Atoms and Molecules in Strong External Fields

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Edited by

P. Schmelcher
University of Heidelberg
Heidelberg, Germany

and

W. Schweizer
University of Tübingen
Tübingen, Germany

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PREFACE

This book contains contributions to the 172. WE-Heraeus-Seminar "Atoms and Molecules in Strong External Fields," which took place April 7–11 1997 at the Physikzentrum Bad Honnef (Germany).

The designation "strong fields" applies to external static magnetic, and/or electric fields that are sufficiently intense to cause alterations in the atomic or molecular structure and dynamics. The specific topics treated are the behavior and properties of atoms in strong static fields, the fundamental aspects and electronic structure of molecules in strong magnetic fields, the dynamics and aspects of chaos in highly excited Rydberg atoms in external fields, matter in the atmosphere of astrophysical objects (white dwarfs, neutron stars), and quantum nanostructures in strong magnetic fields. It is obvious that the elaboration of the corresponding properties in these regimes causes the greatest difficulties, and is incomplete even today.

Present-day technology has made it possible for many research groups to study the behavior of matter in strong external fields, both experimentally and theoretically, where the phrase "experimentally" includes the astronomical observations. Understanding these systems requires the development of modern theories and powerful computational techniques. Interdisciplinary collaborations will be helpful and useful in developing more efficient methods to understand these important systems. Hence the idea was to bring together people from different fields like atomic and molecular physics, theoretical chemistry, astrophysics and all those colleagues interested in aspects of few-body systems in external fields.

In combination or individually, the articles present a broad and timely review of the recent progress and the current state of the art in the theoretical, computational, and experimental studies of atoms and molecules in strong external fields. Astrophysical aspects related to magnetic white dwarfs and neutron stars are discussed. The computational problems in the strong field regime where the valence electrons experience electric and magnetic forces of comparable strength are discussed, and some new and effective methods based on discretization and finite element methods as well as novel basis set approaches are presented.

New experiments of Rydberg states in strong external fields are reported and related theoretical and computational aspects as well as the quest of quantum chaos are discussed. Attention is drawn to the non-separability of the center-of-mass for atomic and molecular systems in strong magnetic fields. This non-separability gives rise to effects important in the Rydberg as well as in the astrophysical region. But not only atoms and molecules in strong magnetic fields are reviewed; this book is rounded off by the discussion of quantum dots and shallow donor states in strong magnetic fields.

Due to the scientific importance of the subject we hope that the articles presented in this book will prove valuable to a wide scientific audience, ranging from the experienced researcher to the newcomer. The 172. WE-Heraeus-Seminar brought together about 50 scientists from many countries. As scientific organizers, we wish to thank them for their participation, their presentation, and their enthusiasm, which created a very stimulating and scientifically fruitful atmosphere. We would like to express our thanks to Jutta Hartmann and Dr. Volker Schafer from the WE-Heraeus-Stiftung for the unbureaucratic procedure of funding, general organization and realization, and, of course, to the founders Dr. Wilhelm Heinrich Heraeus and Else Heraeus. We thank the Deutsche Forschungsgemeinschaft for their financial support for the East-European participants.

Tübingen and Heidelberg

W. Schweizer
P. Schmelcher

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WHITE DWARFS FOR PHYSICISTS

Detlev Koester

Institut für Astronomie und Astrophysik, Universität Kiel
D-24098 Kiel, Germany

INTRODUCTION

A small number of white dwarf stars show extremely high magnetic fields, of the order of 10^8 G. This is the only possibility to observe the behavior of the hydrogen atom in such fields, and to compare energy shifts and transition probabilities with the predictions of theory. These strange objects clearly deserve to be a topic at this meeting, and observations of magnetic white dwarfs as well as theoretical interpretations will be presented in a later talk by S. Jordan. This paper is meant as an introduction for the non-specialist. Using extremely simplified models and avoiding astronomical terminology as far as possible, I will attempt to describe what are white dwarfs, where do they come from, and what are the physical conditions we find in them.

These questions are answered by the theory of stellar structure and stellar evolution, and we understand already the most important facts about stellar evolution, if we realize the overwhelming importance of gravitational forces. The life of a star is dominated by a battle between the gravitational attraction of matter, which attempts to compress the stellar matter to higher and higher densities, and the pressure of the gas, which tries to resist this compression. Since stars are losing energy from the surface into interstellar space, an internal energy source is necessary to maintain the pressure, at least as long as the equation of state is given by the ideal gas law, where pressure depends on density *and* temperature. As we know today, these energy sources are nuclear fusion reactions, and a critical phase in the life of a star comes, when the nuclear fuel is exhausted and stellar evolution reaches the final stages. According to theory there are three different possibilities for these end-products: a black hole, which means the ultimate victory of gravitation, a neutron star, where the pressure of degenerate neutrons (modified by nuclear interactions) supplies the pressure independent of temperature, and, finally, white dwarfs, where the pressure is supplied by the degenerate electron gas.

