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Radiative Transfer in Molecular Clouds

M. Juvela

Department of Physics, FI-00014 University of Helsinki, Finland

Abstract. Information of astronomical objects is obtained mainly through their radiation. Thus, the radiative transfer problem has a central role in all astrophysical research. Basic radiative transfer analysis or more complex modeling is needed both to interpret observations and to make predictions on the basis of numerical models. In this paper I will discuss radiative transfer in the context of interstellar molecular clouds where the main scientific questions involve the structure and evolution of the clouds and the star formation process. The studies rely on the analysis of spectral line and dust continuum observations. After a discussion of the corresponding radiative transfer methods, I will examine some of the current challenges in the field. Finally, I will present three studies where radiative transfer modeling pays a central role: the polarized dust emission, the Zeeman effect in emission lines, and the continuum emission from dense cloud cores.

Keywords. radiative transfer, ISM: clouds, ISM: lines and bands, ISM: molecules, dust, infrared: ISM, radio lines: ISM

1. Introduction

The radiative transfer problem includes both the formation and transport of radiation. Because the radiation field affects the way the medium emits, one must know the radiation field to calculate the emission and vice versa. All parts of an interstellar cloud can interact with each other through radiation and, when optical depths are high, a self-consistent solution may require a lengthy iterative process. This makes the radiative transfer problem hard and computationally demanding.

Interstellar dust interacts with radiation through absorption, emission, and scattering. Monte Carlo (MC) still remains the most common tool for these calculations. After the simulation of the radiation field, the dust temperatures are solved for and, if necessary, the process is repeated until convergence is reached. When small grains are included the calculation of their stochastic heating becomes the dominant cost that limits the size of the models that can be handled. With radiative transfer modeling one can obtain a possible although usually not a unique solution for the cloud structure, the dust properties, and the strength of radiation sources. It is the only way to reliably study more complex phenomena like the spatial variations of dust grain properties.

Line transfer is different in two respects. Firstly, the calculations need to resolve the line profiles and consider the effect of doppler shifts. Secondly, the scattering (induced emission excluded) can usually be ignored so that it is enough to solve the radiative transfer equation along a fixed set of lines. Monte Carlo is often used although non-random ray-tracing methods should be more efficient. Compared to the continuum case, the need for fine discretization of the line profiles tends to make the calculations more time consuming. A large number of energy levels also means large memory requirements that can limit the spatial resolution of the models. The fractional abundances of the studied species are a crucial and often a poorly known parameter. Conversely, radiative transfer modeling of observations is the best way to estimate the abundances and, at the same time, to draw conclusions on the structure and kinematics of the clouds.

2. Radiative transfer methods

I will present a brief review of radiative transfer methods. This is in part biased towards MC methods and the reader is advised to look up the references for a broader view.

2.1. *Methods for continuum radiative transfer*

The Monte Carlo (MC) method simulates actual processes in a cloud: Photons are emitted at random locations (but weighted according to the real emission) and interact with the medium at random positions (but in accordance with the optical depths). This makes MC intuitive and easy to implement, even in the case of arbitrary scattering functions. MC was used already in the 1970's to study the scattering in interstellar clouds (Mattila 1970, Witt 1977) and later also to calculate dust emission (e.g. Bernard *et al.* 1992). Although spherically symmetric models are still used, 2D and 3D models have become common during the past decade (e.g., Wood *et al.* 1998, Dullemond & Turolla 2000, Juvela & Padoan 2003, Pascucci *et al.* 2004). When the radiation field is sampled with random numbers, the noise decreases slowly, $\sim 1/\sqrt{N}$, as the number of photon packages increases. The efficiency can be improved in many ways. When calculating images of scattered light, the method of forced first scattering guarantees that every photon package scatters at least once (Mattila 1970) and the peel-off scheme (Yusef-Zadeh *et al.* 1984) reduces the noise further by registering a contribution from every scattering. In dust temperature calculations, the noise can be decreased by calculating the absorptions explicitly along the photon path (Lucy 1999). Weighting can be applied to the spatial, angular, and spectral distribution of the packages (Watson & Henney 2001, Juvela 2005, Jonsson 2006). For example, in a spherically symmetric model the innermost shells are rarely hit by any of photon packages unless weighted sampling is used. If the same number of packages representing background photons is sent towards each annulus defined by the spatial discretization, the reduced randomness may even lead to a convergence of $\sim 1/N$. Similar improvement can in some cases be obtained with the use of quasi random numbers. Spatial weighting can also be a solution to sampling problems caused by high optical depths. By creating photon packages preferentially close to cell boundaries, one can guarantee that a fixed fraction of the packages crosses the cell boundary and radiative couplings can be determined for any optical depth (Juvela 2005).

