MONTE CARLO RADIATIVE TRANSFER
IN PRESTELLAR CORES AND PROTOSTELLAR DISKS

by

Dimitrios Stamatellos

A THESIS SUBMITTED
TO THE UNIVERSITY OF WALES FOR THE
DEGREE

Doctor of Philosophy

Cardiff, Wales, UK

November, 2003
DECLARATION

This work has not previously been accepted in substance for any degree and is not being concurrently submitted in candidature for any degree.

Signed .................................  (candidate)

Date .................................

STATEMENT 1

This thesis is the result of my own investigations, except where otherwise stated. Other sources are acknowledged by footnotes giving explicit references. A bibliography is appended.

Signed .................................  (candidate)

Date .................................

STATEMENT 2

I hereby give consent for my thesis, if accepted, to be available for photocopying and for inter-library loan, and for the title and summary to be made available to outside organisations.

Signed .................................  (candidate)

Date .................................
This thesis is dedicated to my parents Θεοφάλακτος and Σοφία, my brother Πανταζής, and my wife 静 for their love and support.
“Σα βγεις στον πηγαίμο για την Ιθάκη,
να είχες τη νάνας μακρός ο δρόμος,
γεμάτος περιπέτειες, γεμάτος γνώσεις.”

από το ποιήμα “Ιθάκη” του Κ. Καβάφη (1911)

“When you set out on your journey to Ithaca,
pray that the road is long,
full of adventure, full of knowledge.”

from the poem “Ithaca” by K. Kavafis (1911)
Abstract

MONTE CARLO RADIATIVE TRANSFER
IN PRESTELLAR CORES AND PROTOSTELLAR DISKS

by

Dimitrios Stamatellos

We implement a Monte Carlo radiative transfer method with frequency distribution adjustment (PHAETHON) that uses a large number of monochromatic luminosity packets to represent the radiation transported through a medium. These packets are injected into the medium and interact (i.e. are absorbed and/or scattered) stochastically with it.

We use PHAETHON to study prestellar cores, represented by Bonnor-Ebert spheres, that are directly exposed to the interstellar radiation field (non-embedded cores), and cores that are embedded in molecular clouds. Our models calculate temperature profiles, SEDs and intensity profiles. We find that the temperature profiles in embedded cores are less steep than those in non-embedded cores. Deeply embedded cores (in ambient clouds with visual extinctions larger than 15-25) are almost isothermal at around 7-8 K. The temperatures inside cores in ambient molecular clouds of even moderate thickness ($A_V \sim 5$) are less than 12 K, which is lower than what previous studies have assumed. Thus, previous mass calculations of embedded cores (e.g. in $\rho$ Oph) based on millimetre continuum observations, may underestimate core masses by up to a factor of 2.

We also study non-spherical cores: flattened cores and cores with a “south-pole asymmetry” (the “south” region is denser than the “north” region). These models may represent more realistic density distributions than the commonly used spherically symmetric Bonnor-Ebert model. We find that SEDs of slightly asymmetric cores are essentially independent of the viewing angle. However, isophotal maps depend strongly on the viewing angle. When the core is viewed edge-on it appears elongated on mm and submm maps, which effectively trace column-density. At wavelengths near the peak of the core emission (150-250 $\mu$m), isophotal maps are strongly affected by the temperature of the core and they are not solely column density tracers. There
are characteristic features on these maps which depend on the observer’s viewing angle, and on the detailed density and temperature structure of the core. Hence, they contain complementary information to the mm and submm maps. The predicted characteristic features are on scales 1/5 to 1/3 of the overall core size, and high resolution observations are needed to observe them.

We extend PHAETHON to treat radiative transfer in systems with arbitrary geometries resulting from Smoothed Particle Hydrodynamics (SPH) simulations. We use the SPH tree to construct radiative transfer (RT) cells, i.e. the cells that interact with the radiation. The procedure used creates RT cells with linear size on the order of the SPH resolution. We also develop a method to treat regions close to stars, where the temperature gradients are expected to be very large. The extended version of PHAETHON can be used to perform continuum radiative transfer simulations on SPH snapshots and it is useful for comparing the results of hydrodynamic simulations with observations. We apply this method to model GM Aurigae, a T Tauri star with a circumstellar disk. We examine the case of an axisymmetric disk and the case of a non-axisymmetric, perturbed disk and find that both models are consistent with the observed SED of the system. The results indicate that PHAETHON works reasonably well for treating SPH systems with arbitrary geometries, and thus the two methods can be combined in the future in a self-consistent SPH-RT scheme.
Acknowledgements

I am grateful to Anthony Whitworth for his guidance, advice and encouragement during this project. I would like to thank D. Ward-Thompson and J. Kirk for useful discussions on prestellar cores, and previous and current members of the Cardiff Star Formation group for their help in the past 3 years (Douglas Boyd, Simon Goodwin, Seung-Hoon Cha and Glyn Hosking).

I would also like to thank P. André for suggesting the study of embedded cores, M. Baes for stimulating discussions on Monte Carlo radiative transfer, J. Bouwman for his help in testing the radiative transfer code, and J. Barnes for his tree code. I also thank Z. Ivezic for his benchmarks calculations for the code tests, J. Black for providing a digital version of his estimate of the ISRF, and V. Ossenkopf for useful comments on dust opacities in dense cores.

Finally, I acknowledge help from the EC Research Training Network “The Formation and Evolution of Young Stellar Clusters”.
# Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract</td>
<td>vii</td>
</tr>
<tr>
<td>Acknowledgements</td>
<td>ix</td>
</tr>
<tr>
<td><strong>1 Introduction</strong></td>
<td>1</td>
</tr>
<tr>
<td>1.1 Initial conditions for star formation</td>
<td>2</td>
</tr>
<tr>
<td>1.2 Cloud collapse</td>
<td>4</td>
</tr>
<tr>
<td>1.3 Observational evolutionary sequence</td>
<td>6</td>
</tr>
<tr>
<td>1.4 Disks</td>
<td>8</td>
</tr>
<tr>
<td>1.5 Accretion and outflows</td>
<td>8</td>
</tr>
<tr>
<td>1.6 Binaries and multiple systems</td>
<td>9</td>
</tr>
<tr>
<td>1.7 Star forming regions</td>
<td>10</td>
</tr>
<tr>
<td>1.8 Current issues in star formation</td>
<td>11</td>
</tr>
<tr>
<td>1.9 Thesis outline</td>
<td>15</td>
</tr>
<tr>
<td><strong>2 Monte Carlo Radiative Transfer</strong></td>
<td>17</td>
</tr>
<tr>
<td>2.1 Method overview</td>
<td>17</td>
</tr>
<tr>
<td>2.2 System setup</td>
<td>19</td>
</tr>
<tr>
<td>2.3 Monte Carlo theory</td>
<td>19</td>
</tr>
<tr>
<td>2.4 $L$-packet emission</td>
<td>20</td>
</tr>
<tr>
<td>2.5 Dust properties</td>
<td>22</td>
</tr>
<tr>
<td>2.6 Cell construction</td>
<td>23</td>
</tr>
<tr>
<td>2.7 $L$-packet propagation</td>
<td>24</td>
</tr>
</tbody>
</table>
### 3 Models of Spherical Prestellar Cores

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>Radiative transfer in prestellar cores</td>
<td>54</td>
</tr>
<tr>
<td>3.1.1</td>
<td>Core density profile</td>
<td>54</td>
</tr>
<tr>
<td>3.1.2</td>
<td>The illuminating radiation field</td>
<td>58</td>
</tr>
<tr>
<td>3.1.3</td>
<td>Dust opacities</td>
<td>60</td>
</tr>
<tr>
<td>3.1.4</td>
<td>Code tests</td>
<td>61</td>
</tr>
<tr>
<td>3.2</td>
<td>Non-embedded prestellar cores</td>
<td>62</td>
</tr>
<tr>
<td>3.2.1</td>
<td>Temperature profiles</td>
<td>63</td>
</tr>
<tr>
<td>3.2.2</td>
<td>SEDs and intensity profiles</td>
<td>65</td>
</tr>
<tr>
<td>3.2.3</td>
<td>Effects of dust scattering properties</td>
<td>67</td>
</tr>
<tr>
<td>3.3</td>
<td>Prestellar cores embedded in molecular clouds</td>
<td>69</td>
</tr>
</tbody>
</table>
## 3.3.1 Model description ........................................ 70
## 3.3.2 Temperature profiles and mass estimates .......... 71
## 3.3.3 SEDs and intensity profiles .......................... 74
## 3.3.4 Diagnostics ........................................... 75

### 3.4 Summary .................................................. 79

### 4 Asymmetric Models of Prestellar Cores .................. 81
#### 4.1 Initial system setup .................................. 81

#### 4.2 Flattened prestellar cores (disk-like asymmetry) ........ 83

1. **4.2.1 Non-embedded cores: the model** .......................... 83
2. **4.2.2 Results: core temperatures, SEDs and images** .......... 84
3. **4.2.3 Embedded prestellar cores** ................................ 98
4. **4.2.4 The effect of a UV-enhanced ISRF on embedded cores** 101

#### 4.3 “South-pole” asymmetric cores .......................... 103

1. **4.3.1 The model** ........................................... 103
2. **4.3.2 Results: core temperatures, SEDs and images** .......... 104

#### 4.4 Comparison with observations .......................... 108

#### 4.5 Discussion ............................................. 115

### 5 Monte Carlo Radiative Transfer & SPH ..................... 117
#### 5.1 Smoothed Particle Hydrodynamics (SPH) ............... 119

1. **5.1.1 SPH smoothing kernel** .................................. 120
2. **5.1.2 SPH fluid equations** .................................. 120
3. **5.1.3 Integration scheme & time step setting** .................. 122
4. **5.1.4 The SPH tree** ....................................... 123
5. **5.1.5 SPH: The algorithm** .................................. 124

#### 5.2 Radiative transfer in hydrodynamic simulations ......... 125

1. **5.2.1 Construction of radiative transfer cells** ............... 125
2. **5.2.2 L-packet propagation and interaction** .................. 126
3. **5.2.3 Remark** ............................................. 127

#### 5.3 Tests ...................................................... 127

1. **5.3.1 Sphere embedded in an isotropic blackbody radiation field** 128
2. **5.3.2 Sphere embedded in the ISRF** .......................... 131
5.3.3 Low-temperature source surrounded by a spherical envelope ............. 134
5.4 Stars in SPH-RT simulations ..................................................... 135
  5.4.1 Definition of the problem .................................................. 136
  5.4.2 Solution Method .............................................................. 138
  5.4.3 Tests .............................................................................. 139
5.5 Summary ............................................................................. 144

6 Radiative Transfer in Disks .......................................................... 147
  6.1 Disk initial conditions ............................................................ 148
    6.1.1 Disk surface density ....................................................... 148
    6.1.2 Disk temperature ........................................................... 149
    6.1.3 Disk thickness ............................................................... 150
    6.1.4 Disk volume density ....................................................... 152
    6.1.5 Disk rotation ................................................................. 152
  6.2 SPH disk setup ..................................................................... 154
    6.2.1 Position, mass and initial smoothing length of SPH particles ...... 154
    6.2.2 Azimuthal density perturbations ....................................... 155
  6.3 Models of protostellar disks: GM Aurigae ................................. 156
    6.3.1 Model I: Axisymmetric disk .......................................... 158
    6.3.2 Model II: Perturbed disk ............................................... 161
  6.4 Discussion .......................................................................... 165

7 Discussion & Future Prospects .................................................... 167
  7.1 Monte Carlo radiative transfer with frequency distribution adjustment .. 167
  7.2 Radiative transfer in spherical prestellar cores ........................... 168
  7.3 Models of non-spherical prestellar cores .................................... 170
  7.4 Monte Carlo radiative transfer and SPH .................................... 171
  7.5 Radiative transfer in protostellar disks ...................................... 172
  7.6 Future prospects ................................................................... 172

A L-packet Scattering Angle ........................................................... 175

B Isophotal Maps ........................................................................ 179
  B.1 General case ................................................................. 179
B.2 Spherical case .............................................................. 182

C Photon Injection Angle ................................................. 183

D Distribution of SPH Particles in a Disk ............................. 185

E Fourier Analysis of the Structure of a Disk ....................... 187

F Publications ........................................................................ 189

Bibliography ....................................................................... 191
Chapter 1

Introduction

Star formation is believed to happen when dense regions inside molecular clouds collapse. This occurs when self-gravity dominates over the forces that support the cloud (e.g. thermal pressure, magnetic fields, turbulence). The details of this process are not very well understood but recent observations, theoretical models and numerical simulations indicate that star formation is a dynamical, violent process in which magnetic fields, turbulence, the presence of ionized gas around hot young stars, ejection of mass from newly-born stars and shock waves induced by supernova explosions, may play an important role (see review by Larson 2003). In most cases, the final outcome of the collapse is a cluster or a small group of stars rather than a single star. Most stars have disks that fuel the protostar with material through accretion, and this is thought to power the ejection of material in the form of jets perpendicular to the disk plane. It is speculated that planetary systems form in the late stages of evolution of such disks, but the details of the process are uncertain.

In this thesis we focus on the study of cores in molecular clouds that collapse and form stars. Information about these cores comes from molecular line observations (e.g. Myers & Benson 1983 (NH₃); Myers, Linke, & Benson 1983 (C₁); Stutzki & Guesten 1990 (C₀, CS)) and also from continuum observations at IR, submm and mm wavelengths (e.g. Bacmann et al. 2000 (ISO/ISOCAM ~ 7 μm observations); Ward-Thompson, André, & Kirk 2002 (ISO/ISOPHOT 90, 170 and 200 μm observations); Kirk et al. 2003 (SCUBA 450 and 850 μm observations); Motte, André, & Neri 1998 (IRAM 1.3 mm observations)). We develop a Monte Carlo code to perform continuum radiative transfer simulations of spherical and non-spherical cores illuminated by an ambient radiation field. We then extend this radiative transfer method to study systems with arbitrary geometries resulting from Smoothed Particle Hydrodynamics simulations. The
code solves for the dust temperature and also calculates continuum spectral energy distributions (SEDs) and intensity maps at different wavelengths and at different viewing angles. The SEDs and intensity maps that are calculated by our models can be compared directly with continuum observations.

1.1 Initial conditions for star formation

Molecular clouds are cold regions of gas and dust where the temperature is so low, and the density and column-density so high, that hydrogen exists in the form of molecules. They have typical densities $10^2 - 10^4 \text{ H}_2 \text{ cm}^{-3}$ (or even larger in their cores), temperatures around 10-20 K, and their linear size could be up to 100 pcs and their mass at least up to $10^6 \text{ M}_\odot$. These clouds are concentrated in the Galactic disk, near the dense spiral arms of the Galaxy. Their structure is hierarchical, meaning that smaller subclouds are contained within larger subclouds, and their sizes are irregular and often filamentary (see review by Williams, Blitz, & McKee 2000).