EXTREMELY SIMPLIFIED OVERVIEW OF STELLAR EVOLUTION

Let us start from the beginning, the formation of stars, and a little more quantitatively. We consider a spherical mass of gas, with radial coordinate r measured from

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the center, and m the mass inside a sphere of radius r, dm the mass of a shell between r and $r + dr$. The gravitational force between the sphere and the overlying shell is then

$$F = \frac{G\,m\,dm}{r^2}$$

with gravitational constant G. This force creates an increase of pressure, going inward over a shell dm of

$$dP = \frac{G\,m\,dm}{r^2\,4\pi r^2}.$$

In order to integrate this equation exactly, we would have to know the distribution of matter density $\rho(r)$ inside the sphere. But on dimensional grounds as well as from integrations with simple assumptions (e.g. a homogeneous sphere, $\rho = const$) it is clear that the "gravitational pressure" at the center of the sphere, caused by the "weight" of the matter in the gravitational field, has to be

$$P_{grav} \approx \frac{GM^2}{R^4} \qquad \text{or} \qquad P_{grav} \propto GM^{2/3}\rho_c^{4/3},$$

where M and R are the total mass and radius of the sphere, and for the second form we have used the fact that $\rho_c \propto M/R^3$. The constant of proportionality' in the second expression above is 0.81 for a homogeneous sphere, 0.59 for a quadratic increase of density inward, and always of the order of 1. In our future estimates we will just use 1.

Star formation and early evolution

We can apply this result to study the conditions for the formation of stars out of thin interstellar matter. Considering a spherical cloud of density ρ and temperature T, we estimate that the cloud will start to contract under its own gravity, if at the center the gravitational pressure is larger than the gas pressure

$$GM^{2/3}\rho^{4/3} > \frac{\mathcal{R}}{\mu}\rho T$$

with the gas constant $\mathcal{R}$ and molecular weight μ. A simple calculation determines the minimum mass necessary for this to occur as

$$M > \left[\frac{\mathcal{R}}{G\mu}\right]^{3/2} \rho^{-1/2}T^{3/2},$$

which in astronomy is called the Jeans criterium for star formation. Under typical conditions of the interstellar matter ($\rho = 10^{-24} g\,cm^{-3}, T = 100\,K, \mu = 1$) this corresponds to about 22000 $M_\odot$ (solar masses). Stars are formed in larger groups (clusters) — only when the density gets higher, smaller masses of the order of a solar mass become unstable and the fractionation of the interstellar cloud continues. It should be emphasized again, that this description is extremely simplistic, and that in fact the star formation is rather poorly understood, even by the experts.

What happens next, after the cloud has started to contract, decreasing the radius and increasing the density? That depends on how the two pressures in the balance react to increasing density

$$P_{grav} \propto \rho^{4/3} \qquad \text{and} \qquad P_{gas} \propto \rho T$$

using again the equation of state for an ideal gas. In the beginning the matter is opti-

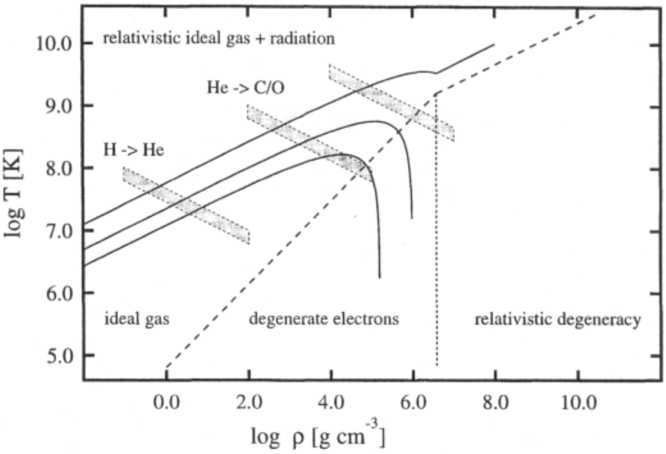

Figure 1. Very schematic evolution of stars with different initial masses in the $T - \rho$ diagram. The path followed by the central parts of the stars is indicated by the continuous lines, from the lower left to upper right. The lower curves correspond to stars with small masses, which, after going through the H- and He-burning stages (shaded areas) reach the domain of electron degeneracy. Here the temperature decreases during the further contraction and the star ends its nuclear life as a white dwarf.