When dust emission has a significant contribution to the radiation field, iterations are needed between the radiative transfer and the re-evaluation of dust temperatures. In optically thin clouds this is not necessary but optically thick dust shells around (proto)stars may require hundreds of iterations. The convergence can be improved by the use of the accelerated MC (AMC) methods (Juvela 2005), sometimes by orders of magnitude. During the iterations only the emission from the medium needs repeated simulation. All the other components of the radiation field can be included as a fixed reference field. When also the dust emission is included in the reference field, simulations are used only to make small corrections to the previously estimated field. As a result, the sampling noise is smaller and is further reduced as the iterations progress (Juvela 2005).

A completely new Monte Carlo scheme was presented by Bjorkman & Wood (2001). In this 'immediate re-emission' method a photon package is initiated in a radiation source. When the package is absorbed, the local temperature is updated and a package is re-emitted from the same location. The package is generated according to a probability distribution that reflects the change in the local SED. The generation of packages follows the natural flow of energy and the method provides automatic weighted sampling. In basic MC, a large number of packages is simulated before the temperatures of all cells are updated at the same time. The immediate re-emission mechanism requires one

temperature update after each interaction but, in the case of grains at an equilibrium temperature, the method is quite competitive with the traditional MC even when the latter is enhanced with weighted sampling, AMC, and the use of a reference field (see Juvela 2005). The situation can change if the cost of temperature updates is increased, for example, by the inclusion of several grain populations, grain size distributions, or stochastically heated grains.

In MC the scattering function is taken into account in a statistical way by drawing scattering angles from the appropriate probability distribution. If the angle is discretized, non-stochastic methods can be used with the expense of somewhat larger memory requirements. Examples of such codes can be found in Steinacker *et al.* (2003), Semionov & Vansevičius (2005), and Ritzerveld & Icke (2006) (see also Pascucci *et al.* 2004 and Steinacker in this volume).

2.2. *Line transfer methods*

In line transfer it is usually enough to solve absorption, emission, and stimulated emission along straight rays, ignoring general scattering processes. However, the optical depths are often high so that the solution needs iterations between the estimation of the radiation field and updates of the level populations.

In Monte Carlo the locations and directions of the rays are selected randomly. The first implementations were made in the 1960s but the history of many of the current codes can be traced back to the paper of Bernes (1979). Bernes employed a fixed reference field to reduce the Monte Carlo noise. Choi *et al.* (1995) introduced an adaptive version where, as iterations progress, the reference field approaches the true field. Other improvements included the handling of overlapping lines (Gonzáles-Alfonso & Cenicharo 1993) and the explicit handling of emission and absorption along the rays (Juvela 1997). The first 3D implementations were also made already in 1990's (Park & Hong 1995, Juvela 1997).

Although the $1/\sqrt{N}$ convergence of Monte Carlo could be improved by using quasi random numbers, it is equally easy to implement a regular grid of rays. In such 'ray-tracing codes' one usually follows intensity instead of photon numbers. In the short characteristic method, the intensity is propagated one layer of cells at a time and interpolation is used to derive the values at exact grid positions (e.g., Kunasz & Auer 1988, Auer & Paletou 1994). Long characteristics are continuous rays from the cloud boundary to a cell. They avoid diffusing the radiation field but cause some duplication of calculations. The ray tracing codes estimate the intensity at grid positions while the Monte Carlo versions estimate an average quantity for a cell volume. By adopting the latter approach, the grid of rays becomes independent of the spatial discretization and the local intensity can be estimated with any rays that cross a cell. The result is essentially a long characteristic method without the need for redundant work (Juvela & Padoan 2005).