Thermal pressure alone cannot support these clouds against gravity, suggesting the presence of other support mechanisms. The internal motions of gas within clouds are supersonic, suggesting that turbulence may be significant in supporting these clouds (e.g. Jijina, Myers, & Adams 1999). Magnetic fields may also play an important role, at least during the initial stages of cloud evolution when the gas is still coupled with the magnetic field (Mouschovias 1976). However, it is possible that molecular clouds are transient rather than equilibrium structures. (e.g. Ballesteros-Paredes, Klessen, & Vázquez-Semadeni 2003). The denser parts of these clouds collapse, when their support against gravity weakens, and form stars, mostly in clusters and associations of $10^2 - 10^6$ stars (clustered star formation) but also in smaller groups with just a few stars (isolated star formation). The whole process of molecular cloud collapse and star formation is very fast and it is expected to last less than 1 Myr.

Observations of molecular clouds have revealed condensations that appear to be on the verge of collapse or already collapsing (e.g. Myers and Benson 1983, Ward-Thompson et al. 1994, Ward-Thompson, André, & Kirk 2002). These condensations are referred to as preprotostellar (or prestellar) cores. They are believed to represent the initial stage of star formation.

Isolated prestellar cores have been observed inside molecular clouds (e.g. L1544; Ward-Thompson et al. 1999). These cores are considered to be precursors of isolated low mass star formation. Isolated prestellar cores have extent $\gtrsim 1.5 \times 10^4 \text{ AU}$ and masses $0.5 - 35 \text{ M}_\odot$ (André,
1.1. INITIAL CONDITIONS FOR STAR FORMATION

Ward-Thompson, & Barsony 2000). They are not in general spherically symmetric and they appear to have flat central density profiles. Magnetic fields are also present and they may play a role in core stability (see André, Ward-Thompson, & Barsony 2000 and references therein).

Prestellar cores have also been observed in young protoclusters, such as ρ Ophiuchi (Motte, André, & Neri 1998, Johnstone et al. 2000) and NGC 2068/2071 (Motte et al. 2001, Johnstone et al. 2001). ρ Ophiuchi is a star-forming cluster of about 1 pc diameter, with estimated average particle density $n(H) \sim 2 - 4 \times 10^4$ cm$^{-3}$ and thermal gas pressure $\sim 10^6$ cm$^{-3}$ K (Liseau et al. 1999). In this region there have been detected ~ 100 structures, 59 of which are identified as prestellar cores and the remaining as embedded young protostellar (Class 0) objects (Motte, André, & Neri 1998). The extent of the prestellar condensations is $2 - 4 \times 10^3$ AU (more compact than isolated prestellar cores), and they have sharp edges. Their estimated masses are 0.05–3 M$_\odot$. NGC 2068/2071 are protoclusters in the Orion B cloud complex. Observations (Motte et al. 2001, Johnstone et al. 2001) have revealed a filamentary structure with ~ 70 starless condensations having small sizes (~ 5000 AU) and masses from ~ 0.3 M$_\odot$ to ~ 5 M$_\odot$.

Many authors have approximated prestellar cores by Bonnor-Ebert (BE) spheres, i.e. isothermal spheres in which gravity is balanced by the gas pressure of the core (Ebert 1955, Bonnor 1956). Barnard 68 (Alves, Lada, & Lada 2001) is an example. However, a recent study of cores in SPH simulations of turbulent molecular clouds by Ballesteros-Paredes, Klessen, & Vázquez-Semadeni (2003), has shown (a) that the non-hydrostatic transient cores which they study, are not spherical and their column density profiles are strongly dependent on the observer’s viewing angle, and (b) that a large percentage (65%) of the cores in their simulations can be approximated by a BE profile, even though these cores are not in hydrostatic equilibrium. In many cases the BE fit is good for just one or two of the three viewing angles they examine. Thus, the usefulness of BE sphere fits for prestellar cores is questionable.

The non-sphericity of prestellar cores is also evident from submillimeter (e.g. 850 μm) continuum maps of prestellar cores, that trace the column density along the line of sight (e.g. Motte, André, & Neri 1998; Ward-Thompson et al. 1999; Kirk 2002). Furthermore, evolutionary models of prestellar core collapse, indicate the formation of flattened (oblate) cores either due to the initial core rotation (e.g. Matsumoto, Hanawa, & Nakamura 1997) or due to flattening along the magnetic field lines of a bipolar magnetic field (e.g. Ciolek & Mouschovias 1994). Other models invoke a toroidal magnetic field to create equilibrium prolate cores (e.g. Fiege & Pudritz 2000), although there are some problems with maintaining a prolate structure. Triaxial structures could
form as a result of complex magnetic fields or turbulent motions in molecular clouds. Gammie et al. (2003), have studied the shapes of condensations arising in hydrodynamic simulations of isothermal, turbulent molecular clouds, including magnetic fields, and conclude that cores are triaxial. This view is supported by recent statistical studies of the projected shapes of a large sample of cores (Jijina, Myers, & Adams 1999), which suggest that prestellar and starless cores are triaxial ellipsoids rather than prolate or oblate spheroids (Jones, Basu, & Dubinski 2001; Goodwin, Ward-Thompson, & Whitworth 2002).

Mass estimates from mm continuum observations, where the cores are optically thin, suggest that the mass function for cores is very similar to the initial mass function (IMF), and therefore the IMF could be determined by fragmentation at the pre-stellar stage of star formation (e.g. André, Ward-Thompson, & Barsony 2000). The question of whether fragmentation can produce the smallest masses in the IMF is still open. Observations of very low mass prestellar condensations are crucial for answering this question but they are beyond the limits of today’s telescopes. Furthermore, current core mass estimates are uncertain, due to our limited knowledge of the properties of the dust in and around these cores, and of the dust temperature.

1.2 Cloud collapse

It has already been mentioned that dense cores in molecular clouds collapse when the gravity dominates over the forces that support the cloud, such as thermal pressure, magnetic fields, turbulent motions, or rotational forces. If we consider just the effects of gravity and thermal pressure, then assuming equilibrium, using the virial theorem we have that

\[ 2E_T + E_G = 0, \]

where \( E_T \) is the thermal energy and \( E_G \) the gravitational energy of the system. The cloud will contract if \( 2E_T < |E_G| \). Substituting for the gravitational and thermal energy of the cloud, we find that the condition for the collapse of a cloud is (Jeans 1902)

\[ r > r_J \simeq \left( \frac{\pi c_s^2}{G \rho} \right)^{1/2}, \]

where \( r \) is the radius of the cloud, \( r_J \) is the Jeans radius, \( \rho \) is the density of the cloud and \( c_s \) is the sound speed. This condition, known as the Jeans criterion, can be expressed in terms of the
mass $M$ of the cloud,

$$M > M_J \simeq \left( \frac{\pi c_s^2}{G} \right)^{3/2} \rho^{-1/2},$$

(1.3)

where $M_J$ is the Jeans mass. More rigorous calculations (e.g. Spitzer 1978) only change the numerical constant in this equation. The effect of other forces opposing the collapse (e.g. turbulence, magnetic fields, rotation) is to increase this minimum mass.

Once the cloud starts to collapse it goes through four main phases. In the first phase (densities $10^{-19}$ to $10^{-13}$ g cm$^{-3}$) the cloud stays almost isothermal at $\sim 10$ K. The thermal pressure is not sufficient to support the cloud, which is nearly free falling, on a timescale $t_{\text{ff}} = (1/G \rho_0)^{1/2}$. During the isothermal collapse phase the Jeans mass decreases since the density increases (see Eq. 1.3). Hence, separate parts of the cloud satisfy the Jeans criterion and start contracting independently, causing the initial cloud to fragment. The resulting fragments may fragment further (hierarchical fragmentation). When the density in the core of the cloud becomes high enough ($\rho \approx 10^{-13}$ g cm$^{-3}$), the core becomes opaque to the radiation it emits and its temperature increases, until the thermal pressure is sufficient to halt the collapse. This happens when the core temperature reaches $\sim 200$ K. The core then contracts quasi-statically (second phase). The rest of the cloud also continues to contract, compressing and heating the core (e.g. Masunaga et al. 1998). When the temperature of the core reaches 2000 K the molecular hydrogen starts to dissociate and the central core starts to collapse again (third phase; e.g. Masunaga & Inutsuka 2000). The core remains isothermal at 2,000 K, because the energy from the collapse is used to dissociate the hydrogen and it does not heat the core. After the hydrogen has been dissociated the collapse continues and the core starts to heat up again, until the temperature becomes high enough ($\sim 20,000$ K) to support the core. The collapse then stops, and the core continues to contract quasi-statically (fourth phase) and to increase its mass by accreting infalling material.

More realistic models include more physics, like rotation (e.g. Cha & Whitworth 2003b), turbulence (e.g. Klessen 2001; Goodwin, Whitworth, & Ward-Thompson 2003), magnetic fields (Vázquez-Semadeni et al. 2000, Hosking & Whitworth 2003), external pressure (Hennebelle et al. 2003). These models show that fragmentation happens under a variety of conditions. The minimum mass of an object produced by fragmentation is uncertain and depends on the assumed physical conditions; it is estimated to be from $10 - 15M_J$ (Rees 1976) down to $3M_J$ (Whitworth & Boyd 2003).
1.3 Observational evolutionary sequence

Star formation begins with the collapse of an unstable prestellar core. Observations during the past two decades have revealed young stellar objects with different characteristics that were subsequently interpreted in terms of an evolutionary sequence (Fig. 1.1, see André, Ward-Thompson, & Barsony 2000 for a review).

*Class 0* objects correspond to the first stage in the evolution of a protostar, where a central luminosity source has been formed in the centre of the core. The protostar cannot be observed because it is highly embedded in the core but its presence can be inferred by compact radio continuum emission, molecular outflows or by the presence of an internal heating source. The core is relatively cold (15-40 K) and the peak of its emission is at 150-250 μm. The embedded protostar accretes mass from the envelope at a high rate ($\gtrsim 10^{-5} \, M_\odot \, yr^{-1}$) and this lasts a few $10^4$ yrs. At the end of this phase the star has acquired at least half of its final mass.

*Class I* objects correspond to a later stage of the collapse where a disk has started to form around the central object but there is also a residual surrounding envelope. Accretion onto the central protostar continues but at a lower rate ($\lesssim 10^{-6} \, M_\odot \, yr^{-1}$). This accretion phase lasts a few $10^5$ yrs, and at the end of this phase the star has almost reached its final mass. The central protostar is still highly embedded, and generally cannot be observed at optical wavelengths but only in the NIR. The surrounding colder envelope emits the bulk of its radiation in the FIR.

*Class II* and *Class III* objects correspond to the classical T Tauri (CTT) and weak-line T Tauri (WT Tauri) stars, respectively. In Class II objects the protostellar envelope has been reduced to a geometrically thin but optically thick disk, with mass $\sim 0.01 \, M_\odot$. The star is now visible at optical wavelengths and the disk produces an infrared excess in the spectrum of the system. Accretion onto the central star continues, as evidenced by the veiling of absorption lines in the UV and strong emission lines from hydrogen ($H_\alpha$). The accretion rate is low ($\sim 10^{-8} \, M_\odot \, yr^{-1}$), although some objects exhibit episodic accretion at rates up to $\sim 10^{-6} \, M_\odot \, yr^{-1}$ (FU Orioni type systems). The age of CTT stars is estimated to be on the order of $10^6$ yrs. WTT stars (Class III objects) show weak $H_\alpha$ emission, and they do not show a significant excess of infrared or UV emission. This suggests that the inner disks have dissipated or the dust has coagulated into larger rocks or protoplanetary objects. The estimated disk mass is less than $3 \times 10^{-3} \, M_\odot$ and the disk is thought to completely disappear after $\sim 10$ Myrs.
Figure 1.1  Evolutionary scenario (from André 1994).
1.4 Disks

Disks are a natural product of cloud collapse because centrifugal forces prevent much of the cloud material from falling directly onto the central protostar. The main evidence for the existence of disks around pre-main-sequence stars comes from the spectral energy distributions (SEDs) of these systems. The disk temperature is lower than the temperature of the parent star and this results in an excess radiation in the IR and, in the case of very extended disks, in the submm region of the spectrum. Furthermore, high spatial resolution optical and near infrared imaging with the Hubble Space Telescope, and ground-based observations with adaptive optics, have provided well-resolved images of disks around T Tauri single and binary stars (e.g. McCaughrean & O'Dell 1996; McCaughrean, Stapelfeldt, & Close 2000). These disks have masses from 0.001 $M_\odot$ to 0.1 $M_\odot$, sizes from 10 to 1000 AU, and it is estimated that they persist for up to 10 Myrs before they dissipate.

Disks are present from the initial stages of protostellar collapse (protostellar disks) to the later stages of evolution, like classical (T Tauri disks) and weak-lined Tauri stars (protoplanetary disks) and even around brown dwarfs.

Protostellar disks have masses comparable with the mass of the protostar since most of the mass of the infalling envelope falls onto the disk rather than directly onto the star. They are susceptible to gravitational instabilities and they may fragment and form a multiple system. They are highly embedded and much of their intrinsic radiation is reprocessed by the surrounding envelope.

T Tauri and protoplanetary disks have masses from at least $10^{-5} M_\odot$ up to a few times $10^{-1} M_\odot$, but these estimates depend strongly on the assumed dust opacities, gas-to-dust ratios and disk density profiles, all of which are poorly determined (Zuckerman 2001). T Tauri disks could be active, i.e. radiate energy generated by viscous dissipation, or passive, i.e. just reprocess stellar radiation. It is also believed that they are flared, and that they do not extend to the surface of the star but are truncated by the star’s magnetic field at a few stellar radii.

1.5 Accretion and outflows

During the first million years from the core collapse, matter accretes onto the central protostar either spherically, during the initial stages of the collapse, or through a disk, during the later
stages. Observations indicate that accretion of material is almost always accompanied by ejection of mass in the form of molecular outflows or stellar jets perpendicular to the disk.

The evidence for accretion in T Tauri stars comes from several features in their spectral energy distributions (see Calvet, Hartmann & Strom 2000). An indicator of accretion is the presence of veiled photospheric absorption lines in the UV and optical. This phenomenon is due to hot continuum emission because of accretion of material onto the stellar surface. There are also specific lines (e.g. H$_\alpha$) that are believed to form when mass flows onto the stellar surface through the magnetospheric accretion columns that connect the disk to the star. The intensity of these lines depends on the density of the material that flows in these columns, which, in turn, depends on the accretion rate.

