using X-ray techniques.The final expression for the pressure dependence of the RI line (the stronger of the two) is (Mao et al., 1978):

$$P[GPa] = 380.8(1 + \frac{\Delta\lambda}{694.2})^5 - 1) \tag{1}$$

The measurement of pressure is in fact indirect:the measured quantity is the change of wavelength of the RI line, and the pressure is calculated from Eq. (1).

The region of phase space accessible to experiments in DACs is limited by $4 \leq T[K] \leq 7000$ and $P \leq 450GPa$ (Čelebonović). Note that the upper limit is of the order of magnitude of the pressure in the center of the Earth.

The applicability of DACs in space science is virtually unlimited. It is well known that the interiors of planets and satellites are inaccessible to direct observation. Some of their observable parameters (for example the magnetic moment or the content of water(Mallin and Edgett, 2000)) critically depend on the conditions in their interiors.The only reliable experimental method for investigating materials under such conditions is the DAC.

In every high pressure experiment one encounters the existence of two "interfering" complex characteristics of this branch of physics. One is the often complicated physical nature of phenomena occurring under high pressure, and the other is the complicated nature of the preparation and actual performing of the experiments. A perfect illustration of this statement, spanning more than 50 years of research and still unsolved, is offered by the behaviour of hydrogen under high pressure.

It has been predicted many times since the mid-thirties of the last century that hydrogen undergoes a phase transition and becomes metallic at a pressure of the order of 250-300 GPa. These predictions have been made so many times, by various authors using different methods of calculation, that the result of all these calculations was taken almost as an experimental value. For a long time so high values of pressure were experimentally unfeasible, but everybody in the researchers community was certain that once they become measurable, they were just going to confirm theoretical predictions.

Results of real experiments came as a complete surprise to the high pressure researchers. It was first shown (Narayana et. al., 1998) that metallization of hydrogen **does not** occur for $P \leq 342GPa$. As a further set-back, came a result from the Lawrence Livermore National Laboratory, that the transition semiconductor → metal in fluid hydrogen occurs at the point $P = 140GPa; T = 3000K$ (Weir et. al., 1996; Nellis et. al., 1997). One possible explanation in "circulating" at the time of writing this paper (summer 2002) invokes effects of disorder (Nellis, 2002).

What can be concluded from this example? Hydrogen is a well known chemical element. It would be logical to expect that everything is known about it, and that the position of a point on its phase diagram can be predicted with arbitrary certainity. It appears that this is not the case, in spite of nearly 60 years of research on the problem.

No definite explanation has been found, but in the oppinion of the present author it should be sought in one of the following directions:

- Some of our theoretical methods and ideas are probably wrong and/or not applicable to hydrogen.
- Perhaps everything is all right with the methodology, but we are making errors in predicting the experimentally measurable consequences of the metallisation transition.

The settling of this "dispute" would have useful consequences for pure astronomy. For example, hydrogen is a constituent of the giant planets of our planetary system. Improvement of its phase diagram under high pressure would enable expanding our knowledge of their interiors.

Experiments in DACs are capable of giving information about the behaviour of various materials in a large region of the $P - T$ plane. A much wider region is accessible theoretically. The remainder of this paper is devoted to a brief review of the main ideas of a semiclassical theory of dense matter, proposed years ago by P. Savić and R. Kašanin. It has been previously discussed (for example Čelebonović, 2000 and references given there), so we shall not go into detailed considerations.

3. Semiclassical studies of dense matter:a particular theory

A specimen of a solid, although it may appear macroscopically small, is actually a typical example of a many-body system. It is a standard practice in statistical physics to describe the state of such a system by a Hamiltonian, which has the following general form:

$$H = \sum_{i=1}^{N}(-\frac{\hbar^2}{2m})\nabla_i^2 + \sum_{i=1}^{N} V(\vec{x_i}) + \sum_{i,j=1}^{N} v(\vec{x_i} - \vec{x_j}) \qquad (2)$$

The first term in this expression denotes the kinetic energy, the second is the interaction of the system with a possible external field, and the third denotes the pair-wise interaction of the particles. According to the rules of statistical mechanics, proceeding from a Hamiltonian of the general form given by Eq. (2), one should calculate the free energy and all the other thermodynamic potentials. Singularities in these potentials would be identified with the phase transition points of the system under consideration.

This algorithm may seem clear and straightforward, but scientific reality is exactly the opposite. Sums in Eq. (2) go over all the particles of the system, and this number is usually of the order of Avogadro's number $N_A \approx 10^{23}$. It follows that these sums can not be performed for systems containing realistic numbers of particles, and that various approximate methods have to be found. One of such approximate methods is the semi-classical approach proposed by Pavle Savić and Radivoje Kašanin (Savić and Kašanin 1962/65).

At the beginning of the sixties they have started developing a semiclassical theory of dense matter. The starting point was astronomical one: they have shown that the mean volumetric planetary densities can be related to the mean solar density by a simple relationship:

$$\rho = \rho_0 2^{\varphi} \tag{3}$$

where $\rho = \frac{4}{3}$ is the mean solar density, and φ an integer. By choosing suitable values of this integer, it becomes possible to reproduce the measured values of the densities. Using this result, and a fact known from geophysics and high pressure experiments that at certain values of pressure abrupt changes of the mass density occur, they came to the conclusion that the atomic structure changes under the influence of high external pressure.