The similarity of Monte Carlo and ray tracing codes is evident also by looking at the methods used to accelerate the convergence. If emitted photons are absorbed locally, the flow of energy between cells becomes small. This is reflected in the iterations as slow convergence. The core saturation method improves the situation by a specific handling of the optically thick part of the line. The method that was originally developed by Rybicki 1972 was first implemented in the Monte Carlo context by Hartstein & Liseau (1998). In accelerated Λ-iteration (ALI) one explicitly takes into account the emission-absorption cycle within each cell (diagonal Λ operator) or even the radiative couplings between neighboring cells (Scharmer 1981, Olson *et al.* 1986). On the Monte Carlo side the term Accelerated Monte Carlo (AMC) is used for essentially identical methods (Juvela & Padoan 1999; Hogerheijde & van der Tak 2000).

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3. Current challenges

Better integration with models of other physical processes and the quest for higher spatial resolution through the use of adaptive grids are some of the current challenges in the radiative transfer modeling.

3.1. *Models of chemistry and interstellar dust*

A complete model of an interstellar cloud should include self-consistent calculations of cloud dynamics, thermal equilibrium, and chemistry. Molecular clouds are cooled through atomic and molecular emission lines and dust continuum emission and, with the exception of the densest cores, heated mainly through the photoelectric effect. Therefore, radiative transfer plays a central core in the thermal balance. Similarly, the chemical photo-reaction rates can be estimated only if the radiation field is known.

The chemical abundances are a major source of uncertainty for a quantitative analysis of line observations. The abundances can vary by orders of magnitude and depend on many parameters like the density, the temperature, and the local radiation field. The large spread in the time constants of the chemical reactions means that a chemical equilibrium may be reached only after several million years. In a dynamic environment the equilibrium is never attained and the prediction of line emission would require the tracing of the chemical history of each gas element. In the setting of turbulent clouds, the dissipation of turbulent energy may produce very localized abundance variations for species like HCO+ (Falgarone *et al.* 2006) while even for the most important observational tracer molecule, CO, the time dependence leads to a large scatter in the abundances found for given density and temperature (Glover *et al.* 2010). These could affect our view of the large scale statistics of the density and velocity fields and need to be studied further, also with high resolution simulations.

In dense regions of the clouds, depletion poses additional problems. For CO, the complementarity of the gas phase phase and solid state abundances has been demonstrated (e.g. Whittet *et al.* 2010) but the general modeling of the depletion process still contains many uncertainties. This is particularly relevant for pre-stellar cores where the depletion is eventually almost complete for most of the commonly observed species and where the depletion time scales are not very different from those of the dynamic core evolution. Although some emission lines can be observed towards even the coldest of cores (e.g., H_2D+, N_2H+, and ammonia) one cannot be quite sure how they probe the different regions of the cores (see, e.g., Walmsley *et al.* 2004; Sipilä *et al.* 2010). This makes it difficult to draw definite conclusions even on the basic core kinematics.

In the case of dust, dense cores are again associated with the strongest effects with an almost complete disappearance of small grains, the accumulation of ice mantles, and the possible formation of fluffy, very large grains (e.g., Ossenkopf & Henning 1994, Stepnik *et al.* 2003). These are used to explain the variations in the ratio of mid-infrared and far-infrared emission and the sub-millimeter emissivity that, at least in some dense clouds, appear to have increased several fold (Bernard *et al.* 1999, Lehtinen *et al.* 2007). The temperature dependence of the spectral index (e.g., Dupac *et al.* 2003) has also been seen in laboratory measurements (Boudet *et al.* 2005) and can be explained by properties of the grain material itself (Meny *et al.* 2007). When these effects are included in dust models (e.g., DUSTEM, Compiègne *et al.* 2010) their effect on the interpretation of far-infrared and sub-millimetre observations must be studied with radiative transfer models. From a technical point of view, the temperature dependence of the dust opacities is a fundamental change that requires modifications in many algorithms and may prove impractical in connection of some previously used methods.