Theoretical studies of accretion disks indicate that the disk material rotates in almost Keplerian orbits around the star, slowly drifting inwards due to the effects of viscosity (Lynden-Bell & Pringle 1974). The origin of disk viscosity is uncertain. Theoretical models suggest that the viscosity could be due to turbulence generated either by convection (Lin & Papaloizou 1980) or by magnetic fields (magneto-rotational instability; Balbus & Hawley 1991).

The accretion seems to power jets in the form of bipolar outflows of mass, along the rotation axis of the star (Eisloffel et al. 2000; Richer et al. 2000). These jets are highly collimated, have velocities of hundreds of km sec$^{-1}$, and eject mass at a rate up to 10$\%$ of the accretion rate (Hartigan et al. 1995). Their relation to accretion is suggested by the fact that they are observed only when there is evidence for accretion. Thus, the presence of jets is an indicator of stellar youth. The mechanism that produces the jets is not yet clear and models suggest that they originate either from the disk (disk winds; see Königl & Pudritz 2000) or from the interface of the star disk system (X-winds; see Shu, Najita, Shang, & Li 2000).

1.6 Binaries and multiple systems

It is well established that more than 50$\%$ of the pre-main sequence (PMS) systems are binaries or multiple systems (e.g. Mathieu 1994, Mathieu 1995, Mathieu et al. 2000), and this suggests that most stars form in multiple systems. There are binaries with separations from a few solar radii up to 1 pc with an average binary separation 20-50 AU (i.e. with period ~ 200 yrs). Surveys of different star forming regions (e.g. Duchêne, Bouvier, & Simon 1999; White & Ghez 2001; Bouvier et al. 2001) indicate that the binary frequency varies from region to region. This could
mean either that the binary population evolves in time, or that the binary formation efficiency varies among different star forming regions (see Kroupa, Petr, & McCaughrean 1999).

Binaries form during the collapse and fragmentation of prestellar cores. The detailed products of the collapse are determined by the initial conditions of the core, such as shape, density, angular momentum, and the presence of magnetic fields or turbulence. The collapse of a core usually produces binaries or multiple systems (e.g. Goodwin, Whitworth, & Ward-Thompson 2003), with the formation of just a single star being the exception, when fragmentation is suppressed, e.g. by feedback processes (Boyd 2003) or magnetic fields (Hosking 2002).

If fragmentation does not occur during the cloud collapse and the outcome of the collapse is a disk or a ring around a central object, then it is possible that the disk or the ring could still fragment due to gravitational instabilities to form a binary (Bonnell 1994; Rice et al. 2003; Cha & Whitworth 2003b). An important quantity for disk fragmentation is the Toomre parameter,

\[ Q = \frac{\kappa c_s}{\pi G \sigma} \]  

where \( \kappa \) is the epicyclic frequency, \( c_s \) is the isothermal sound speed, and \( \sigma \) is the local surface density. If \( Q < Q_c \) (\( Q_c \approx 1 \), depending on the conditions assumed) then the disk is unstable to gravitational instabilities. If \( Q > Q_c \) then the disk is stable against axisymmetric gravitational instabilities, but it can be unstable to non-axisymmetric instabilities for \( Q_c < Q < 3 \). Disk fragmentation also depends on the radiative processes in the disk. If the disk does not cool fast enough (\( t_{\text{cooling}} > 3/\Omega_{\text{disk}} \)) then fragmentation is suppressed (Gammie 2001; Rice et al. 2003).

Binaries could also form via capture, i.e. from two initially unbound stars. This requires the loss of significant kinetic energy from the stars, which could be due to three-body interactions or dissipation of energy due to the presence of disks around the stars (Boffin et al. 1998; Watkins et al. 1998a; Watkins et al. 1998b). This mechanism might be important in dense, small clusters of young stars with disks.

### 1.7 Star forming regions

The best studied star forming regions are Taurus, Orion and Ophiuchus, mainly due to their proximity to Earth. These regions have different characteristics (e.g. gas density, binary fraction, star formation efficiency), which suggests that star formation depends on the initial conditions and/or the dominant forces during the star formation process. Taurus is at distance \( \sim 150 \) pc
with mass \( \sim 10^4 M_\odot \) and an extent of \( \sim 20 \) pc. It has a low star and gas density and high binary fraction. Orion is at distance \( \sim 450 \) pc, with mass \( \sim 10^5 M_\odot \) and an extent of \( \sim 100 \) pc. It is characterised by a large star density and contains several OB associations. Ophiuchus is at the same distance as Taurus, and has about the same mass and overall size.

### 1.8 Current issues in star formation

Many problems of star formation remain unsolved. In this section we summarize some of the current issues in star formation.

**Initial conditions for protostellar collapse**  Observations of condensations in molecular clouds in dust continuum (e.g. submm and mm) and in molecular lines (e.g. NH\(_3\), CO) are crucial in determining the initial conditions for star formation. Prestellar cores are generally asymmetric with density profiles that are flat near the centre and fall off as \( r^{-2} \) at larger distances. Their column density profiles resemble an isothermal sphere (Bonnor-Ebert sphere), although numerical simulations suggest that this may be a coincidence. The asymmetric profiles of molecular lines observed in some of these cores (e.g. L1544) suggest that their outer parts are collapsing while the inner parts are almost stationary. Observations with better resolution are needed to determine the density profiles near the centres of the these cores and to establish whether they have an internal energy source.

**Planet formation**  It is generally believed that planets form from coagulation of dust particles into larger bodies (planetesimals) that merge to form rocky (terrestrial) planets. The giant planets form the same way as rocky planets but at larger distances from the parent star. They subsequently accrete gas from the disk and increase their masses (e.g. Bodenheimer & Pollack 1986). Planet formation models indicate that this process could take at least 10 Myr. However, disks around young stars are estimated to persist for only about 3-6 Myrs. It is also suggested that planets could form via gravitational fragmentation of disks (Gammie 2001; Rice et al. 2003), if the disk can cool efficiently. Since the discovery of the the first extrasolar planet in 1995 (51 Pegasi; Mayor & Queloz 1995), a large number (\( \sim 100 \)) of candidate extrasolar planets have been detected, mainly from measurements of the periodic radial velocity variation of the parent star, but also from transit events (Charbonneau et al. 2000). Most of them are gaseous giant planets at distances very close to the parent star, in contrast with the solar system paradigm. Current
ideas suggest that these planets were formed farther away from the central star and then migrated inwards due to interactions with the residual disk (e.g. Nelson et al. 2000).

**Origin of brown dwarfs** Brown dwarfs are low-mass objects ($13 \, M_J < M < 80 \, M_J$). The temperatures in their centres do not rise enough for the burning of hydrogen to start, but they are able to burn deuterium (see Oppenheimer, Kulkarni, & Stauffer 2000). They are very faint objects ($L < 10^{-4} \, L_{\odot}$), and therefore difficult to observe. It is believed that they are fundamentally different from planets but quite similar to stars. They have disks, exhibit flares indicative of magnetic activity and exist in brown dwarf binary systems, all suggesting a common formation mechanism with stars, i.e. formation from fragmentation during the collapsing of a core or fragmentation in an unstable disk (unlike planets, which are thought to form from coagulation of dust in disks). Recent theories suggest that brown dwarfs may form as ejected embryos in three-body interactions in fragmenting cores (Reipurth & Clarke 2001; Goodwin, Whitworth, & Ward-Thompson 2003). This may explain the lack of brown dwarf companions around main-sequence stars (the brown dwarf desert).

**Brown dwarfs vs planets debate** There has been a debate in the past few years about the distinction between brown dwarfs and planets. This debate has been initiated by the discovery of planetary mass objects free floating in young stellar clusters (Lucas & Roche 2000; Zapatero Osorio et al. 2000). These are objects with masses $< 13 \, M_J$ but with more similarities to brown dwarfs than planets. It is still unclear whether these objects were formed in a disk and then somehow ejected into the cluster (e.g. Nelson 2003), or whether they have been formed directly by fragmentation during the collapse of a core (e.g. Whitworth & Boyd 2003).

**Low-mass initial mass function** The initial mass function (IMF) refers to the distribution of masses of objects within a cluster when the stars reach the main sequence. The IMF is well determined at masses $\gtrsim 0.4 \, M_{\odot}$ but poorly determined at the low-mass end, i.e. in the brown dwarf region, due to the fact that low-mass, low-luminosity objects are very difficult to observe. In Fig. 1.2, we present a schematic view of the the probability $\phi(M) \, dM$ of forming a star with mass between $M$ and $M + dM$. For $0.4 \leq M_{\odot} \leq 10 \, M_{\odot}$ the probability function can be approximated by a power law (Salpeter 1955)

$$\phi(M) dM \approx K M^{-2.35}.$$  

(1.5)
At masses above $10 \, M_\odot$ the IMF steepens on the log-log plot, whereas below $< 0.4 \, M_\odot$ observations suggest that it may flatten down to the limits of detection. New observations with telescopes having better sensitivity have pushed this limit into the brown dwarf regime. However, the low-mass end of the IMF is still uncertain. It is also uncertain whether the IMF is universal, or depends on the initial conditions of cloud collapse.

**Figure 1.2** Schematic view of the initial mass function (IMF).

**Angular momentum problem** Observations suggest that molecular cloud cores rotate slowly ($v \lesssim 0.1 \, \text{km s}^{-1}$), and hence possess angular momentum. If this angular momentum were conserved minutely during the star formation process then the resulting stars would rotate extremely rapidly, contrary to observation. Thus, a large amount of this initial angular momentum must somehow be extracted from the system. This is the angular momentum problem (e.g. Mestel 1965 a,b). It is speculated that magnetic fields may play an important role in removing angular momentum during the initial stages of the collapse when the gas is coupled to the magnetic field. It is also believed that dissipative processes in a disk could transport angular momentum outwards, but the sources of disk viscosity are uncertain. It is also possible that a forming planet could extract angular momentum from the disk. Another option could be the formation of a binary or a multiple system, or the ejection of material in the form of molecular outflows and protostellar jets.
\textbf{Origin of very close binaries}  Binaries with separation \(< 1 \text{ AU}\) represent 10\% of the total number of binaries. Their formation mechanism is quite uncertain since a large amount of angular momentum needs to be taken away from the system. Numerical studies (e.g. Bate, Bonnell, \\& Bromm 2002) suggest that close binaries could form from wider binaries by accretion of gas with lower angular momentum, by dynamical interactions within a multiple system (e.g. the ejection of a brown dwarf) or by tidal interactions between the binary and the circumbinary disk. They could also form via disk fragmentation (e.g. Bonnell \\& Bate 1994).

\textbf{Origin of protostellar jets}  Jets are a common phenomenon during star formation. In most cases, ejection of material seems to be connected with the accretion process. The ejection area and mechanism are uncertain (Garcia, Fey, \\& Thiébaut 2002, Shepherd 2003). They may emanate from the star, the disk (disk winds) or the star-disk interaction zone (X-winds), with the latter two possibilities being more favourable. In the X-wind theory (e.g. Shu, Najita, Shang, \\& Li 2000), the infalling material accretes through the disk until it reaches the inner truncation radius where a part of it is redirected outwards in a helical orbit by the effect of magnetic fields. In the disk wind theory (e.g. Königl \\& Pudritz 2000) material is driven outwards centrifugally from a magnetised disk.

\textbf{Role of magnetic fields in star formation}  Magnetic fields are believed to be present from the prestellar phase to the later phases of cloud collapse. Their role is expected to be important initially when the gas is coupled to the magnetic field. According to the theory of ambipolar diffusion neutral gas can diffuse through the ions, but the ions cannot move perpendicular to the magnetic field lines (Mouschovias 1976). Simulations of collapsing cores indicate that the presence of magnetic fields suppresses fragmentation (Hosking \\& Whitworth 2003). During the later stages of star formation (T Tauri phase) strong magnetic fields are generated by dynamo action in the central star and they may truncate the disk close to the star, account for the disk viscosity, and be responsible for the production of protostellar jets.

\textbf{Formation of massive stars}  Massive stars are usually observed at the centres of both low and high-mass clusters (see review by Stahler, Palla, \\& Ho 2000). Their formation mechanism could be similar to that of low-mass stars. However, there are two problems: (i) most massive stars have larger masses than the Jeans mass in the clouds within which they form, and thus during the cloud collapse process they should have fragmented into a number of stars, and (ii) the radiation
1.9. THESIS OUTLINE

pressure from the star should stop subsequent accretion of material from the infalling envelope. Massive stars may also form in mergers of lower-mass stars, or from runaway accretion processes in the denser regions of a protocluster.

Origin of the Sun The Sun and the solar system are atypical in many aspects. The Sun is a single, isolated star, though most stars form in binaries and clusters. Its high metallicity in comparison with the local galactic environment indicates an origin closer to the centre of the Galaxy or in an OB association. The gas-giant planets of extrasolar planetary systems are close to the central star, contrary to the gas planets of our solar system. Furthermore, the tilt of the ecliptic with respect to the Sun's equatorial plane suggests an encounter with another star.

1.9 Thesis outline

In this thesis we implement a Monte Carlo radiative transfer code with frequency distribution adjustment and use it to perform continuum radiative transfer simulations in spherical and non-spherical prestellar cores. We also extent the code to treat systems with arbitrary geometry resulting from SPH hydrodynamic simulations.

In Chapter 2, we implement the Monte Carlo radiative transfer method. This method uses a large number of monochromatic luminosity packets to represent the radiation transported through a medium. The luminosity packets are injected into the medium and interact (i.e. are absorbed and/or scattered) stochastically with it. When a packet is absorbed it is immediately reemitted so as to conserve energy. The frequency of the reemitted packet is chosen from a probability distribution function so as to correct from the packets reemitted previously from an incorrect frequency distribution. Thus, at the end of the simulation the correct temperature and SED of the medium is obtained, without iteration. The method is computationally efficient and can be applied to systems with arbitrary geometries for continuum radiative transfer calculations. We also perform several tests which show that the method is very accurate.

In Chapter 3, we apply the Monte Carlo radiative transfer code to study prestellar cores. These cores do not have an internal heating source; the heating is provided by the ambient interstellar radiation field. Initially, we study non-embedded cores, i.e. cores that are directly heated by the interstellar radiation field, and we compare our results with those of other authors. We then study cores that are embedded inside molecular clouds. We calculate dust temperature
distributions, SEDs and radial intensity profiles. We find that the temperatures of embedded prestellar cores are lower than the temperatures of non-embedded cores.

In Chapter 4, we extend our study to non-spherical prestellar cores. We examine two kinds of asymmetries: disk-like asymmetry (slightly flattened cores) and south-pole asymmetry (cores that are denser on one side). Our models predict features on the isophotal maps of such cores at wavelengths near the peak of the core emission (150-250 µm) indicative of the core structure and orientation. The resolution of current FIR telescopes is not high enough to observe these features but future space probes (e.g. Herschel, to be launched in 2007) should be able to detect them.