Proceeding from these ideas, they proposed a set of 6 postulates which govern the behaviour of materials under high pressure. Each of them is based on known experimental results. Developing further these postulates, they have set up a computing scheme, which gives the possibility of theoretical studies of dense matter physics. Full details about their postulates and the ensuing algorithm for calculation were recently discussed by Čelebonović (2000). In the remainder of this section we shall describe the applicability of their theory in astronomy.

Input data needed for modelling the internal structure of a planet, satellite or asteroid are the mass and the radius of the object. Starting from this pair of values, it is possible to determine the following characteristics of the body:

- the number of zones in the interior and their thickness ;
- the distribution of P, ρ, T within each of the zones ;
- the magnetic moment of the object ;
- the mean atomic mass of the chemical mixture which the object is made of ;
- the allowed interval in which the speed of axial rotation of the object must be.

Numerous examples of astronomical applications of this theory exist in the literature ([11] and references given there) and the reader interested in details is advised to consult these publications.

All the planets except Saturn and Pluto, as well as the satellites of the Earth, Jupiter and Uranus, and the asteroids 1 Ceres and 10 Hygiea have been modelled so far. Assembling the values of the mean atomic masses of all these objects one gets the following tables - which in fact show the spatial distribution of the chemical

Table 1: The chemical composition of the Solar System

object	A
Sun	1.4
Mercury	113
Venus	28.12
Earth	26.56
Mars	69
1 Ceres	96
Jupiter	1.55
Saturn	/
Uranus	6.5
Neptune	7.26
Pluto	/

elements in the planetary system and within the Jovian and Uranian satellite systems (Čelebonović, 2000).

Although Table 1. is incomplete, several physically interesting conclusions can be drawn from it. It shows, for example, that the planetary system is chemically inhomogeneous. The well known qualitative difference between the terrestrial and Jovian planets is reflected in their mean atomic masses. Striking similarities are visible in Table 1; they can be interpreted as consequences of violent events in the early history of the Solar system. It turns out that Ceres and Mercury and Triton and Mars have similar values of the mean atomic mass. As they are at present in widely different regions of the solar system, it is almost certain that they have moved out of regions in which they have been formed. The physical causes of such migrations are at present an open subject of research (for example Kuchner and Lecar, 2002).

Values of gradients of A found in the Jovian and Uranian satellite systems (see Table 2) have been interpreted as a consequence of various transport processes in the respective circumplanetary accretion disks. The values of A found for the Earth and Mars suggest that the Moon is a result of a "deep impact" into the Earth of a body which originated somewhere near the present orbit of Mars. A completely open question is the physical mechanism which provoked this impact. Judging by pure physical "'intuition"' it must have been some sort of a close encounter or direct collision of two bodies in the asteroid belt.

4. What now?

The aim of this lecture was to describe some results in two field of dense matter which have direct applications in astronomy. The choice of the material included was of course subjective - it was conditioned by the author's research experience and by work being performed in the author's laboratory in the Institute of Physics (IoP) in Belgrade.

On of the topics covered is the ruby scale for measurements of pressure in DACs. Although it is widely used, research work is going on with the aim of finding new

Table 2: The chemical composition of some satellites

satellite	A
Moon	71
J1	70
J2	71
J3	18
J4	19
U1	38
U2	43
U3	44
U4	32
U5	32
Triton	67

materials which could be used as pressure sensors. Some work along these lines is going on in IoP ((Jovanić et. al, 1996 and later work). Experiments along these lines could be performed jointly with colleagues from Bulgaria.

At the time of writing of this text (April 2002 in draft form) new results have emerged concerning the behaviour of hydrogen under high pressure (Amer. Inst. of Physics, 2002). They were obtained in the United States, in two big national laboratories:Sandia and Livermore, and concern the compressibility of hydrogen under high pressure. As it could have been expected (by experience with previous research on this topic), the preliminary results are contradictory. These results show once more that the problem of the behaviour of hydrogen under high pressure is far from being solved, in spite of some 60 years of research on the subject. As such, it could be a possible subject for collaboration of physicist and astronomers from Serbia and Bulgaria. Taking into account the experimental facilities needed, it would have to be theoretically oriented.

Another interesting line of research, actively pursued in Belgrade, concerns high pressure metrology. Basically, the problem is to find a replacement for the ruby scale. In view of the experimental equipment which exists both in Serbia (IoP) and Bulgaria (Institute of Solid State Physics), it seems that a fruitful experimental collaboration could be initiated.

Concerning astronomy as such, it would be very interesting to measure optical reflection spectra and the behaviour under high pressure of various materials which enter in the composition of asteroids and planets.

The theory proposed four decades ago by Savić and Kašanin needs a major "modernization". Ongoing work shows that according to modern data Eq. (3) can be replaced by

$$\rho = \frac{7}{5}\exp[\theta] \tag{4}$$

where the exponent θ is non-integer. Details are currently being elaborated, and will be discussed elsewhere.

The list of problems presented here is certainly not exhaustive, which anyhow was not the aim of this contribution. Much simpler, the aim of this lecture was to describe to some extent two basic notions and indicate some open problems, which could form the basis for further collaboration.

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