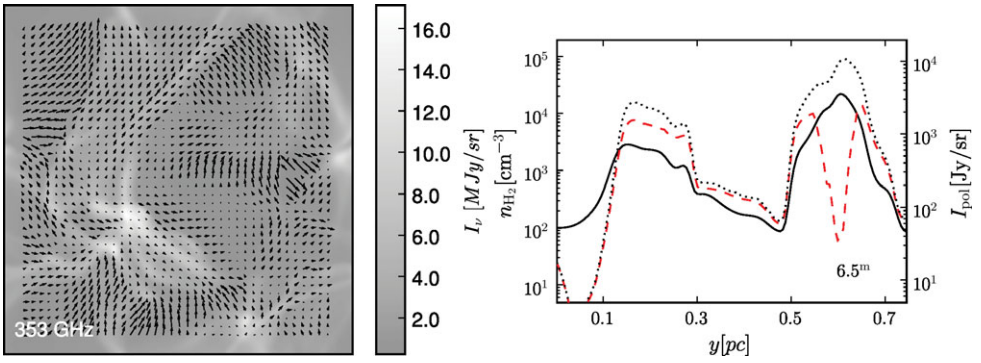

Figure 1. *Left:* Simulated dust polarization map of an interstellar cloud at 353 GHz. The vectors show the polarization degree on a map of total intensity (Pelkonen *et al.* 2007). *Right:* The gas density (solid line) and the polarized intensity at 353 GHz for normal (dashed line) and doubled dust grain size (dotted line) along a line of sight. Without significant grain size increase, the densest core does not contribute significantly to the polarized intensity (see Pelkonen *et al.* 2009).

3.2. *High spatial resolution*

The star formation process involves size scales spanning more than seven orders of magnitude. It is possible to study separately phenomena at large scales (clouds) and at small scales (cores or protostars) but there is clear need for methods with adaptive spatial resolution. This possibility already exists in many codes (e.g., Steinacker *et al.* 2003, Juvela & Padoan 2005, Ritzerveld & Icke 2006, Niccolini & Alcolea 2006).

The implementation of variable resolution using a hierarchy of grids provides advantages beyond the improved effective resolution. Each grid can be processed relatively independently providing a basis of parallel implementations and sequential programs with very low memory usage. However, more interesting is the way the grid structure can help the organization of the calculations. Most effort is usually spent on optically thick regions that fill a small fraction of the full model volume. Optical depth causes problems for the sampling of the radiation field (especially for MC) and for the convergence. When the spatial resolution only changes between well defined grids, simple ray splitting/joining at the grid boundaries ensures that the sampling of the radiation field always corresponds to the spatial discretization. In MC weighted sampling of the emission from the medium can be implemented with any discretization. However, for external radiation this is easier if the incoming energy is first stored on the grid boundary. The effect of the external field on the grid or a subtree in a grid hierarchy can then be estimated by sampling this information with any number of photon packages.

If the information of the external radiation is stored (explicitly on the grid boundary or, in MC, in the form of a reference field) it is trivial to carry out sub-iterations on arbitrary parts of the grid hierarchy. This can results in very large savings in the modeling of inhomogeneous clouds. The overhead of basic ALI/AMC is small enough so that these methods can be used throughout the models. However, the radiative couplings between neighboring cells already require a significant amount of storage. Because higher order ALI/AMC methods are not helpful in optically thin medium, their use can be safely limited to the grids with the highest optical depths. In dust continuum calculations, if a subgrid contains only a few thousand cells, it becomes feasible to store the couplings between most or even all the cells within the grid. So far as the external field remains unchanged, the temperatures can then be solved for that grid almost without any iterations. Only if the dust opacities are temperature dependent, iterations cannot be avoided.