In Chapter 5, we use the Monte Carlo radiative transfer method to perform radiative transfer calculations in systems resulting from Smoothed Particle Hydrodynamics simulations. We use the SPH tree to construct the cells needed for the radiative transfer simulation, so that the Monte Carlo code could be implemented in future within SPH without much additional computational expense. We also develop a method to treat regions with large temperature gradients, i.e. regions near stars. We thoroughly test our method against previous calculations. The tests indicate that the method works reasonably well.

In Chapter 6, we study protostellar disks resulting from SPH simulations. We construct realistic models of protostellar disks and evolve them using SPH. We also perform 3-dimensional radiative transfer simulations on the disks. To test our radiative transfer method, we model the the GM Aurigae star/disk system and compare our results with those of previous studies.

Finally, in Chapter 7 we summarise the most important results of our study and discuss the future prospects for using Monte Carlo radiative transfer in hydrodynamic simulations.
Chapter 2

Monte Carlo Radiative Transfer

The Monte Carlo approach for equilibrium radiative transfer (Lefèvre et al. 1982, 1983; Wolf et al. 1999; Lucy 1999; Bjorkman & Wood 2001; Misselt et al. 2001; Ercolano et al. 2003a; Niccolini, Woitke & Lopez 2003), provides a way to study systems with arbitrary geometries. The method has been applied to a variety of systems, including stellar atmospheres (Lucy 1999), dusty galaxies (Bianchi et al. 2000; Misselt et al. 2001), planetary nebulae (Ercolano et al. 2003b), prestellar cores (Stamatellos & Whitworth 2003), protostellar envelopes (Whitney et al. 2003), and protostellar disks (Wood et al. 2002b). However, as with any Monte Carlo method, it is computationally expensive, especially when iteration is used.

Bjorkman & Wood (2001), extended an idea by Lucy (1999) and proposed a method to avoid iteration, by remitting photons as soon as they are absorbed, with a frequency distribution adjustment technique (see Baes et al. 2003, for a critical review of the method) that corrects for the incorrect spectrum of the previously re-emitted \( L \)-packets. This method avoids iteration and it is fast when compared to the traditional Monte Carlo radiative transfer methods.

2.1 Method overview

We implement a Monte Carlo continuum radiative transfer method that uses a large number of monochromatic luminosity packets (\( L \)-packets) to represent the radiation being transported through the computational domain. This radiation originates from discrete sources within the computational domain (i.e. stars), from diffuse emission within the domain (i.e. radiative cooling) and from the background radiation field incident on the boundary of the computational domain.
The $L$-packets are injected into the medium and interact stochastically with it (see Fig. 2.1). The medium itself is divided into a number of cells with given mass and uniform temperature. Each time an $L$-packet is scattered by a cell, a new direction is chosen using the Henyey & Greenstein (1941) scattering phase function. Each time an $L$-packet is absorbed by a cell, it raises the cell’s temperature and the packet is directly reemitted, so that the dust is in radiative equilibrium. The temperature of the cell is determined by equating the absorbed to the emitted luminosity. The frequency of the reemitted $L$-packet is chosen using a probability distribution function (PDF) which corrects for the $L$-packets that were emitted previously from the cell with an incorrect frequency distribution (Bjorkman & Wood 2001; Baes et al. 2003). Using this procedure the correct temperature distribution and spectrum of the system are obtained at the end of the simulation, when all packets have been propagated through the medium and escaped. The method does not use iteration, it accounts for both absorption and scattering, it is robust, it is very accurate (see tests by Bjorkman & Wood 2001, Stamatellos & Whitworth 2003), it conserves energy exactly, it can be parallelised easily and can treat systems with arbitrary geometries. In the next sections we describe the details of the method.

**Figure 2.1** Schematic representation of the Monte Carlo radiative transfer method. Luminosity packets are injected into the computational domain and interact stochastically with it until they escape.
2.2 System setup

Initially, we specify the system under study (both the medium where the \( L \)-packets propagate and the luminosity sources), so we need to define the following:

1. The physical extent of the system (see Fig. 2.1).

2. The position \( \mathbf{r}_* \) and the monochromatic luminosity \( L_\lambda \) of the sources inside and outside the computational domain. For example, in the case of a star, if we know the radius \( R_* \) and the temperature \( T_* \) of the star then \( L_\lambda = 4\pi R_*^2 \pi B_\lambda (T_*) \).

3. The monochromatic luminosity of the background radiation incident on the system \( L^B_\lambda \).

For example, in the case of an isotropic radiation field illuminating a spherical structure \( L^B_\lambda = 4\pi R_{\text{sphere}}^2 F^B_\lambda \). If the background radiation field has a blackbody spectrum with temperature \( T_B \), then \( F^B_\lambda = \pi B_\lambda (T_B) \).

4. The monochromatic luminosity of any diffuse sources of radiation \( L^{\text{diff}}_\lambda \), e.g. cooling radiation from the medium.

5. The properties of the dust (absorption and scattering opacities, scattering phase function) and the dust density distribution \( \rho(\mathbf{r}) \).

2.3 Monte Carlo theory

We make use of the fundamental principle of Monte Carlo methods, according to which we can sample a quantity \( \xi \in [\xi_1, \xi_2] \), from a probability distribution \( p_\xi \) using uniformly distributed random numbers \( \mathcal{R} \in [0, 1] \), by picking \( \xi \) such that

\[
\frac{\int_{\xi_1}^{\xi_2} p_\xi d\xi'}{\int_{\xi_1}^{\xi_2} p_\xi d\xi'} = \mathcal{R} \, . \tag{2.1}
\]

We use the above equation to chose a frequency for the emitted \( L \)-packets, their direction, their mean free path, the kind of interaction they have with the medium (absorption or scattering), and finally the new direction of a scattered \( L \)-packet or the new direction and frequency of a re-emitted \( L \)-packet.
2.4 \textit{L}-packet emission

\textit{L}-packet luminosity

We divide the luminosity of the source \( L \) into a large number \( N \) of monochromatic packets emitted in time \( \Delta t \). Therefore, the luminosity of each packet is

\[
\delta L = \frac{L}{N},
\]

and its energy

\[
\delta E = \frac{L \Delta t}{N}.
\]

We assign each \( L \)-packet a frequency \( \nu \), a direction \( \mathbf{k} \) and an optical depth \( \tau_{\nu} \), and then inject it into the medium.

\textit{L}-packet frequency

The specific intensity of the luminosity source serves as the probability distribution \( p_{\nu} d\nu \) of an \( L \)-packet to be emitted with frequency between \( \nu \) and \( \nu + d\nu \):

\[
p_{\nu} d\nu = I_{\nu} d\nu.
\]

Using the Monte Carlo fundamental principle (Eq. 2.1), we get

\[
\frac{\int_0^{\nu_0} I_{\nu}(T) d\nu}{\int_0^{\infty} I_{\nu}(T) d\nu} = R_{\nu},
\]

where \( R_{\nu} \) is a random number (\( R_{\nu} \in [0,1] \)). Solving the above for \( \nu_0 \), we obtain the frequency for each \( L \)-packet. Alternatively, we can reproduce the intensity distribution by dividing the frequency spectrum into a large number of bins, with each bin having a characteristic frequency \( \nu_{\text{bin}} = (\nu_1 + \nu_2)/2 \), where the frequencies \( \nu_1, \nu_2 \) define the beginning and end of the bin. Each bin corresponds to an integrated intensity \( I_{\text{bin}} = \int_{\nu_1}^{\nu_2} I_{\nu}(T) d\nu \). The total integrated intensity across the entire spectrum is \( I = \int_{0}^{\infty} I_{\nu}(T) d\nu \), so the fraction of \( L \)-packets that should be emitted with frequency \( \nu_{\text{bin}} \) is \( I_{\text{bin}}/I \), and the actual number of \( L \)-packets is \( n_{\text{bin}} = \text{INT}\{(NI_{\text{bin}}/I) + 0.5\} \). For systems with more than one source (e.g. another star, background radiation) we repeat the above procedure for each source.
24. L-PACKET EMISSION

L-packet initial position and direction

L-packets are emitted from a given point (point source), from the surface of a star or from the boundaries of the computational domain for a background radiation field. In the case of a point star, if we assume that it emits isotropically, then all directions are equally probable. In this case, the probability that an L-packet is emitted at polar angle between $\theta$ and $\theta + d\theta$ is

$$p_\theta d\theta = \frac{\sin(\theta) d\theta}{2}, \quad 0 \leq \theta \leq \pi,$$

and at azimuthal angle between $\phi$ and $\phi + d\phi$, is

$$p_\phi d\phi = \frac{d\phi}{2\pi}, \quad 0 \leq \phi < 2\pi.$$

Thus, applying the general Monte Carlo formula (Eq. 2.1) we get:

$$\theta = \cos^{-1}(1 - 2R_\theta),$$

and

$$\phi = 2\pi R_\phi,$$

where $R_\theta$ and $R_\phi$ are random numbers between 0 and 1. Thus, the direction of an emitted L-packet is

$$\hat{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z},$$

where

$$k_x = \sin \theta \cos \phi,$$

$$k_y = \sin \theta \sin \phi,$$

$$k_z = \cos \theta.$$

If an L-packet is launched from the boundary of the computational domain, as for example when a core is embedded in a isotropic background radiation field, then we specify using random numbers the position and the direction of the L-packet as it enters the computational domain (see Chapter 3).
Optical depth

The probability $p(\tau)$ that the optical depth an $L$-packet travels, before it interacts with the medium, is between $\tau$ and $\tau + d\tau$, is

$$p(\tau)d\tau = e^{-\tau}d\tau. \quad (2.12)$$

Thus, using Eq. (2.1), we have:

$$\int_0^\tau p(\tau)d\tau = R_\tau, \quad (2.13)$$

from which we obtain

$$\tau_\nu = -\ln R_\tau, \quad (2.14)$$

where $R_\tau \in [0,1]$.

### 2.5 Dust properties

The dust properties determine the opacity of the medium in which the radiation is propagating. We assume a single dust grain model (our code can easily be modified for treatment of multi-grain dust), with dust radius $r_d$ and dust internal density $\rho_d$. The geometric cross section of a dust grain is

$$\sigma_d = \pi r_d^2. \quad (2.15)$$

The cross sections for absorption and scattering are the following:

$$\sigma_{abs}(\lambda) = \sigma_d Q_{abs}(\lambda), \quad (2.16)$$

$$\sigma_{scat}(\lambda) = \sigma_d Q_{scat}(\lambda), \quad (2.17)$$

where $Q_{abs}(\lambda)$ and $Q_{scat}(\lambda)$ are the relevant efficiencies. For the calculations we use the opacity (i.e. cross section ) per unit mass $\kappa_{abs}(\lambda)$ and $\kappa_{scat}(\lambda)$:

$$\kappa_{abs}(\lambda) = \frac{\sigma_d Q_{abs}(\lambda) Z_d}{m_d}, \quad (2.18)$$

$$\kappa_{scat}(\lambda) = \frac{\sigma_d Q_{scat}(\lambda) Z_d}{m_d}, \quad (2.19)$$
where \( m_d = 4\pi r_d^3 \rho_d / 3 \) is the mass of one dust grain and \( Z_d \) the dust-to-gas ratio by mass. Finally, the total mass opacity (total extinction per unit mass) is

\[
\kappa(\lambda) = \kappa_{\text{abs}}(\lambda) + \kappa_{\text{scat}}(\lambda).
\] (2.20)

The value of \( Z_d \) in the general interstellar medium is estimated to be 1/100 but in circumstellar disks this ratio may be a factor of two or so larger, due to grain growth by depletion.

To implement the Monte Carlo radiative transfer method we need to know:

- The mass absorption opacity \( \kappa_{\text{abs}}(\lambda) \).
- The mass scattering opacity \( \kappa_{\text{scat}}(\lambda) \) or the albedo \( \gamma_\lambda \).
- The mean scattering cosine \( g_\lambda \).

The choice of the above depends on the system under study.

### 2.6 Cell construction

The computational domain in which the \( L \)-packets propagate is divided into a number of cells \( N_{\text{cells}} \), with volume \( V_i \) and mass \( m_i \), where \( i \) is the cell identifier (Fig. 2.1). Cell construction is very important for the accuracy of the results and also for the running time of the code. A cell defines a subregion of the computational domain in which the density and temperature are assumed to be uniform. In regions where the density or the temperature gradients are large, more cells are needed. Generally, we know the density beforehand and we can construct the cells accordingly. However, we do not know the temperature beforehand. Therefore, we must either make an educated guess about the temperature gradients, or we perform a first run to get an idea about how temperature varies from cell to cell and then re-adjust the computational grid.

We can fulfil both of the above conditions by constructing cells with dimensions \( S_{\text{cell}} \) less than, or on the order of, the local directional scale-heights,

\[
S_{\text{cell}} \lesssim \text{MIN} \{ h_\rho, h_T \}.
\] (2.21)

In the direction given by the unit vector \( \mathbf{k} \), the directional scale heights are

\[
h_\rho = \left( \frac{\left| \mathbf{k} \cdot \nabla \rho \right|}{\rho} \right)^{-1},
\] (2.22)
\[ h_T = \left( \frac{|k \cdot \nabla T|}{T} \right)^{-1}. \]  

(2.23)

Thus, theoretically, we can construct a grid with a very large number of cells to satisfy the accuracy requirements in calculating temperature. Unfortunately, as usually happens with computational methods, we have to lower the demands on accuracy if we want to get results in an acceptable amount of time. If we have a large number of cells we need a large number of \( L \)-packets to interact with these cells so that the statistical noise of the calculation (of the order of \( 1/\sqrt{N_{\text{abs}}} \)) is small. This means that we have to use a larger number of \( L \)-packets if we want to have better statistical results, but, of course, more \( L \)-packets means an increase in the computational time. We should note here that the number of \( L \)-packets required for good statistical results also depends on the optical depth of the computational domain. If the optical depth is large, then \( L \)-packets experience many interactions before they exit the computational domain, and, so fewer \( L \)-packets are required than in the case of a small optical depth computational domain, with the same number of cells. Following the same reasoning we can have smaller cells in regions where there are more \( L \)-packets (e.g. close to the luminosity source). Finally we should emphasise that the above are only general guidelines which give a rough idea of how to construct cells. Each problem has individual characteristics that affect accuracy and computational time, and should be treated accordingly.