cally thin, meaning that photons can freely escape and carry away the heat produced by contraction and release of gravitational binding energy. The temperature remains approximately constant, and therefore $P_{gas} \propto \rho$. Gravitational forces increase steeper with density and very soon dominate completely over the gas pressure. This leads to a free-fall collapse of the cloud. The timescale for this collapse is the dynamical timescale, which can be estimated in several different ways (for example from the time a sound wave needs to travel the radius of the cloud R). The typical result is always

$$\tau_{dyn} = \frac{1}{\sqrt{G\rho}},$$

which in the case considered means a few million years.

When the density becomes high enough, photons can no longer escape freely and a better model is the opposite extreme of adiabatic changes (no exchange of heat with the outside world). For a monatomic gas (e.g. neutral hydrogen), we then get $P_{gas} \propto \rho^{5/3}$. This is a steeper increase than for the gravitational pressure, and the protostar can find a new hydrostatic equilibrium, where both pressures are in complete balance, $P_{grav} = P_{gas}$.

As the energy loss from the surface continues (called L, the luminosity, by astronomers), the protostar continues to contract, transforming gravitational binding energy into heat, but the evolution is slow and the object always remains extremely close to mechanical equilibrium. Such a phase is called gravitational contraction. The gravitational binding energy of a protostar or star is approximately

$$\Omega \approx -\frac{GM^2}{R} \approx P_{grav} R^3.$$

The release of this energy could supply the luminosity L of a star for a time called the thermal or Kelvin-Helmholtz timescale

$$\tau_{th} \approx \left|\frac{\Omega}{L}\right|$$

which is about 10^7 years for our sun.

Evolution in the density-temperature plane

The key point to understanding the essentials of stellar evolution, and especially the formation of white dwarfs, is the study of the behavior of the central parts in a density-temperature diagram (Fig. 1). Using the hydrostatic equilibrium condition $P_{grav} = P_{gas}$, we find

$$GM^{2/3}\rho^{4/3} = \frac{\mathcal{R}}{\mu}\rho T \longrightarrow T = \frac{G\mu}{\mathcal{R}}M^{2/3}\rho^{1/3}$$

or

$$\log T = \frac{1}{3}\log\rho + \frac{2}{3}\log M + const.$$

The central parts move on a straight line with slope 1/3 in the double-logarithmic diagram, and therefore the temperature increases, until the conditions necessary for "hydrogen burning", the fusion of hydrogen to helium, are reached. This marks the change from protostar to star; nuclear fusion provides so much energy that the star changes very little for several billion years (nuclear timescale). For a star like our sun this is the longest phase in its life.

When finally the hydrogen in the central parts is transformed to helium, the energy generation moves farther out, to a shell around the helium core. This core again starts gravitational contraction, until conditions for He burning are reached. For a massive star, e.g. $15\ M_\odot$, this pattern of nuclear burning and gravitational contraction continues until the central parts consist of the most tightly bound element iron, and no further energy source is available. The interior then collapses to a neutron star or black hole, releasing so much energy in one second that we observe it as a very spectacular event, a supernova.

What is different for less massive stars? According to our condition for gravitational contraction less massive stars evolve at lower temperature and higher density. They eventually reach regions in the $T - \rho$ diagram, where the assumption of a classical ideal gas for the equation of state is no longer valid. The matter in the interior is completely ionized, consisting of the heavy nuclei and electrons. When the electrons are squeezed into a smaller and smaller volume by the overall gravitational forces, they start to feel the effect of the quantum mechanical Pauli principle. Because all low lying states for the momenta are occupied, they are forced into higher and higher states, increasing the pressure (= transfer of momentum) provided by the electron gas. In the extreme case of complete degeneracy, the pressure does not depend anymore on temperature, but only on density as

$$P \propto \rho^{5/3} \qquad \text{or} \qquad P \propto \rho^{4/3}$$

depending on whether the velocities of the electrons are non-relativistic (5/3) or relativistic (4/3). We can estimate the location of the transition region by equating the pressure of the limiting expressions ideal gas, and completely degenerate, non-relativistic electron gas

$$\rho T \propto \rho^{5/3} \longrightarrow T \propto \rho^{1/3}.$$

The slope of this line marking the transition is obviously steeper than the slope of the path during gravitational contraction (2/3), so sooner or later a low-mass star will reach this region.

