Diffusion coefficients in white dwarfs

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Abstract. Models of diffusion in white dwarfs universally rely on the coefficients calculated by Paquette et al. (1986). We present new calculations of diffusion coefficients based on an advanced microscopic theory of dense plasmas and a numerical simulation approach that intrinsically accounts for multiple collisions. Our method is validated against a state-of-the-art method and we present results for the diffusion of carbon ions in a helium plasma.

1. Introduction

The spectral type, atmospheric composition, and spectral evolution of white dwarfs (WDs) is largely determined by the diffusion of elements in the envelope of the star. Modern models of WDs universally rely on the diffusion coefficients of Paquette et al. (1986). Advances in the theory of dense plasmas and in computational capabilities in the last three decades motivate a re-evaluation of the coefficient of ionic diffusion in WD envelopes, particularly under physical conditions that are challenging to model. Our physical model and computational approach are very different from those of Paquette et al. (1986). We have developed a new microscopic model of dense, partially ionized, multi-component plasmas. When combined with a molecular dynamics simulation of the ions in the plasma mixture, the diffusion coefficient can be evaluated. We discuss our model and methods and contrast them with the approach of Paquette et al. (1986). Finally, we present our first calculation of the diffusion coefficient in WDs for a mixture of carbon and helium.

1.1. Microscopic model for dense plasmas

Starrett & Saumon (2013) and Starrett & Saumon (2014) describe a detailed and realistic microscopic model for dense, partially ionized, multi-component plasmas that accounts for strong interactions between ions, partial electron degeneracy, bound states, pressure ionization, and non-linear electron screening. For clarity of the following discussion, we will consider a plasma consisting of a single species of ions and free electrons although the model can describe a mixture of species equally well (Starrett et al. 2014). The model consist of two main elements which are coupled. First the ions are modeled within the framework of an average atom model. This assumes that all ions in the plasma are identical and imposes spherical symmetry on the distribution of bound and free electrons around the nucleus. The electronic states (bound and free) are obtained by solving the Schrödinger (or Thomas-Fermi) equation within the density functional formalism. The potential in which the electrons evolve accounts for the central nucleus, the other electrons belonging to the ion, and the distribution of other
charges in the surrounding plasma. Thus non-ideal effects on the electronic structure of the ion (such as pressure ionization) are naturally included. This part of the model provides the average ion charge and the distribution of the continuum electrons around the ion (the screening cloud of electrons). The second part of the model uses those two quantities to calculate the structure of the surrounding plasma. In the dense plasmas found in WDs, the ion-ion interactions can be very strong. While the fluid is disordered, the positions of the particles are not random but correlated. The statistical average of the relative positions of particles in the plasma is described by correlation functions that are calculated with the integral equations formalism of fluid theory. This in turn provides the external plasma distribution needed to solve the Schrödinger equation of the average atom. A consistent solution of the two coupled parts of the model is obtained by numerical iteration and provides the ion-ion interaction potential to be used in molecular dynamics simulations (see below). This model is physically self-consistent and has no adjustable parameters.

1.2. Evaluation of the diffusion coefficient

All the equations describing the above plasma model are time independent. On the other hand, diffusion is an inherently dynamic process that describes how a particle drifts from an initial position. For the purpose of evaluating the coefficient of ionic diffusion, we resort to the numerical simulation method of molecular dynamics (MD, Allen & Tidesley (1989)). In a MD simulation, a fluid of classical particles interacting with a pair potential at a given density and temperature is represented by \( N \) particles (typically a few thousands) in a cubic box of fixed volume. After the position and velocity of each particle in the box have been initialized, the total force on each particle is calculated from the sum of the pair interactions. The position and velocity of each particle are updated by integrating Newton’s law \( F = ma \) over a small time step. The forces are then recalculated. This simple scheme is repeated to let the system evolve in time. The diffusion coefficient can be evaluated from the trajectories of the particles in the simulation. An infinite system is approximated by using periodic boundary conditions at the surface of the box.