2.7 \( L \)-packet propagation

\( L \)-packets propagate into the medium, according to their optical depth until they reach an interaction point. If \( \tau_{\text{total}} \) is a \( L \)-packet’s total optical depth then in order to calculate the distance it propagates into the computational domain before it interacts with it, we need to calculate the line integral along the path of the \( L \)-packet,

\[ \Delta S = \int_0^{\tau_{\text{total}}} \frac{d\tau}{\kappa_\lambda \rho}. \]  

(2.24)

If the opacity \( \kappa_\lambda \rho \) is uniform then the above equation becomes \( \Delta S = \tau_{\text{total}} / (\kappa_\lambda \rho) \), but in the general case it is not possible to calculate the preceding integral analytically. Our approach is to approximate this integral with a sum,

\[ \Delta S = \sum_i \frac{\delta \tau_i}{\kappa_\lambda \rho_i} = \sum_i \delta S_i. \]  

(2.25)
2.8. THERMAL EQUILIBRIUM OF DUST GRAINS

The element step $\delta S_i$ through which $L$-packet propagates should be small so that along this step the density remains almost constant. Also the element optical depth, $\delta \tau_i = \kappa \lambda \rho_i \delta S_i$, should not be larger than the remaining total optical depth of the $L$-packet $\tau_i$. $\tau_i$ is just the optical depth that the $L$-packet still has to propagate after $i$ steps,

$$\tau_i = \tau_{\text{total}} - \sum_{j=0}^{i} \delta \tau_j . \quad (2.26)$$

To satisfy the above requirement we chose an element step according to the following condition:

$$\delta S_i = \text{MIN} \{ \eta_{\rho} h_{\rho}, \eta l, (\tau_i + \epsilon) l, \eta_{\gamma} |r| \} , \quad (2.27)$$

where $l = (\kappa \lambda \rho_i)^{-1}$, and $\eta_{\rho}$, $\eta$, $\eta_{\gamma}$ are constants that determine the accuracy we demand (typical values are between 0.1 and 1). The first term $(\eta_{\rho} h_{\rho})$ ensures that the density does not change much in one element step (where $h_{\rho}$ is the density scale height in the direction that the $L$-packet propagates), the second term $(\eta l)$ ensures that the element step is less than the mean free path of the $L$-packet and the third term $[(\tau_i + \epsilon) l]$ takes effect on the last step ($\epsilon$ is a very small number). The last term $(\eta_{\gamma} |r|)$ ensures that the distance the $L$-packet travels in one element step is less than the distance from the luminosity source. This term comes into effect when a gap exists around the source. The smaller the factors $\eta_{\rho}$, $\eta$, $\eta_{\gamma}$ are chosen, the better the accuracy in propagating packets, but the larger the computational time.

We propagate the $L$-packet following the above procedure until $\tau_i \leq 0$ or until the $L$-packet escapes from the computational domain. If the $L$-packet escapes, then it is placed in frequency and direction bins. If, after propagating, it is still in the computational domain, it is either scattered or absorbed, depending on the albedo. We generate a random number $\mathcal{R}_{\gamma} \in [0, 1]$, and if it is less than the albedo then the $L$-packet is scattered, otherwise it is absorbed.

2.8 Thermal equilibrium of dust grains

2.8.1 $L$-packet absorption

When an $L$-packet is absorbed in a cell its energy raises the cell’s temperature, and then it is reemitted with a new frequency. The new temperature is calculated by the balance between
absorbed and emitted energy, assuming LTE,

\[ E_i^{\text{abs}} = E_i^{\text{em}} \]  

(2.28)

If \( N_i \) is the total number of \( L \)-packets absorbed by a cell, then the total energy absorbed by the cell is

\[ E_i^{\text{abs}} = N_i \delta E = N_i (L \Delta t / N) , \]  

(2.29)

and the total energy emitted

\[ E_i^{\text{em}} = 4 \pi \Delta t \int_{\text{cell}} j_\nu \, d\nu \, dV_i = 4 \pi \Delta t \int_0^\infty \kappa_\nu B_\nu (T_i) \, d\nu \int_{\text{cell}} \rho \, dV_i \Rightarrow \]

\[ E_i^{\text{em}} = 4 \pi \Delta t \, m_i \int_0^\infty \kappa_\nu B_\nu (T_i) \, d\nu \]  

(2.30)

where \( T_i \) the temperature of the cell and \( m_i \) its mass. Equating the absorbed with the emitted energy, we obtain (Bjorkman & Wood 2001)

\[ \sigma T_i^4 = \frac{N_i (L/N)}{4 \kappa_P(T_i) m_i} , \]  

(2.31)

where

\[ \kappa_P(T_i) = \frac{\int_0^\infty \kappa_\nu B_\nu (T_i) \, d\nu}{\sigma T_i^4 / \pi} , \]  

(2.32)

is the Planck mean opacity. This equation has to be solved for a given cell every time an \( L \)-packet is absorbed by that cell.

2.8.2 \( L \)-packet reemission

Solution using iteration

In the standard approach to Monte Carlo radiative equilibrium computations all source luminosity packets are launched and followed until they leave the computational domain or are absorbed, while recording the cell in which each absorption takes place. Then the dust temperature of each cell is calculated from the radiative equilibrium condition (Eq. 2.28). In order to conserve energy, each absorbed luminosity packet is reemitted according to the new emissivity of the dust cell by which it was absorbed, \( j_\nu = \kappa_\nu B_\nu (T) \). Each of these re-emitted \( L \)-packets is again followed through the computational domain until it is either absorbed or escapes. The
temperature of each cell is then updated taking into account the additionally absorbed packets. Afterwards, a new set of $L$-packets is re-emitted and so on. This procedure hence naturally leads to an iteration, which stops when the temperature of each cell converges.

**Solution using the frequency distribution adjustment (FDA) method**

Lucy (1999) argues that a much faster convergence could be achieved by applying a temperature correction and re-emission immediately after each individual absorption event. Thus, every time an $L$-packet is absorbed, the cell acquires a new temperature $T + \Delta T$ and a new $L$-packet is re-emitted with the new emissivity of the cell $\kappa_\nu B_\nu (T + \Delta T)$. This $L$-packet is followed until it either leaves the computational domain or it is absorbed again. The re-emitted $L$-packets hence enter the radiative transfer alongside the source $L$-packets, and also contribute to the heating of the dust. As a consequence, the temperature distribution and the radiation field after the last $L$-packet leaves the computational domain, are closer to the equilibrium state, and fewer iterations are necessary to reach convergence.

An extension of the idea of Lucy (1999) has been proposed by Bjorkman & Wood (2001). In the Bjorkman & Wood scheme the frequency of the reemitted $L$-packet is chosen so as to correct for the $L$-packets that were reemitted previously with an incorrect spectrum. Consider some stage in the Monte Carlo process, where $k$ $L$-packets have already been absorbed and reemitted in a certain cell. The temperature of the cell has been gradually increasing from zero to $T$, and assume that we have somehow managed to fine-tune the re-emission frequencies such that collectively they correspond to the emissivity $\kappa_\nu B_\nu (T)$. Now assume a $(k+1)$th $L$-packet is being absorbed, which increases the dust cell temperature to $T + \Delta T$, such that the emissivity changes to $\kappa_\nu B_\nu (T + \Delta T)$. To preserve radiative equilibrium, a new $L$-packet packet must be emitted with luminosity $\delta L$. Its frequency must be chosen in such a way that the ensemble of the $k+1$ re-emitted $L$-packets from this cell correspond to the new emissivity $\kappa_\nu B_\nu (T + \Delta T)$. Bjorkman & Wood (2001) argue that this can be satisfied if the $(k+1)$th frequency corresponds to the emissivity difference

$$
\Delta j_\nu = \kappa_\nu \left[ B_\nu (T + \Delta T) - B_\nu (T) \right].
$$

(2.33)
The \((k + 1)\)th frequency should hence be drawn from the normalised PDF

\[
p_{\nu} (\nu) \, d\nu = \frac{\kappa_\nu [B_\nu(T + \Delta T) - B_\nu(T)] \, d\nu}{\int_0^\infty \kappa_\nu [B_\nu(T + \Delta T) - B_\nu(T)] \, d\nu}.
\] (2.34)

This PDF is everywhere positive, because the Planck function is an increasing function of temperature. When the difference \(\Delta T\) between the two temperatures is small, this expression can be approximated by

\[
p_{\nu} \, d\nu \approx \frac{\kappa_\nu B'_\nu(T) \, d\nu}{\int_0^\infty \kappa_\nu B'_\nu(T) \, d\nu},
\] (2.35)

where \(B'_\nu(T)\) is the temperature derivative of the Planck function (see Fig. 2.2 for a demonstration). The re-emitted \(L\)-packet is also given a new optical depth and a new direction, and continues its voyage until it escapes from the computational domain.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2_2.png}
\caption{The frequency of the reemitted \(L\)-packet is chosen from the difference of the cell emissivities before and after the absorption of the packet. \textbf{Left:} Emissivity before absorbing a \(L\)-packet (e.g., cell temperature 400K) and after absorbing a \(L\)-packet (e.g., cell temperature 600K). \textbf{Right:} Difference in the emissivities (400-600 K) (Note: We have exaggerated the difference in cell temperature before and after the absorption of a \(L\)-packet for demonstration purposes).}
\end{figure}

Bjorkman & Wood (2001) tested their method on a set of benchmark models presented by Ivezić et al. (1997). They found good agreement with the benchmark results, and concluded that their FDA method works well. There are two arguments, however, that made us doubt whether
this method is really an exact rigorous method, or whether it is just a very good and convenient approximation:

1. Eq. (2.34) suggests that one can always adjust the spectrum of $k$ emitted frequencies from one PDF (corresponding to $T$) to another one (corresponding to $T + \Delta T$) by just adding one single frequency. We intuitively expect that this can be possible if the difference between these two temperatures is small, but that this is very hard or impossible if the temperature difference is large.

2. It seems logical that adjusting a sampled distribution by adding one more data point is much harder if many frequencies have been sampled before, than when only a small number of frequencies have been sampled. Therefore, one would in general expect that the adjustment PDF $p_{\text{adj}}(\nu)d\nu$ would be an explicit function of $k$.

In order to investigate this in detail, we study the issue of adjusting the behaviour of a set data points by adding new data points in a more general context in the next section, and then apply the results to Monte Carlo radiative transfer.

2.9 The adjustment probability distribution function

2.9.1 Adjusting a sampled distribution for a general PDF

Assume $p(x)dx$ and $p'(x)dx$ are two arbitrary PDFs, and consider the following question: is it possible to construct a third PDF $p_{\text{adj}}(x)dx$ which satisfies the condition that any set of $n + m$ data points, where the $n$ first data points are drawn randomly from $p(x)dx$ and the last $m$ ones are drawn randomly from $p_{\text{adj}}(x)dx$, represents a set of data drawn randomly from $p'(x)dx$? In other words, can we find an adjustment PDF that adjusts an arbitrary original PDF into an arbitrary altered PDF?

The solution of this problem is based on the definition that the probability that any data point drawn randomly from a PDF $p(x)dx$ lies between $x$ and $x + dx$ equals $p(x)dx$. Hence, when we draw $n$ random data points from this PDF, the expected number of them between $x$ and $x + dx$ equals $np(x)dx$. Applying this to the total data set of $m + n$ data points, we can find the form of the required PDF. Because we can simply add the number of data points in each interval, the expected number of data points between $x$ and $x + dx$ is be given by

$$dN(x) = np(x)dx + m p_{\text{adj}}(x)dx.$$  (2.36)
On the other hand, this sample of \( m + n \) data points should represent a sample drawn randomly from the PDF \( p'(x)dx \), and therefore we also obtain

\[
dN(x) = (n + m)p'(x)dx.
\] (2.37)

From these two expressions, we find that the adjustment PDF should have the form

\[
p_{\text{adj}}(x)dx = \left( 1 + \frac{n}{m} \right)p'(x)dx - \frac{n}{m}p(x)dx.
\] (2.38)

However, it is not always guaranteed that this function is a valid PDF, because there is no a priori guarantee that it is positive over its entire domain. If this function does become negative, this means that it is impossible to adjust the PDF \( p(x)dx \) to \( p'(x)dx \) by adding \( m \) data points.

Whether or not it is possible to adjust one PDF into another one depends both on the particular PDFs involved and on the ratio \( k \equiv n/m \) of the number of data points already sampled to the number of data points which can be added. Logically, it should be easier to transform one PDF into another one if the distributions are very similar, than when they are very different. Also, it should in general be easier to change one distribution into another one if many data points can be added to a few sampled before \( (m \gg n) \), than when only a few ones can be added to a large set of already existing data \( (n \gg m) \).

Baes et al. (2003) demonstrate the adjustment of one PDF to another for gaussian distributions. They show that if we want to adjust the original gaussian distribution into another gaussian distribution with the same dispersion but a different mean, the resulting adjustment PDF is always negative at some point, no matter how small is the shift in the mean or the relative number of data points to add. On the other hand, if we want to alter the original PDF to a PDF with the same mean but a larger dispersion, they find that this is possible in some cases. When the relative number of data points to add is too small or when the dispersion increase is too large, however, the adjustment is not possible.

### 2.9.2 Application to Monte Carlo radiative transfer

In the Monte Carlo radiative transfer problem, we want to adjust a sample of \( k \) frequencies drawn randomly from the PDF

\[
p(\nu)\,d\nu = \frac{\kappa_{\nu} B_{\nu}(T)}{\int_0^{\infty} \kappa_{\nu} B_{\nu}(T)\,d\nu} \,d\nu
\] (2.39)
2.9. **THE ADJUSTMENT PROBABILITY DISTRIBUTION FUNCTION**

to a sample of \( k + 1 \) frequencies drawn from the PDF

\[
p'(\nu) d\nu = \frac{\kappa_\nu B_\nu(T + \Delta T)}{\int_0^\infty \kappa_\nu B_\nu(T + \Delta T) d\nu},
\]

by adding just one \( L \)-packet. Applying Eq. (2.38), we find that the last emitted \( L \)-packet should have a frequency drawn from the adjustment PDF

\[
p_{adj}(\nu) d\nu = (1 + k) \frac{\kappa_\nu B_\nu(T + \Delta T)}{\int_0^\infty \kappa_\nu B_\nu(T + \Delta T) d\nu} - k \frac{\kappa_\nu B_\nu(T)}{\int_0^\infty \kappa_\nu B_\nu(T) d\nu}.
\]

This formula can easily be interpreted in a physical way. When the \((k+1)\)th \( L \)-packet is absorbed the temperature rises from \( T \) to \( T + \Delta T \). This last \( L \)-packet should then be re-emitted with a frequency sampled from the PDF corresponding to the new temperature, i.e.

\[
P_{k+1}(\nu) d\nu = \frac{\kappa_\nu B_\nu(T + \Delta T)}{\int_0^\infty \kappa_\nu B_\nu(T + \Delta T) d\nu}.
\]

Additionally, we must compensate for the \( k \) \( L \)-packets that were emitted previously with the incorrect frequency distribution. The required correction to this frequency distribution is simply the difference between the new and the old PDF

\[
P_k(\nu) d\nu = \frac{\kappa_\nu B_\nu(T + \Delta T)}{\int_0^\infty \kappa_\nu B_\nu(T + \Delta T) d\nu} - \frac{\kappa_\nu B_\nu(T)}{\int_0^\infty \kappa_\nu B_\nu(T) d\nu}.
\]

The above procedure is equivalent to emitting just one \( L \)-packet with the combined propability distribution function \( P_{k+1} + kP_k \), as given by Eq. (2.41).