Once the central parts reach the region of degeneracy, this results in a profound change of evolution. We can understand this qualitatively with a simple approximation to the equation of state in the transition region by taking the sum of both contributions. In the limiting cases this is correct, while in the transition region the error may be a factor of 2, but that is good enough to understand the basic principle. The equilibrium condition becomes

$$GM^{2/3}\rho^{4/3} = \frac{\mathcal{R}}{\mu_0}\rho T + \frac{K_1}{\mu_e^{5/3}}\rho^{5/3},$$

where some new symbols are constants from the exact formulation of the equation of state, but not important for our argument here. The evolution in the $T-\rho$plane is given by

$$T = \frac{GM^{2/3}\mu_0}{\mathcal{R}}\rho^{1/3} - \frac{K_1\mu_0}{\mathcal{R}\mu_e^{5/3}}\rho^{2/3}.$$

The first term is the well known result for the ideal gas, with the temperature increasing with contraction. However, when the region of electron degeneracy is reached, the second term will gradually become more and more important, the central temperature will go through a maximum and then start to *decrease* steeply upon further contraction. This is still a gravitational contraction with some release of gravitational binding energy, but since the star cools down internally, no new nuclear energy source will be reached and this is a final state of evolution. Our current theory predicts that most stars, including our own sun, will reach this stage after the He burning phase. Their interior will then be composed of the ashes of this process, that is carbon and oxygen.

WHITE DWARFS — COOLING HIGHLY DEGENERATE CONFIGURATIONS

The astronomical objects called "white dwarfs" arc identified with these theoretical configurations, which do not reach iron in the sequence of nuclear burning phases, but enter the regime of electron degeneracy (in most cases after the He burning) and then quietly cool down into invisibility. Observationally they were recognized about 90 years ago as stars with normal surface temperatures, but much lower total energy output (luminosity). The only explanation was a small radius, of the order of 1/100 of the solar value. In the case of binary stars, e.g. the famous example of Sirius A and its companion Sirius B the mass was known to be about one solar mass, which meant extremely high densities. This puzzle was only solved in 1926, after the discovery of quantum mechanics and the degenerate electron gas.

Masses, radii, cooling times

Typical parameters of these stars arc masses around 0.6 $M_\odot$ sun, with a rather narrow distribution, although a few stars are known below 0.4 and above 1.0 $M_\odot$. Average densities are then 10^5 to 10^6 $\mathrm{g\,cm^{-3}}$, and typical luminosities around 0.01 $L_\odot$. This luminosity ultimately comes from the change of gravitational binding energy

$$\Delta\Omega \approx \frac{GM^2}{R}\frac{\Delta R}{R}$$

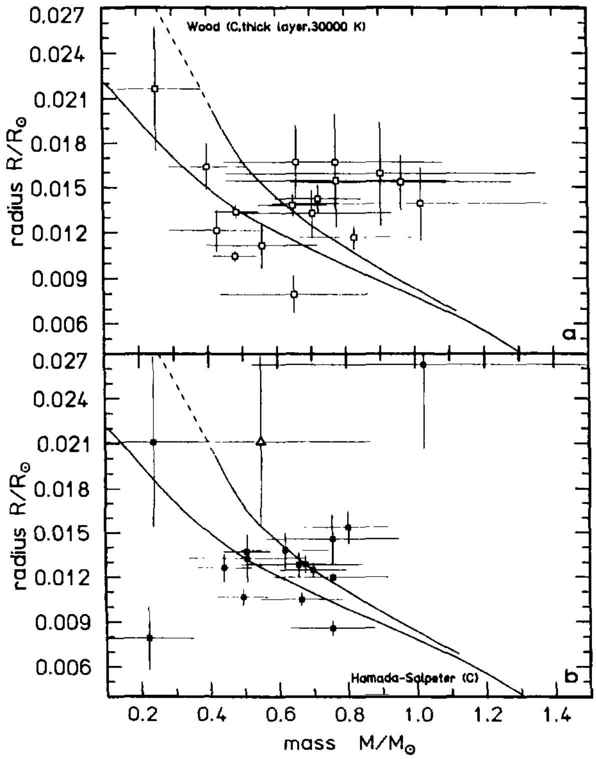

Figure 2. Masses and radii obtained using ground-based distances (top) compared to data derived from the recent HIPPARCOS space mission. The continuous lines are more sophisticated versions of the MRR, including non-ideal effects like Coulomb interactions in the equation of state, and the effect of finite temperatures (non-complete degeneracy). The results generally agree with the theoretical relations (with a few exceptions, which can be understood as perturbation of the measurement by a very close companion star), but due to the clustering of points around 0.6 $M_\odot$ they cannot confirm the detailed shape. From Vauclair et al. (1997)