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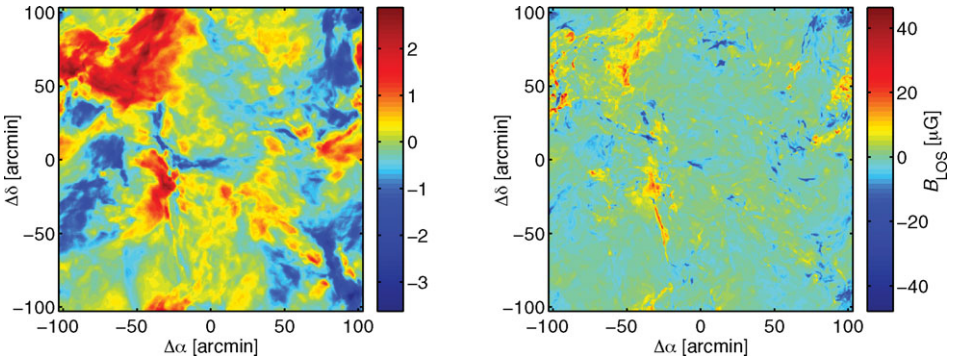

Figure 2. *Left:* Mean line-of-sight magnetic field in the MHD model used for simulations of the Zeeman splitting of OH lines. *Right:* Line-of-sight magnetic field strength determined from the simulated Zeeman observations. The derived magnetic field estimates are strongly weighted towards the densest regions (Lunttila et al. 2009).

4. Examples of radiative transfer studies

Below are given three examples of studies of interstellar clouds where radiative transfer modeling plays a major role.

Polarized dust emission. If dust grains are aligned with the magnetic field in interstellar clouds, they will polarize background starlight (excess intensity along the magnetic field), and will themselves emit polarized thermal radiation (excess intensity perpendicular to the magnetic field). Different grain alignment mechanisms have been debated since the 1950's (see Lazarian 2007). The current favorite is alignment by radiative torques (RATs) where a grain that reacts differently to left- and right-handed circularly polarized light is spun up even when subjected to unpolarized but anisotropic light. Draine & Weingartner (1997) demonstrated with numerical simulations that radiative torques are able to spin up and, importantly, also align the dust grains with respect to the magnetic field. When polarized dust emission of interstellar clouds is modelled, radiative transfer calculations are needed not only to determine the total intensity of the dust emission but also to estimate the anisotropic illumination of the grains and, thus, the degree of grain alignment. Using spherically symmetric model clouds, Cho and Lazarian (2005) showed that RATs lead to the observed drop in the polarization degree as a function of intensity. The conclusion has been confirmed by the subsequent studies with more realistic cloud models (Pelkonen *et al.* 2007) and, in addition, with more realistic grain alignment modeling (Bethell *et al.* 2007, Pelkonen *et al.* 2009) that employs radiative transfer calculations to derive the radiation field inside clumpy clouds.

The grain growth may be of critical importance for dense cores to contribute to polarized emission (see Fig.1). Pelkonen *et al.* (2009) added two caveats. Firstly, grain growth is a slow process and thus not all dense cores might be observable in polarization. Secondly, previous studies assumed that the magnetic field direction and the anisotropic radiation field direction were identical. Hoang & Lazarian (2009) showed that when the angle between these two directions increases, the efficiency of the grain alignment by RATs weakens. When this effect is included the ability of polarization to trace the magnetic field is limited to much lower A_V (see Pelkonen *et al.* 2009).