However, it is not guaranteed that the function in Eq. (2.41) corresponds to a valid PDF, because it can be negative. This is illustrated in Fig. 2.3, where we plot the adjustment PDF \( p_{adj}(\nu) \) for \( T = 20 \) K and different values of the parameters \( \Delta T \) and \( k \). The opacity function adopted is a simple power law of frequency, \( \kappa_\nu \propto \nu^2 \). For small values of \( k \), the adjustment PDF is positive for a large range of temperature shifts. However, when the number of previously generated frequencies \( k \) is high, the adjustment PDF is positive only for the smallest values of \( \Delta T \). This behaviour is also illustrated in Fig. 2.4, where we explicitly show the region in \((k, T, \Delta T)\) parameter space where the adjustment in possible. The red diagonal lines (different lines are shown for different values of \( T \), but there is hardly any dependence on \( T \)) mark the border between positive and negative adjustment PDFs. For each number of data points \( k \) and each temperature \( T \), there is a maximum temperature increase \( \Delta T_{max}(T, k) \) that can be allowed
Figure 2.3  Examples of the adjustment PDF (2.41) for \( \kappa_\nu \propto \nu^2 \) and \( T = 20 \) K. The four different panels show the adjustment PDF for various values of \( k \), as noted on the graph. In each panel, the different curves correspond to different values of the temperature increase, increasing from \( \Delta T = 0.02 \) K (cyan) to \( \Delta T = 2 \) K (red).

for adding one \((k + 1)\)th frequency \( L \)-packet packet. As expected, this maximum temperature increase decreases strongly with increasing \( k \).

2.9.3  Comparison with the Bjorkman & Wood (2001) adjustment PDF

The calculation in the previous subsection has shown that the adjustment PDF in Eq. (2.34) proposed by Bjorkman & Wood is in general not the same as the adjustment PDF (Eq. 2.41). Moreover, we showed that the latter does not represent a proper PDF for all of the parameters \((k, T, \Delta T)\), as for a given \( k \) and \( T \) there is a critical value of \( \Delta T \), above which the adjustment PDF becomes negative. This observation suggests that an exact FDA procedure in Monte Carlo radiative transfer might not always be possible.

It is important to realise, however, that not the entire \((k, T, \Delta T)\) parameter space is covered during the simulation. Indeed, if a dust cell has a given temperature \( T \) after absorbing and re-emitting \( k \) \( L \)-packets, and the \((k + 1)\)th \( L \)-packet is absorbed, the temperature rise \( \Delta T \) is determined by the requirement of radiative equilibrium (Eqs. 2.29-2.30),

\[
\int_0^\infty \kappa_\nu B_\nu(T + \Delta T) \, d\nu = \frac{(k + 1) \, \delta L}{4\pi M}.
\]  

(2.44)

For the opacity function \( \kappa_\nu \propto \nu^2 \), the temperature increase \( \Delta T \) can be calculated explicitly for each \( T \) and \( k \). Using the expression

\[
\int_0^\infty \nu^2 B_\nu(T) \, d\nu \propto T^6,
\]  

(2.45)
Figure 2.4 Region in \((k, T, \Delta T)\) parameter space in which the adjustment PDF (Eq. 2.41) is positive (for opacity \(\kappa_\nu \propto \nu^2\)). Different solid lines correspond to different values of the temperature \(T\), but there is hardly any dependence on \(T\). Each line shows for a given \(T\) and \(k\) the maximum temperature increase \(\Delta T\) such that the adjustment PDF is positive. Hence, underneath the solid diagonal lines, adjustment is possible, above these lines, adjustment is impossible. The dotted line indicates the relative temperature increase expected from the radiative equilibrium requirement (see Section 2.9.3).

One obtains after some algebra

\[
\Delta T(T, k) = T \left[ \left( 1 + \frac{1}{k} \right)^{1/6} - 1 \right].
\] (2.46)

This function is plotted as the dotted line in Fig. 2.4. This plot shows that \(\Delta T(T, k) < \Delta T_{\text{max}}(T, k)\), i.e. at every step in the Monte Carlo simulation, the temperature increase is always small enough that the adjustment PDF is positive. This assures us that the FDA method is applicable to radiative equilibrium Monte Carlo transfer computations.

Knowing that the adjustment PDF (Eq. 2.41) is always positive for the expected temperature increase, we can compare the results with those of Bjorkman & Wood. From Eq. (2.44), we obtain

\[
\frac{\int_0^\infty \kappa_\nu B_\nu(T + \Delta T) \, d\nu}{\int_0^\infty \kappa_\nu B_\nu(T) \, d\nu} = \frac{k + 1}{k}.
\] (2.47)

If we use this expression to eliminate \(k\) from the adjustment PDF (Eq. 2.41), we find

\[
p_{\text{adj}}(\nu) \, d\nu = \frac{\kappa_\nu [B_\nu(T + \Delta T) - B_\nu(T)] \, d\nu}{\int_0^\infty \kappa_\nu [B_\nu(T + \Delta T) - B_\nu(T)] \, d\nu} \equiv p_{\text{nW}}(\nu) \, d\nu,
\] (2.48)

where \(p_{\text{nW}}(\nu)\) is the original radiative equilibrium PDF.
i.e. we recover the adjustment PDF proposed by Bjorkman & Wood (2001).

2.10 \textbf{L}-packet scattering

If the scattering is isotropic then all we have to do is to choose a new random direction, using two random numbers, the same way we did for the case of emitting an \textit{L}-packet from a point radiation source. However, in many cases scattering is not isotropic, meaning that some directions are more favourable than other directions. Anisotropic scattering can be described using the scattering phase function \(p(\theta_{\scat})d\theta_{\scat}\) that gives the probability that an \textit{L}-packet of wavelength \(\lambda\) is scattered through an angle between \(\theta_{\scat}\) and \(\theta_{\scat} + d\theta_{\scat}\). We use an analytic scattering phase function due to Henyey & Greenstein (1941),

\[
p(\theta_{\scat}) d\theta_{\scat} = \frac{(1 - g^2) \sin(\theta_{\scat})}{2 \left[ (1 + g^2) - 2g \cos(\theta_{\scat}) \right]^{3/2}} d\theta_{\scat}, \tag{2.49}
\]

where \(g\) is the mean scattering cosine,

\[
g \equiv \langle \cos(\theta_{\scat}) \rangle = \int_0^\pi \cos(\theta_{\scat}) p(\theta_{\scat}) d\theta_{\scat}. \tag{2.50}
\]

In general \(g\) is a function of wavelength. If \(g > 0\) then the scattering is mainly in forward directions, and if \(g < 0\) then the scattering is mainly backwards. Isotropic scattering corresponds to \(g = 0\).

To choose the direction of the \textit{L}-packet in the case of anisotropic scattering we use the Monte Carlo fundamental theorem and we set the integrated probability equal to a random number \(\mathcal{R}_\theta \in [0, 1]\):

\[
P(\theta_{\scat}) = \int_0^{\theta_{\scat}} p(\theta) d\theta = \mathcal{R}_\theta. \tag{2.51}
\]

We then solve for the scattering angle cosine,

\[
\cos(\theta_{\scat}) = \frac{1}{2g} \left[ 1 + g^2 - \left( \frac{1 - g^2}{1 + g - 2g\mathcal{R}_\theta} \right)^2 \right]. \tag{2.52}
\]

We should point out that the scattering angle \(\theta_{\scat}\) refers to the change in the direction of the \textit{L}-packet relative to its previous direction, so this angle is measured in the \textit{L}-packet’s pre-
scattering idiosystem*. This means that we need to find the new direction of the $L$-packet in the coordinate frame of the computational domain. For this calculation see Appendix A.

2.11 SEDs and isophotonal maps

While an $L$-packet propagates through the computational domain we keep a record of its position, direction and frequency, but also other information, such as (i) how many times it has interacted with the computational domain and how it has interacted, (ii) the position of the last interaction, (iii) the total distance travelled. Once the $L$-packet escapes from the computational domain we record its frequency, position and direction. When all the $L$-packets have escaped we construct the spectral energy distribution (SED) of the system at different viewing angles by placing the $L$-packets in frequency and direction-of-observation bins. To construct an isophotonal map of the system is a little more complicated (see Appendix B).

2.12 Code implementation and efficiency

The general flowchart of the radiative transfer code (named PHAETHON, after a Greek mythical hero) is shown in Fig. 2.5. Phaethon was the son of Helios (the Sun God) and the nymph Clymene. He grew up not knowing who his father was, but when he finally discovered his noble descent he was very excited and set off to meet his father to the east where the Sun rises. His father was so delighted to meet him that he promised to offer him anything he wanted. Phaethon asked to ride the chariot of the Sun along the sky for one day. Helios was very reluctant to do that because driving the chariot of the Sun is not an easy task; he tried to change his son’s mind but finally he had to give in since he had already given his word. The next day Phaethon climbed into the golden chariot, but the horses sensed the inexperienced hands of the young boy and started running way off their usual tracks, too far away from or too close to the Earth. The Earth was overheated and vast areas were turned into desert. Humans were devastated and asked for help from Zeus. Zeus had no other option but to kill him with a thunderbolt saving the Earth from destruction.

The shaded parts in this diagram refer to procedures that, in general, need to be done more than once for each luminosity packet and consequently are those that dictate the efficiency of

*From the Greek word ἰδιοστυξια that means self-system.
Figure 2.5 PHAETHON: Code flow chart. Luminosity packets are injected into the computational domain, propagate, interact and finally escape. The shaded parts in this diagram refer to procedures that, in general, need to be done more than once for each \textit{L}-packet. The propagation routine is the most computationally expensive routine.

the code. The calculations indicate that the \textit{L}-packet propagation routine takes about 25-50\% of the computational time, depending on the specific problem. Thus, this is the routine that should be targeted by any efforts to diminish the running time of the code. Time efficiency is very important since a large number of \textit{L}-packets is needed for good statistical results. Some general strategies that can help reduce the computational time of the code, whilst maintaining good results, are listed here:

1. \textit{The specific nature of the system we examine should be taken into account}. For example, in the case of a uniform density sphere we can propagate each \textit{L}-packet in a single step, saving a huge amount of computational time.

2. \textit{Any kind of symmetry should be exploited}. When the system is symmetric we need fewer \textit{L}-packets to have good statistical results, and fewer \textit{L}-packets means less computational time. One dimensional problems (e.g. spherically symmetric systems) require far fewer \textit{L}-packets than three dimensional problems.
3. Use look-up tables to solve equations. The use of tables to solve for the cell temperature after absorbing an $L$-packet and then to calculate the reemission frequency of the new $L$-packet, can reduce the computational times especially in cases where each $L$-packet undergoes a large number of interactions (e.g. in a large optical depth environment).

4. Code parallelisation. The nature of this radiative transfer method means that each $L$-packet is treated independently. To calculate the temperature of a cell we just need to know the number of luminosity packets absorbed in that cell; the order does not matter. Thus, each processor of a parallel machine could be used to treat a single $L$-packet until it escapes from the computational domain, meaning that it would be quite easy to parallelise the code using an automated parallelisation protocol such as OPENMP. The only problem would arise when an $L$-packet were absorbed by a cell while another $L$-packet had just been absorbed by the same cell and calculations of the cell temperature and $L$-packet reemission were ongoing. The problem that would arise is that during the calculation the value of the cell luminosity variable changes. The probability of this happening would be relatively small, and even in this case the absorption of one more $L$-packet would change the luminosity absorbed by the cell only by a small fraction and, consequently, the temperature would also change only by a small fraction. Thus, we could be confident that the frequency of the re-emitted $L$-packet would be calculated with high precision.

Computational details

The code is implemented in C. It comprises 3 different parts: (i) the code to calculate the re-emission probabilities from the mass opacity, (i) the code to construct the radiative transfer grid (i.e. construct RT cells, and calculate the density and mass of each cell), and (iii) the main radiative transfer code, which emits, propagates and interacts $L$-packets, and finally places the escaping packets in direction-of-observation bins and calculates SEDs and isophotal maps.

The running time of the code depends on the number of $L$-packets used and on the specific system under study (we use a dual 2.4 GHz processor PC with 1 GB RAM). Typical running times for obtaining temperatures and SEDs with low statistical noise are $\sim 50 - 100$ minutes (using around $10^7$ packets). For producing isophotal maps with low statistical noise we need $> 10^8 - 10^9$ packets, and the computational time could be up to 7 days. These runnings times are comparable with other Monte Carlo and ray-tracing radiative transfer methods. The memory requirements of the code are average ($\sim 200$ MB).


2.13 Code tests

We test PHAETHON against benchmark calculations proposed by Ivezić et al. (1997) for a star surrounded by a spherical envelope, first with constant density, and then for density decreasing as \( r^{-2} \). The code reproduces the results of Ivezić et al., and also the results of Bjorkman & Wood (2001) for disk-like structures embedded in an envelope. We also test the code against the “thermodynamic equilibrium test”, in which a system is illuminated by a uniform blackbody radiation field of a certain temperature. All tests indicate that the code is very accurate. In the next subsections we present these tests.

2.13.1 Test 1: Spherical structures (Ivezić et al. 1997)

We perform the test developed by Ivezić et al. (1997) in which they used three different, well established radiative transfer codes, with different numerical schemes, to solve a set of benchmark spherical geometry problems. In all cases these methods gave differences smaller that 0.1% and so, as Ivezić et al. noted, the solution can be considered exact. This test was adapted to this method by Bjorkman & Wood (2001).