leading to a cooling timescale of

$$\tau_{cool} \approx \frac{\Delta\Omega}{L} \approx \frac{GM^2}{RL}\frac{\Delta R}{R} \approx 10^{11}\frac{\Delta R}{R} \qquad \text{years.}$$

Even a very small change in R is sufficient to supply the luminosity of a white dwarf for billions of years; this is another long-lived phase for low-mass stars.

The best-known fact about the physics of white dwarfs is probably the existence of a mass-radius relation (MRR) and of a limiting mass. We can understand this qualitatively using the same argumentation as before for the mechanical equilibrium, but now using the equation of state for the degenerate electron gas and the form including the radius instead of density

$$\frac{GM^2}{R^4} \propto \rho_c^{5/3} \propto \left(\frac{M}{R^3}\right)^{5/3} \propto \frac{M^{5/3}}{R^5}.$$

This leads to a relation $R \propto M^{-1/3}$, valid for non-relativistic electrons, that is low-mass white dwarfs. The radius decreases with increasing mass and increasing central density.

When the electrons become relativistic, we have

$$\frac{GM^2}{R^4} \propto \rho_c^{4/3} \propto \frac{M^{4/3}}{R^4},$$

and equilibrium is now possible for one single mass only, but arbitrary radius. This is, however, not a stable equilibrium; a small perturbation would either lead to a collapse to infinite density at radius zero, or to an expansion. In such an expansion the electrons in the outer parts will become non-relativistic and a stable equilibrium is possible. The single solution for the mass in the ultra-relativistic case is the critical, or Chandrasekhar mass. It is the upper limit for white dwarf masses, and for an interior composition of carbon or oxygen its value is 1.4 $M_\odot$.

Although this MRR and the limiting mass are firmly established theoretically, the empirical evidence is still not very convincing. The most important reasons are that the observed white dwarfs seem to cluster around 0.6 $M_\odot$, making it difficult to establish the relation for small and large masses, and the difficulty to measure distances to these objects, which are necessary for the determination of masses and radii. In recent years the European Space Agency ESA has used the satellite HIPPARCOS, to measure accurate distances to a large number of stars, including about 20 white dwarfs. Fig. 2 shows the results for the MRR obtained with these new data, compared to the use of ground-based measurements only. Because the white dwarfs are very faint, the improvement is not as obvious as for other, brighter stars. The general agreement with the theoretical calculations is considered satisfactory, although the observations certainly do not prove the detailed shape of the relation, nor distinguish between different versions for slight differences in the internal structure of white dwarfs.

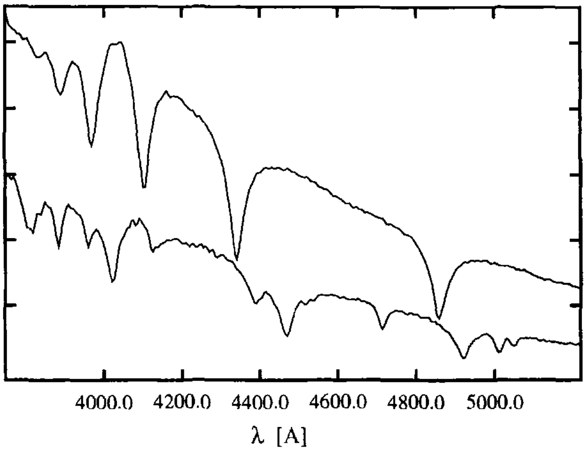

Figure 3. Optical spectra of typical DA (upper curve, Balmer lines of hydrogen only) and DB (lower curve, HeI lines only). Vertical axis is intensity in arbitrary units.