Zeeman effect in emission lines. Measurements of the Zeeman effect provide information on the absolute value of the line-of-sight component of the magnetic field. This is crucial input for theories of cloud dynamics and prestellar core formation but the complex structure of molecular clouds makes the interpretation of observations difficult. Lunttila

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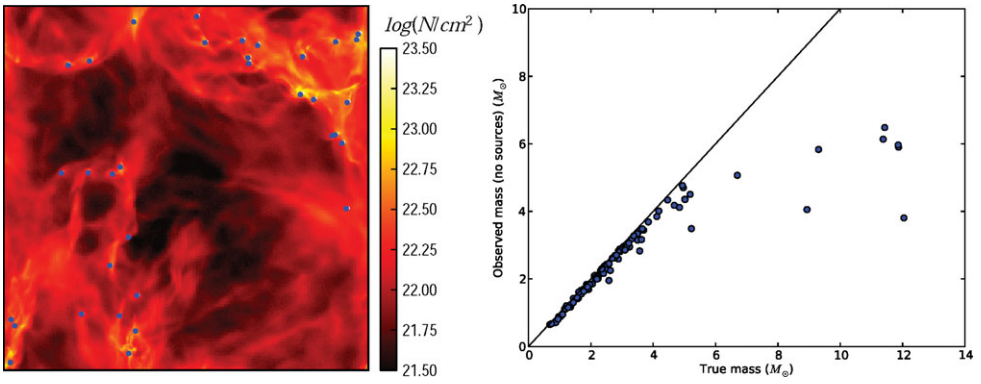

Figure 3. *Left:* Column density in a MHD run that is used to study the accuracy of the mass estimates of cloud cores. The mean extinction through the cloud is $A_{\rm V} = 13^{\rm m}$. The locations of the self-gravitating cores are marked with blue circles. *Right:* Comparison of the observed and real masses within a fixed radius of 0.05 pc around the core positions. The masses are derived from observations of dust emission at 250 and 500 μm. The cores contain no internal heating sources. The mass estimates are found to be biased only for cores that are more compact than stable Bonnor-Ebert spheres (Malinen *et al.* 2010).

et al. (2009) used radiative transfer calculations to simulate Zeeman splitting observations of a MHD model cloud. By closely following the procedures used by observers, some key parameters of the models were compared with observations. The cores were selected with the clumpfind algorithm from simulated maps of OH line intensity. The Zeeman splitting of OH 1665 and 1667 MHz lines was calculated by integrating the coupled radiative transfer equations along the line of sight. The simulated observations were done using a beam size and noise level similar to recent OH Zeeman surveys (Troland & Crutcher 2008). The OH Zeeman splitting observations were found to be sensitive to the magnetic field strength in dense cores, where the magnetic field is strong (see Fig. 2). The observations significantly overestimate the mean magnetic field, a conclusion that might be further strengthened if variations in the fractional abundance of OH were considered. Despite the low mean magnetic field of that particular model, $< B >= 0.34$ μG, the properties of the simulated cores were found to agree with observations.

Dust emission from pre-stellar cores. Star formation takes place in the dense cores of molecular clouds. The mass spectrum and internal structure of the cores can be determined with far-infrared and sub-millimetre observations. The accuracy of such determinations can be examined with radiative transfer modeling. Malinen *et al.* (2010) are studying these issues using adaptive mesh refinement (AMR) MHD simulations (Collins et al. 2010) with effective resolutions up to 4096^3. The radiative transfer calculations are conducted on the same AMR grids (for the methods, see Lunttila *et al.* 2010). For the type of observations made by the Herschel satellite, the extracted core masses are usually quite accurate and the possible errors result mainly from the uncertainty in the dust properties, its mass absorption coefficient and spectral index. This is true for stable, Bonnor-Ebert type cores. However, in the 3D simulations some of the gravitationally bound cores are more opaque and have densities that significantly exceed the densities found in stable cores. This will lead to strong temperature gradients in the cores. The observed color temperatures may overestimate the average dust temperature and, consequently, lead to underestimation of the core masses (see Fig. 3). If cloud collapse can proceed without any internal heating, the observed masses will eventually be underestimated by one order of magnitude. It still remains open if such extremely dense and at

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the same time cold cores exist in nature. When a core is heated internally by a formed protostar, the dust that was previously hidden in the cold central core again becomes visible. In that situation, despite large temperature variations, the mass estimates are not strongly biased. Although some errors are seen in the case of individual cores, the core mass spectra are found to be quite robust against such observational effects, even in the case of dust property variations that are correlated with density.

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