Table 2.1  Ivezić et al. (1997) test parameters

<table>
<thead>
<tr>
<th>( p )</th>
<th>( \tau_{\mu m} )</th>
<th>( R_{\text{dust}}/R_* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>8.44</td>
</tr>
<tr>
<td>0</td>
<td>10</td>
<td>8.46</td>
</tr>
<tr>
<td>0</td>
<td>100</td>
<td>8.60</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>9.11</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>11.37</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>17.67</td>
</tr>
</tbody>
</table>

The system under study is a spherical cloud, with a star in the centre and a central cavity devoid of dust. We assume that the temperature of the star is \( T_* = 2500K \) and the dust destruction temperature \( T_{\text{sub}} = 800K \). We use the dust destruction radii \( R_{\text{dust}} \) listed in Table (2.1). These radii have been chosen to match the parameters used by Ivezić et al. (1997). The cloud extends out to radius \( R_{\text{max}} = 10^3 R_{\text{dust}} \). We investigate two different density profiles,

\[
\rho = \rho_0 \left( \frac{R_{\text{dust}}}{r} \right)^p ,
\]  

(2.53)
for $p = 0$ (uniform density envelope) and $p = 2$, where

$$
\rho_0 = \frac{\tau_\lambda}{(\kappa_\lambda + \sigma_\lambda)(1 - R_{\text{dust}}/R_{\text{max}})} \begin{cases} 
1/R_{\text{max}}, & p = 0 \\
1/R_{\text{dust}}, & p = 2
\end{cases}.
$$

(2.54)

Like Bjorkman & Wood (2001), we divide the cloud into $N_r = 200$ radial cells, and choose equal radial optical depth cells with radii

$$
\frac{r_i}{R_{\text{dust}}} = \begin{cases} 
i\Delta r + 1, & p = 0 \\
N_f/(N_f - i), & p = 2
\end{cases},
$$

(2.55)

where $\Delta r = (R_{\text{max}}/R_{\text{dust}} - 1)/N_r$ and $N_f = N_r/(1 - R_{\text{dust}}/R_{\text{max}})$. For this test we use an analytical law for the opacity, that corresponds to spherical amorphous grains with radius 0.16 $\mu m$ (see Fig. 2.6, left),

$$
\frac{\kappa_\nu}{(\kappa + \sigma)_{1\mu m}} = 0.5 \begin{cases} 
1, & \lambda < 1 \mu m \\
1/\mu m/\lambda, & \lambda > 1 \mu m
\end{cases}
$$

(2.56)

$$
\frac{\sigma_\nu}{(\kappa + \sigma)_{1\mu m}} = 0.5 \begin{cases} 
1, & \lambda < 1 \mu m \\
(1/\mu m/\lambda)^4, & \lambda > 1 \mu m
\end{cases}.
$$

(2.57)
Figure 2.7  Left: SED of a spherically symmetric envelope with uniform density, for different optical depths ($\tau_{\mu\mu}=1, 10, 100$). The dotted line represents the intrinsic spectrum of the star. Right: Temperature profiles of the structures described.

Figure 2.8  Left: SED of a spherically symmetric envelope with density $\rho \propto r^{-2}$ for different optical depths ($\tau_{\mu\mu}=1, 10, 100$). The dotted line represents the intrinsic spectrum of the star. Right: Temperature profiles of the structures described.
In Fig. 2.6, right, we show the cumulative re-emission probability. The cumulative re-emission probability at a given wavelength for a given temperature shows the fraction of \( L \)-packets that must be re-emitted with wavelengths down to the specified wavelength. As the temperature increases, the re-emission cumulative probability moves towards shorter wavelengths (see Fig. 2.6).

The results of the calculations for surrounding envelopes with different optical depths (\( \tau_{\mu m} = 1, 10, 100 \)) are seen in Fig. 2.7, for a uniform density envelope and in Fig. 2.8 for an envelope with density \( \rho \propto r^{-2} \). We note that:

- There is a long-wavelength excess in the spectrum caused by emission from the envelope.
  The envelope absorbs \( L \)-packets emitted from the star and re-emits those \( L \)-packets at longer wavelengths because its temperature is much less than the star’s temperature.
- The larger the optical depth of the envelope the more radiation is absorbed and re-emitted at longer wavelengths.
- The larger the optical depth, the lower the temperature of the envelope. This is because when the optical depth of the envelope is large, the photons emitted by the central source are absorbed very close to the centre and then they are reemitted at long wavelengths and escape the computational domain without interacting with the outer parts of the envelope.
- There is more FIR radiation emitted from the uniform density sphere than from the \( \rho \propto r^{-2} \) sphere with the same optical depth.
- These results are in excellent agreement with the calculations of Ivezić et al. (1997) and Bjorkman & Wood (2001).

### 2.13.2 Test 2: Disk-like structures (Bjorkman & Wood 2001)

For this test, we use a star with \( T_* = 3500K \) at the centre of an envelope with density profile

\[
\rho = \rho_0 \frac{(R_{\text{dust}}/r)^2}{1 + f^2 \cos^2 \theta},
\]

(2.58)

where \((r, \theta)\) are the polar coordinates and \( f = \sqrt{(\rho_{\text{equator}}/\rho_{\text{pole}}) - 1} \), is the flattening factor. The dust destruction radius is set to be \( R_{\text{dust}} = 10R_* \) and the cloud extends out to radius \( R_{\text{max}} = 10^3R_{\text{dust}} \). We use the standard MRN (Mathis, Rumpl, & Nordsieck 1977) interstellar grain mixture (53\% silicate & 47\% graphite) with optical constants from Draine & Lee (1984) (Fig. 2.9, left).
Figure 2.9  Left: The absorption opacity (dashed line), the scattering opacity (dotted line) and the total opacity (solid line), normalised to the total opacity at $\lambda_V = 0.55 \ \mu\text{m}$.
Right: The cumulative reemission probability for a wide range of temperatures (as marked on the graph).

We construct a grid with $N_r = 100$ radial and $N_\mu = 8$ latitudinal grid points, so that both radial and latitudinal optical depths are the same for each cell. To accomplish this, Bjorkman & Wood (2001) have chosen the radius $r_i$ and the polar angle $\theta_j$ for each cell such as

$$r_i = \frac{N_f}{N_f - i} R_{\text{dust}}, \ i = 0, \ldots, N_r - 1,$$

and

$$\mu_j \equiv \cos \theta_j = \frac{1}{\sqrt{1 + (\rho_{\text{equator}}/\rho_{\text{pole}}) \tan^2 (\pi j/2N_\mu)}}, \ j = 0, \ldots, N_\mu - 1,$$

The results for $\rho_{\text{equator}}/\rho_{\text{pole}} = 1000$, for 2 different equatorial optical depths ($\tau_V = 20$, $\tau_V = 200$) and for 5 different viewing angles (see captions) are shown in Fig. 2.10 and Fig. 2.11. We also plot for the second case ($\tau_V^{\text{equator}} = 200$) the different components of the spectrum at 4 different viewing angles (Fig. 2.12). Additionally, we examined the case for a less well-defined disk, i.e. for $\rho_{\text{equator}}/\rho_{\text{pole}} = 10$ (Fig. 2.13, Fig. 2.14).

The features seen in these figures are typical of a star/disk system embedded in an envelope (e.g. young T Tauri stars):

- There is a long-wavelength excess that is due to emission from the disk and the envelope.

They both absorb radiation from the star and then re-emit this radiation at longer wave-
lengths. We note that most of the radiation at optical and NIR wavelengths is direct or scattered star emission (see Fig. 2.12).

- When the the disk is viewed edge-on less direct star radiation reaches the observer.
- More FIR radiation radiation is emitted by a system with a more optically thick disk.
- The temperature is lower near the midplane ($\mu = 0$).
- The silicate feature at 10$\mu$m appears in emission in all cases apart from the last case (see Fig. 2.14), where it appears either in emission or in absorption depending on the viewing angle.

The results are in good agreement with the results of Bjorkman & Wood (2001).

2.13.3 Test 3: System in thermodynamic equilibrium

Consider a system that is exposed to a uniform, isotropic blackbody radiation field of temperature $T$. Thermodynamic equilibrium dictates that every part of the system will adopt the same temperature $T$. This also means that the intensity of the radiation coming from the system is the same as that of the illuminating blackbody field. It is easy to see this from a simple radiative transfer calculation:

$$I_{\nu}(D) = I_{\nu}(0)e^{-\tau_{\nu}(D)} + B_{\nu}(T)[1 - e^{-\tau_{\nu}(D)}] = B_{\nu}(T),$$  \hspace{1cm} (2.61)

where $D$ is the distance travelled within the system. Practically this means that the system is invisible to an observer.

We note here that this test can be applied to any structure (e.g. disks, non-symmetric structures) and it is a way to check the main radiative transfer code (i.e. $L$-packet propagation, absorption, temperature correction and reemission) but also the specifics of each problem (e.g. $L$-packet injection angle into a core to simulate an isotropic ambient radiation field). This test is a very robust one, and we suggest that any continuum radiative transfer code should be tested in this way.

We perform this test for a uniform density sphere, with radius $R = 10^6R_\odot$, density $\rho = 1.6 \times 10^{-16}g \text{ cm}^{-3}$, optical depth $\tau_V = 11.1$, using 50 radial equal depth cells. We illuminate this sphere with isotropic blackbody radiation fields having temperature $T =$ 50, 100 and 200 K,
Figure 2.10  **Left:** SED of a disk-like envelope with $\rho_{\text{equator}}/\rho_{\text{pole}} = 1000$ and $\tau_V^{\text{equator}} = 20$ for different viewing angles ($\mu = 1, 0.7, 0.5, 0.3, 0.1$; the highest curve corresponds to $\mu = 1$ and the lowest curve to $\mu = 0.1$). The dotted line represents the intrinsic radiation of the star.  **Right:** Temperature profile as a function of radius for the 8 latitudinal cells (as defined by Eq. 2.60; the highest curve corresponds to $\mu = 1$ and the lowest curve to $\mu = 0$).

Figure 2.11  The same as in Fig. 2.10 but for $\tau_V^{\text{equator}} = 200$. 
Figure 2.12  SED of a disk-like envelope with $\rho_{\text{equator}}/\rho_{\text{pole}} = 1000$ and $\tau_{\text{equator}} = 200$, for different viewing angles $\theta$. The dotted line represents the intrinsic stellar SED, the red line is the total SED of the system, the green line represents the $L$-packets that escape without interacting with the envelope, the blue line is the scattered starlight and the cyan line represents the reprocessed $L$-packets.
Figure 2.13 Left: SED of a disk-like envelope with $\rho_{\text{equator}}/\rho_{\text{pole}} = 10$ and $\tau^\text{equator}_V = 20$, for different viewing angles ($\mu = 1, 0.7, 0.5, 0.3, 0.1$; the highest curve corresponds to $\mu = 1$ and the lowest curve to $\mu = 0.1$). The dotted line represents the intrinsic radiation of the star. Right: Temperature profile as a function of radius for the 8 latitudinal cells (as defined by Eq. 2.60; the highest curve corresponds to $\mu = 1$ and the lowest curve to $\mu = 0$).

Figure 2.14 The same as in Fig. 2.13 but for $\tau^\text{equator}_V = 200$. 
2.14. Extensions and Optimisations

![Image of graphs showing temperature and spectrum](image)

**Figure 2.15** Thermodynamic equilibrium test for a uniform density sphere. The sphere is illuminated by a blackbody radiation field with a given temperature and acquires the same temperature. **Left:** Temperature versus distance from the centre of the sphere. **Right:** Spectrum of the incident and the emergent radiation in units of $B = \sigma T^4 / \pi$ (there is no difference at all with the expected spectrum).

respectively, and we calculate the spectrum and temperature of the sphere. We see (Fig. 2.15) that the sphere acquires the same temperature as the blackbody radiation field in which it is embedded, and the spectrum is a blackbody spectrum with the corresponding temperature. In other words the sphere and the surrounding radiation field are in thermodynamic equilibrium. This test indicates that PHAETHON is very accurate.

2.14 Extensions and optimisations

The method proposed by Bjorkman & Wood (2003) is a clever way to avoid iteration in Monte Carlo continuum radiative transfer calculations using a correction PDF to reemit absorbed luminosity packets. However, we have shown that its correct behaviour is due to the additional requirement of local radiative equilibrium (Eq. 2.44). We now examine whether this method can be combined with other ideas of Monte Carlo radiative transfer, such as the weighted luminosity packets technique (e.g. Witt 1977) and the continuous absorption of photons technique (Lucy 1999). We also explore the adaptivity of the method to systems with small non-thermal dust grains and with additional non-radiative luminosity sources.
2.14.1 Weighted $L$-packets

We have assumed so far that all $L$-packets have the same luminosity $\delta L$. When an $L$-packet is absorbed, a new packet must be re-emitted with a different frequency but with the same luminosity. As such, the method can be very inefficient in regions with low density. One option is to make the cells bigger so that more absorptions occur, but this decreases the spatial resolution. A better option is to introduce $L$-packets with different luminosities, i.e. weighted packets. Then other methods can be used to reduce the Poisson noise in the isophotal maps, such as the forced interaction or the peel-off technique (Cashwell & Everett 1959; Yusef-Zadeh et al. 1984).

We consider whether such techniques are compatible with the FDA technique. To answer this question, we assume that $k$ $L$-packets with luminosity $\delta L$ have been absorbed in a particular cell, that the temperature of the cell is $T$, and that a $(k + 1)$th $L$-packet is absorbed with a different luminosity $w \delta L$. Clearly, a packet with this luminosity has to be re-emitted, but what must be the shape of the adjustment PDF in this case? In Section 2.9.1 we showed that the adjustment PDF corresponding to adding $m$ data points to a set of $n$ existing data points only depends on the relative number $k = n/m$ of existing data points. Translating this to the current case means that the adjustment PDF corresponding to adding an $L$-packet with luminosity $w \delta L$ to a set of $k$ $L$-packets with luminosity $\delta L$, is equivalent to adding one $L$-packet with luminosity $\delta L$ to a set of $k/w$ $L$-packets with luminosity $\delta L$. The same formula (Eq. 2.41) is appropriate but with $k$ replaced by $k/w$. We should in general not consider $k$ as an integer number corresponding to the number of $L$-packets absorbed by the dust cell before the last absorption event, but rather as a real number corresponding to the ratio of the total luminosity absorbed by the dust cell before the last absorption event to the luminosity of the last absorbed $L$-packet. Because $k$ has the same meaning in Eq. (2.44) for the absorption rate, the Bjorkman & Wood adjustment PDF is still valid. $L$-packet weighting can hence easily be combined with the FDA method.

2.14.2 An alternative estimate for the absorption rate

In our method, we estimate the absorption rate by multiplying the number of $L$-packets that have been absorbed with the luminosity $\delta L$ of each packet. (Eq. 2.29). However, this way of estimating the absorption rate performs rather poorly in low density environments. A better way could be to estimate the absorption rate from the mean intensity of the radiation field,

$$L_{\text{abs}} = 4\pi M \int_0^\infty \kappa_\nu J_\nu \, d\nu.$$  \hspace{1cm} (2.62)
As Lucy (1999) argues, the mean intensity in a given cell can be estimated through its relation to the energy density of the radiation field. We only have to add a path length counter in each cell and determine the total path length covered by all $L$-packets in the cell (see also Niccolini et al. 2003). The advantage of this method is that all $L$-packets entering the dust cell contribute to the estimate of the absorption rate. Because in general only a small number of the $L$-packets entering a cell are absorbed, it is clear that this method is superior to estimate the absorption rate, and hence the temperature of the dust cells.