Observable Atmospheres

Directly observable are only the atmospheres, the outermost layers of white dwarfs, which are accessible to photometry (measuring brightness through different filters) and spectroscopy. From the observed spectra we distinguish two main spectral groups of white dwarfs. By far the largest subgroup ($\approx 80\%$) shows only spectral lines of hydrogen; this is the type DA, and the surface layers consist indeed of extremely pure hydrogen. On the other hand, in the remaining 20 %, the atmospheres are almost pure helium and show only spectral lines of neutral or ionized helium (spectral types DB, DO, + some smaller groups). Fig. 3 shows typical representatives of these two spectral groups; the most apparent features are extremely broad lines (broadened by pressure broadening) due to either hydrogen (DA) or helium (DB). These mono-elemental compositions are unknown in any other object in the universe; the basic explanation for this is "gravitational separation", an effect known since almost 50 years. In the strong gravitational fields on the surfaces of these stars the heavy elements sink down, leaving the lightest element present floating on top. The physical process is element diffusion, and it seems to work efficiently in white dwarfs, because there are no other velocity fields (due to convection, circulation, stellar winds) to disturb it.

Of the few white dwarfs with very strong magnetic fields, all objects with identified features belong to the DA class. Whether this is a selection effect due to small numbers, or whether helium is responsible for some objects with unidentified features, is currently unknown, and will probably only be understood, when calculations for He in extreme fields become available.

This concludes our journey from interstellar matter to the surfaces of magnetic white dwarfs. White dwarfs are very interesting objects from an astronomical point of view, since they are the most common end-product of stellar evolution, and since they offer the opportunity to study important astrophysical processes as convection, diffusion, pulsation, accretion. But they are also fascinating for a physicist, because they offer conditions that cannot, or not easily be achieved in terrestrial laboratories. We can study macroscopic effects of quantum mechanics with the equation of state, various aspects of line broadening theories, and, finally, the effect of extremely strong magnetic fields on atoms, which is the topic of this meeting. In the spirit of this very elementary physical discussion 1 have given almost no references in the text; however, for the reader interested in more of the physical or astronomical details I include below a few review papers and the most relevant recent conference proceedings.

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MAGNETIC WHITE DWARFS: OBSERVATIONS IN COSMIC LABORATORIES

Stefan Jordan

Institut für Astronomié und Astrophysik, Universität Kiel
D-24098 Kiel, Germany

INTRODUCTION

Magnetic white dwarfs are the only known physical system in which the behaviour of spectral lines, especially of hydrogen, in the presence of very strong magnetic fields (up to 10^9 G) can directly be studied. Presently, the analysis of the radiation from neutron stars is much more complicated and less unique. As discussed in the paper by Detlev Koester (this conference) the atmospheres of white dwarfs (i.e. the layers in which the observed radiation originates) are often of very simple chemical composition (almost pure hydrogen or helium); the reason is element separation due to the strong gravitational accelaration of about $g = 10^8\,\mathrm{cm\,sec^{-2}}$. Therefore the shifted line components of hydrogen and helium can be observed, often without taking into account a complicated mixture of different elements.

MAGNETIC FIELD ON STARS

Magnetic fields have been measured in many different types of stars. For obvious reasons the first star on which magnetic fields could be detected was the sun on which Hale (1908) observed the magnetic splitting of spectral lines in sunspots. The solar magnetic field is quite complex and mostly concentrated in magnetic flux tubes with field strengths of a few kG. Babcock (1947) discovered a large ($\approx 1500\,\mathrm{G}$) and variable magnetic field on 78 Vir. With spectral type A1 p this star belongs to the peculiar A and B main sequence stars (hot stars, burning hydrogen to helium in their center) on which magnetic fields up to 16 kG have been found (Landstreet 1992). It was not until 1980 when Robinson et al. discovered magnetic fields of about 2000 G on limited parts ($\approx 10\%$) of the stellar surface of cooler main sequence stars (spectral type G and K).

MAGNETIC FIELD ON WHITE DWARFS

Blackett (1947) predicted that much stronger magnetic fields ($\approx 1\,\mathrm{MG}$) could exist in white dwarfs if the magnetic moment of a star is proportional to its angular momentum,

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which he assumed to be conserved during the stellar evolution and the collapse. This is, however, probably not the case since most isolated white dwarfs seem to be relatively slow rotators ($v \lesssim 40\,\mathrm{km/sec}$, e.g. Koester & Herrero 1988, Heber et al. 1997), although a few exceptions from this rule exist (e.g. REJ 0317-853, see below). The fact that white dwarfs are typically slow rotators is rather surprising since most of the known white dwarfs stem from progenitors with masses $> 1.5\ M_\odot$ which had typical rotational velocities of $v_{rot} \approx 100\,\mathrm{km/sec}$; if angular momentum is completely conserved during the evolution we would expect the white dwarf remnant to have $v_{rot} \approx 10,000\,\mathrm{km/sec}$.