At the microscopic level, diffusion describes the drift in the position of a particle from its initial position due to its thermal motion and collisions with other particles. From the particle’s trajectory \( \vec{r}(t) \), the coefficient of self-diffusion is expressed as (Hansen & McDonald 1986)

\[
D = \lim_{t \to \infty} \frac{1}{6t} \langle (\vec{r}(t) - \vec{r}(0))^2 \rangle \tag{1}
\]

where \( \vec{r}(0) \) is its initial position and \( <> \) represent the thermal average over all particles in the simulation. Equation (1) says that after a large number of collisions, the particle has traveled a distance that is proportional to \( \sqrt{t} \) (the well-known random walk result), and that the proportionality constant is six times the diffusion coefficient. For a plasma of two species, which is of interest in WDs, the coefficient of inter-diffusion can be obtained from \( D_{12} = J(x_2 D_1 + x_1 D_2) \), where \( D_i \) is the self-diffusion coefficient of species \( i \), \( x_i \) is its number fraction (\( x_2 = 1 - x_1 \)), and \( J \) is the so-called thermodynamic factor (Hansen, Joly & McDonald 1985). For ideal gases and for trace diffusion (\( x_1 \to 0 \)), \( J = 1 \). Otherwise, our calculations show that \( J \) can be as large as 1.5. This expression for \( D_{12} \) is an approximation that neglects cross-correlation terms. It has been shown to be fairly accurate to a few percent for some systems (Hansen, Joly & McDonald 1985).
1985; Daligault 2012) but should to be re-evaluated for the conditions of interest here (Haxhimali et al. 2014).

### 1.3. Comparison with the approach of Paquette et al. (1986)

Our approach to evaluate the coefficient of inter-diffusion in WDs is compared with that of Paquette et al. (1986) in Table 1. For the diffusion of a trace element (Ca, for example) in a plasma dominated by one species (typically H or He), the most significant advantages of our calculation are 1) the ion-ion potential is calculated from a microscopic model of the plasma and does not have an assumed functional form, 2) the use of MD to evaluate the diffusion coefficient, which is not limited to low densities, and 3) the self-consistency of the approach that uses a single model to generate the EOS and the diffusion coefficients. Furthermore, for non-dilute mixtures our approach properly accounts for the thermodynamic factor $J$.

| Assumption / Approximation | Paquette et al. (1986) | This work |
|----------------------------|-----------------------|-----------|
| Equation of state (EOS)    | Ideal gas             | Fully non-ideal |
| Order of the collisions    | 2-body collisions only | N-body collisions |
| Ion-ion pair potential     | Static screened Coulomb “Debye-Hückel” | self-consistent with plasma model |
| Diffusion coefficient      | Collision integrals (theory for dilute gases) | Molecular dynamics (valid for dense fluids) |
| Thermodynamic factor ($J$) | $J = 1$               | From non-ideal EOS |

### 1.4. Accuracy and application to carbon/helium plasmas in white dwarfs

The diffusion of C in He at the core/envelope interface and its dredge up by the He convection zone is responsible for the presence of C in the spectra of DQ WDs (Pelletier et al. 1986). A change in the diffusion coefficient would affect the quantitative modeling of this process and estimates of the mass of the He layer in DQ stars.

Thomas-Fermi Molecular Dynamics (TFMD, Zérah, Cléroul & Pollock (1992)) is a state-of-the-art method for simulating hot, dense plasmas. It explicitly accounts for the electrons of the plasma (with the Thomas-Fermi model) and the nuclei with a minimal set of approximations. TFMD is more accurate than the present model but is computationally too expensive to generate large tables of diffusion coefficients. A comparison with TFMD validates our calculations of $D_{12}$ for C/He mixtures over a wide range of conditions to better than 5% (Fig. 1). Along a WD envelope profile, our diffusion coefficients for C/He are in excellent agreement with those of Paquette et al. (1986) at depth ($\log T > 6.4$ or $\log q > -6.9$) but are up to factors of 3 larger in the upper envelope (Fig. 1).

### 1.5. Conclusions

We have developed a realistic model of the plasmas found in the envelopes of WDs that provides a self-consistent description of the equation of state and diffusion coefficients.
Figure 1.  Left: Solid curve: Envelope profile of a DB WD model ($T_{\text{eff}} = 20000$ K, $\log g = 8$). Dots show the points where we validated our approach against TFMD simulations. Right: Comparison of the diffusion coefficient of a trace of C in He with Paquette et al. (1986) along the profile shown in the left panel. Error bars are estimates of the uncertainty in our calculation ($\pm 5\%$).

Our approach relaxes several of the approximations of Paquette et al. (1986) that are not well justified in WD envelopes. Our initial results for inter-diffusion in C/He mixtures show that our calculations of the diffusion coefficient are accurate to better than 5%. Along a model envelope of a WD, we find excellent agreement with Paquette et al. (1986) at depth but large deviations in the upper envelope of up to a factor of three.

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