Another possibility was proposed by Ginzburg (1964) and Woltjer (1964). They argued that if the magnetic flux, which is proportional to BR^2, is conserved during evolution and collapse, very strong magnetic fields can be reached in degenerate stars. A main sequence star with a radius $R \approx 10^{11}\,\mathrm{cm}$ and a surface magnetic field of 1-10 kG can therefore become a white dwarf ($R \approx 10^9\,\mathrm{cm}$) with a magnetic field strength of $10^7 - 10^8$ G.

The search for magnetic white dwarfs began in 1970 when Preston looked for quadratic Zeeman shifts in the spectra of DA white dwarfs. Due to the extremely strongly Stark broadned Balmer lines and the limited spectral resolution he was only able to place upper limits of about 0.5 MG for the magnetic fields in several white dwarfs.

A rather sensitive method to detect magnetic fields in white dwarfs is the measurement of circular polarization. Kemp (1970) proposed that a field of $10^6 - 10^7$ G would produce detectable circular polarization due to circular dichroism, caused by different free-free opacities for the ordinary and extraordinary mode of radiative propagation. After his failure to find polarization in DA white dwarfs he applied his method to several of the almost featureless white dwarfs (classified as DC). In Grw +70°8247, an object that was known for its rather shallow and unidentified "Minkowski bands" (Minkowski 1938, Greenstein 1956, Wegner 1971), he detected circular polarization of several percent. With the help of a magnetoemission model he derived a magnetic field strength of 10 MG, although the circular polarization was not proportional to the wavelength as predicted by Kemp's model. Later his value for the magnetic field strength turned out to be much too low (due to the fact that the free-free opacity is not the dominating absorption process in Grw +70°8247); his idea that the strange spectrum of Grw +70°8247 can be explained by a strong magnetic field was, however, correct. Nevertheless, all attempts to identify the Minkowski bands with various atoms or molecules in magnetic fields of a few MG failed.

Even for the simplest atoms, hydrogen and helium, accurate calculations for the line components did not exist at that time for field strengths above 20-100 MG (depending on the line transitions, Kemic 1974a, 1974b); only for extremely intense fields ($10^9 - 10^{10}$ G) data were available again (Garstang 1977), but none of the predicted line positions were in agreement with the wavelengths of the Grw +70°8247 features. For this reason Angel (1979) proposed that the star must possess a field strength above 100MG (but below the intense-field regime).

For hydrogen the intermediate-field gap has been closed partly during the last twelve years with numerical calculations of energy level shifts and transition probabilities for bound-bound transitions by groups in Tübingen and Baton Rouge (Forster et al. 1984; Rösner et al. 1984; Henry and O'Connell 1984, 1985).

Since the magnetic field on the surface of a white dwarf normally is not homogeneous but often better described by a magnetic dipole, the variation of the field strengths from the pole to the equator (a factor of two in the case of a pure dipole field) smears out most of the absorption lines; this explains why the spectral features

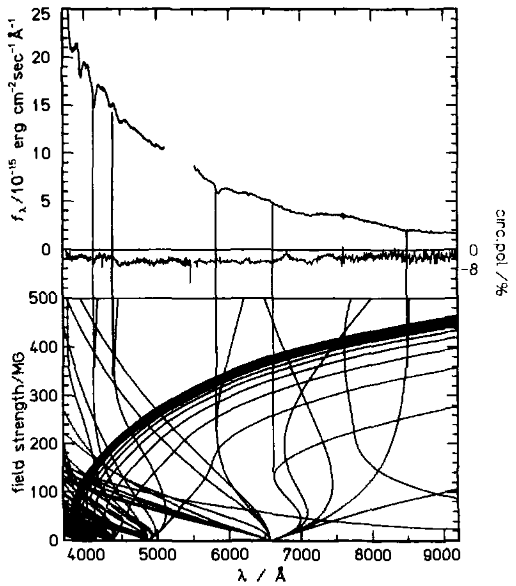

Figure 1. Spectrum and circular polarization of Grw +70°8247 (Obs. A. Putney). The star has a magnetic dipole with a polar field strength of about 320 MG (Wickramasinghe & Ferrario 1988, Jordan 1988). The variation of the wavelengths of the line components of hydrogen with magnetic field strength is indicated below. Some of the stronger features can be identified with stationary line components of hydrogen, others are a superposition of components which vary only moderately between about 160 and 320 MG

on Grw +70°8247 are so shallow for strong magnetic fields. However, a few of the line components become stationary, i.e. their wavelengths go through maxima or minima as functions of the magnetic field strength. These stationary components are visible in the spectra of magnetic white dwarfs despite a considerable variation of the field strengths.

It was a great confirmation for the correctness of the theoretical calculations that indeed the unidentified features in the optical and UV spectrum of Grw +70°8247 could be attributed to stationary components of hydrogen in fields between about 150 and 500 MG (Greenstein 1984, Greenstein et al. 1985, Angel et al. 1985, Wunner et al. 1985, cf. Fig. 1).

These identifications allowed an estimation of the approximate range of field strengths covering the stellar surface. However, the detailed field structure could not be inferred. This was only possible by simulating the radiative transfer through magnetized stellar atmospheres using the line opacities published by the groups in Baton Rouge and Tübingen. Wickramasinghe & Ferrario (1988) have obtained a good fit to most of the Minkowski bands by assuming a pure dipole model with a polar field strength of 320 MG. This result was confirmed by Jordan (1988; 1989) who used more recent atomic data and made improvements to the treatment of the bound-free opacities.

Up to now on about 50 (2%) of the 2100 known white dwarfs (McCook & Sion 1996) magnetic fields have been detected with fields ranging from about 40 kG up to 1 GG. A list of all currently known magnetic white dwarfs is found in Jordan (1997). Although some selection effects may exist (e.g. shallow features are not easily recognized in faint stars) we believe that the number statistics is consistent with the assumption that Ap stars are the progenitors of magnetic white dwarfs, in which the field strengths are enhanced by magnetic flux conservation during the evolution.

The goal of magnetic white dwarf spectroscopy is to determine the field strength, the detailed geometry of the magnetic field, and the rotational period of the star (which is very difficult to measure in non-magnetic white dwarfs). The results provide important constraints for the theory of the origin of magnetic white dwarfs.

MODELS FOR THE RADIATIVE TRANSFER

The spectrum and polarization of a magnetic white dwarf is the superposition of the radiation originating from all different parts of the visible hemisphere of a white dwarf (which may vary due to rotation). Observations of the spectra and wavelength dependent polarization can be analyzed by simulating the transport of polarized radiation through a magnetized stellar atmosphere. The methods for the calculations of synthetic spectra and the wavelength dependent linear and circular polarization are described by Jordan (1988, 1992). The basis is the solution of the four coupled radiative transfer equations (Beckers 1969) for the four Stokes parameters which describe the intensity and polarization of the radiation. With the help of the atomic data the absorption coefficients for $\Delta m = -1, 0$, and $+1$ and the magneto-optical parameters for Faraday rotation and Voigt effect are calculated for a given magnetic field strength and orientation. With these values the radiative transfer equations are solved for the temperature and pressure structure of a (currently zero-field) white dwarf model atmosphere.

For the line data of hydrogen we use the data from the Tübingen group (Forster et al. 1984, Rösner et al. 1984, Wunner et al. 1985). For the bound-free opacities either a simple and probably unrealistic approximation (Lamb & Sutherland 1974) with some improvements by Jordan (1988, 1992) is used or complex energy eigenvalues and dipole matrix elements calculated by Merani et al. (1995) were utilized in order to study the influence of the bound-free opacities on the polarization (Jordan & Merani 1995).

The magnetic field configuration cannot be derrived from the observed flux and polarization in a unique way by a simple inversion process, since different magnetic geometries can in principle lead to the same observational data. The current strategy is to assume that the global field can be described by a magnetic dipole, which does not necessarily need to be located in the center of the star, or by a dipole+quadrupole combination. In principle higher order multipoles could be included, but this would increase the number of fit parameters. After the magnetic geometry has been fixed, the stellar surface is divided into a large number (typically 1000-10 000) of surface elements on which the radiative transfer equation are calculated. Finally, the Stokes parameters are added up according to the projected size of the surface elements.

RESULTS OF THE ANALYSES

The main result of the analyses of magnetic white dwarfs is that many spectra and polarization measurements can be sucessfully reproduced with our models. In order to do so it is, however, often necessary to assume off-centered dipoles or dipole+quadrupole configurations for the magnetic field geometry (e.g. Putney & Jordan 1995, see Fig. 2). One important questions is, how the higher order multipoles of the magnetic field can survive during the cooling time of a white dwarf.

Chanmugam & Gabriel (1972) and Fontaine et al. (1973) have calculated the time scale for the decay of magnetic fields of white dwarfs. They showed that the decay