However, if we estimate the absorption rate in this way, the relation (Eq. 2.44) is not generally valid anymore, and there is no reason why the adjustment PDF (Eq. 2.41) should be equal to the Bjorkman & Wood PDF (Eq. 2.34). Hence, for the FDA method to work correctly, it may be necessary to estimate the absorption rate as in Eq. (2.29), which may be rather inefficient.

### 2.14.3 Additional heating sources

Up to now, we have considered dust grains, which are in radiative equilibrium with the radiation field. In realistic astrophysical situations, heating by the ambient radiation field is often not the only source of dust heating. Dust grains can be heated by a variety of other astrophysical processes, such as viscous or compressional heating, collisions with hot electrons in an X-ray halo or collisions with cosmic rays. In this case, the condition of radiative equilibrium (Eq. 2.28) is not satisfied, and should now be replaced by a more general equation

$$E_i^\text{em} = E_i^\text{abs} + E_i^\text{add},$$

(2.63)

where $E_i^\text{add}$ represents the amount of energy gained by the dust cell due to other processes. If we assume that this factor in general depends on the position, size, etc. of the dust cell, but not on its temperature, it remains constant during the Monte Carlo simulation.

Although radiative equilibrium is not satisfied, it is straightforward to see that the FDA method is fully compatible with such additional heating sources. Indeed, it suffices to consider $k$ as the ratio of the total luminosity gained by the dust cell before the last absorption event to the luminosity of the last absorbed $L$-packet. In particular, this means that the temperature $T_0$ of the dust cell at the beginning of the simulation is not zero, but is determined by

$$\int_0^\infty \kappa_\nu B_\nu(T_0) \, d\nu = \frac{L_\text{add}}{4\pi M},$$

(2.64)
where $L_{\text{add}} = E_i^{\text{add}} / \Delta t$. Thus, the FDA method can easily be combined with additional heating sources.

### 2.14.4 Very small dust grains

Another case where the condition (2.44) is not satisfied occurs when the contribution of small dust grains is important. These dust grains undergo transient heating to temperatures well above the equilibrium temperature (Guhathakurta & Draine 1989). This means that the grains within a dust cell have a range of time-dependent temperatures characterised by a temperature probability function $P(T)dT$ rather than a single temperature. The Monte Carlo method can also be applied to this problem (e.g. Misselt et al. 2001). However, it is possible that the relative temperature increase of small dust grains may be too large, so that the adjustment PDF (Eq. 2.41) is negative. In that case iteration may be a more appropriate method to use.

### 2.15 Discussion

In this chapter, we have described the Monte Carlo radiative transfer method we have implemented. It is an inherently three-dimensional method and can be used to study systems with arbitrary geometries. It conserves energy exactly and it does not require iteration, due to reemitting previously absorbed luminosity packets with a corrected frequency distribution function. Thus it is much faster than traditional iterative Monte Carlo radiative transfer methods. It can be combined with the weighted photons technique, can treat additional non-radiative heating such as accretion energy in circumstellar disks or compression in collapsing molecular clouds, and can give polarisation maps (e.g. Wolf et al. 1999). Different dust properties can also be treated. Currently the dust properties enter the calculation through the total absorption and scattering cross sections, but the code could be modified to treat systems with two or more different dust components having different temperatures. Each $L$-packet can be followed during its journey inside the computational domain, and thus can be traced back to its origin, giving us detailed information about the transport of radiation in specific parts of the system.

The main disadvantage of this method is that, as in any Monte Carlo method, a large number of $L$-packets must be simulated for good statistical results. This can be time consuming and makes the construction of the radiative transfer cells that represent the computational domain, crucial for the efficiency of the method. The method may be problematic in regions of low density
where not many luminosity packets are absorbed per cell, and also in high density regions where the packets propagate slowly, but special techniques can be used to tackle such problems.

The method can be applied to a variety of symmetric and asymmetric problems in the field of star formation and early stellar evolution, such as

- **Prestellar cores and protostars embedded in molecular clouds:** The Monte Carlo approach is the best choice for treating these systems since they are generally asymmetric (e.g. flattened cores, turbulent molecular clouds, non-isotropic background radiation field when the core is near the edge of the cloud or when the core is near OB stars).

- **Star/Disk systems:** This is a 2D problem if the disk is axisymmetric around the central star. The symmetry breaks when the system is perturbed by another object, e.g. a passing star from the same cluster, or when there is an embedded protoplanet in the disk.

- **Binaries with circumstellar and/or circumbinary disks:** This is a non-axisymmetric problem because of the presence of the binary, but also because of density perturbations induced in the disk. The Monte Carlo method we have described is highly suitable for treating such systems.

- **Arbitrary structures resulting from hydrodynamic simulations:** This is also an asymmetric problem and radiative transfer calculations in such systems could be used to compare the results of hydrodynamic simulations directly with observations.

- **Coupling hydrodynamics with radiative transfer:** Most hydrodynamics simulation codes do not include radiative transfer because radiative transfer codes are very time consuming and geometry dependent. The method we describe here is computationally efficient, and could in principle be integrated into SPH. However, this requires further optimisation.
Chapter 3

Models of Spherical Prestellar Cores

Prestellar cores are condensations in molecular clouds that are either on the verge of collapse or already collapsing (e.g. Myers & Benson 1983; Ward-Thompson, André & Kirk 2002). They represent the initial stage of star formation and their study is important since theoretical models of star formation are very sensitive to the initial conditions. Prestellar cores have been observed both in isolation and in protoclusters. Isolated prestellar cores (e.g. L1544, L43, L63; Ward-Thompson, Motte & André 1999) have extents $\gtrsim 1.5 \times 10^4$ AU and masses $0.5 - 35 \, M_\odot$ (see also André, Ward-Thompson, & Barsony 2000). On the other hand, prestellar cores in protoclusters (e.g. in $\rho$ Oph, NGC2068/2071) are generally smaller, with extents $\sim 2 - 4 \times 10^3$ AU and masses $\sim 0.05 - 3 \, M_\odot$ (Motte, André & Neri 1998, Motte et al. 2001).

Mass estimates from mm continuum observations, where the cores are optically thin, are uncertain due to our limited knowledge of the properties of the dust in and around these cores, and of the dust temperature. Previous studies have assumed isothermal dust at 12-20 K (e.g. Motte et al. 1998, Johnstone et al. 2000). More recent radiative transfer studies (Evans et al. 2001, Zucconi et al. 2001) model cores that are illuminated directly by the isotropic interstellar radiation field, and find that the temperature decreases towards the centre of the core. However, these studies cannot be applied to embedded cores, because in this case the illuminating radiation field is not the interstellar one, and, in general, it is not isotropic.

In this chapter, we present a more realistic model that treats cores that are embedded in molecular clouds. We use the PHAETHON Monte Carlo radiation transfer code to study cores approximated by Bonnor-Ebert (BE) spheres. In Section 3.1, we discuss how we adapt our code to treat radiation transfer in externally illuminated spheres, and present the tests we have performed. In Section 3.2, we study BE spheres exposed directly to the Black (1994) interstellar
radiation field and compare our results with those of Evans et al. (2001) and Zuconi et al. (2001), which were obtained using different radiative transfer methods. In Section 3.3, we study the more realistic case of cores embedded in molecular clouds; we calculate the dust temperatures in their interiors, their spectra and their intensity profiles at different observing wavelengths. Finally, we summarise our results in Section 3.4.

3.1 Radiative transfer in prestellar cores

3.1.1 Core density profile

A simple approach to modelling prestellar cores is to assume that they are isothermal spheres in which gravity is balanced by gas pressure (Bonnor-Ebert spheres; Bonnor 1956, Ebert 1955). Recent observations (e.g. Alves et al. 2001, Ward-Thomson et al. 2002) show that this may be a good approximation for many cores. In this chapter, we focus our study on cores represented by BE spheres.

Bonnor-Ebert spheres

If we take into account gravity and gas pressure and forget any other contribution (e.g. rotation, magnetic fields, turbulent motions), the equation of hydrostatic balance for the core is

\[
\frac{dP(r)}{dr} = -\frac{GM(r)}{r^2} \rho(r),
\]  

where \(P(r)\) is the pressure at distance \(r\) from the centre, \(M(r)\) the mass contained within this radius, and \(\rho(r)\) the density. The conservation of mass can be written as

\[
\frac{dM(r)}{dr} = 4\pi r^2 \rho(r) .
\]

Assuming isothermality, we have

\[
P(r) = c_s^2 \rho(r) ,
\]

where \(c_s = \sqrt{\frac{kT}{\mu m_H}}\) is the sound speed. Combining the above three equations we obtain (Bonnor 1956, Ebert 1955)

\[
1 \frac{d}{dr} \left[ \frac{r^2 c_s^2 d\rho(r)}{dr} \right] = -4\pi G \rho(r) .
\]
3.1. RADIATIVE TRANSFER IN PRESTELLAR CORES

If we set \( r = r_0 \xi \) and \( \rho(r) = \rho_c e^{-\psi(\xi)} \), where \( r_0 = c_s/(4\pi G \rho_c)^{1/2} \), Eq. (3.4) reduces to

\[
\frac{1}{\xi^2} \frac{d}{d\xi} \left[ \xi^2 \frac{d\psi}{d\xi} \right] = e^{-\psi},
\]

with the boundary conditions \( \psi(0) = 0 \) and \( \left[ \frac{d\psi}{d\xi} \right]_{\xi=0} = 0 \). This equation must be solved numerically, although there are some analytic approximations to the solution (Liu 1996, Natarajan & Lynden-Bell 1997). We follow the numerical approach and solve the equation using a Runge-Kutta integration scheme (Fig. 3.1).

![Figure 3.1](image)

Figure 3.1  Numerical solution for the isothermal sphere using a Runge-Kutta integration scheme. **Left:** Parameter \( \psi \) with respect to \( \xi \) (scaled radius). **Right:** Density \( \rho \) (in unit of central density \( \rho_c \)) with respect to \( \xi \).

The mass \( M_{\text{BE}} \) of a Bonnor-Ebert sphere with radius \( r_b = r_0 \xi_b \) is

\[
M_{\text{BE}} = \int_{r=0}^{r=r_b} \rho(r) 4\pi r^2 dr = \int_{\xi=0}^{\xi=\xi_b} \rho_c e^{-\psi(\xi)} 4\pi r_0^2 \xi^2 d\xi = 4\pi r_0^2 \rho_c \left[ \xi^2 \frac{d\psi}{d\xi}(\xi) \right]_{\xi=0}^{\xi=\xi_b} \Rightarrow (3.6)
\]

\[
M_{\text{BE}} = \frac{c_s^3}{(4\pi \rho_c)^{1/2} G^{3/2} \xi_b^6 \frac{d\psi}{d\xi}(\xi_b)}.
\]

From the above we can calculate the central density,

\[
\rho_c = \frac{c_s^6}{4\pi G^3 M_{\text{BE}}^2} \left[ \xi_b^2 \frac{d\psi}{d\xi}(\xi_b) \right]^2.
\]
Using $\rho(r) = \rho_c e^{-\psi(\xi)}$ we get for the pressure at the boundary $\xi_b$

$$P_b = P(\xi_b) = \rho_c c_s^2 e^{-\psi(\xi_b)} = \frac{c_s^8}{4 \pi G^3 M_{BE}^2} \left[ \xi_b^2 \frac{d \psi}{d \xi} (\xi_b) \right]^2 e^{-\psi(\xi_b)} .$$  \hfill (3.9)

**Figure 3.2** Left: Dimensionless pressure $\mathcal{P}$ versus $\xi$ for Bonnor-Ebert spheres. Right: Dimensionless pressure $\mathcal{P}$ versus dimensionless radius $\mathcal{R}$.

It is useful to define the dimensionless radius $\mathcal{R}(\xi_b)$ and pressure $\mathcal{P}(\xi_b)$,

$$\mathcal{R}(\xi_b) = \left[ \xi_b^2 \frac{d \psi}{d \xi} (\xi_b) \right]^{-1} \xi_b = \frac{c_s^2}{G M_{BE}} r(\xi_b) .$$ \hfill (3.10)

$$\mathcal{P}(\xi_b) = \left[ \xi_b^2 \frac{d \psi}{d \xi} (\xi_b) \right]^2 e^{-\psi(\xi_b)} = \frac{4 \pi G^3 M_{BE}^2}{c_s^8} P(\xi_b) ,$$ \hfill (3.11)

In the $\mathcal{P} - \xi$ plot (Fig. 3.2, left), there is a maximum at $\xi_c = 6.451$, corresponding to a maximum external pressure $P_{\text{MAX}}$,

$$P_{\text{MAX}} = 1.40 \frac{c_s^8}{G^3 M_{BE}^2} ,$$ \hfill (3.12)

above which there is no equilibrium solution. The corresponding radius is

$$R_{\text{MIN}} = 0.41 \frac{G M_{BE}}{c_s^2} .$$ \hfill (3.13)
3.1. RADIATIVE TRANSFER IN PRESTELLAR CORES

This means that for a given core mass there is a maximum external pressure that can be balanced by the gas pressure. Stability analysis (Bonnor 1958) shows that if \( \xi_b < \xi_c \) (\( \rho_{\text{center}} / \rho_{\text{edge}} < 14.1 \)) the equilibrium is stable, whereas for \( \xi_b > \xi_c \) (\( \rho_{\text{center}} / \rho_{\text{edge}} > 14.1 \)) the equilibrium is unstable. Spheres with \( \xi_b = \xi_c \) are referred to as critical Bonnor-Ebert spheres. It is easy to calculate (using \( P < P_{\text{MAX}} \) and Eq. 3.12) that the condition for the existence of an equilibrium solution is

\[
\frac{PM^2}{T^3} \leq \frac{1.40}{G^3 \mu^4 m^4_H} k^4.
\]

(3.14)

It is also interesting to examine the \( P - R \) plot (Fig. 3.2, right). If the external pressure \( P \) is greater than \( P_{\text{MAX}} \) then, as mentioned before, there is no equilibrium solution. If the external pressure is small

\[
P < P' = 0.48 \frac{c^5}{G^3 M^2_{\text{BE}}},
\]

(3.15)

then there is only one solution for the outer radius \( R \), corresponding to a stable sphere. A more complex region is that between \( P' \) and \( P_{\text{MAX}} \), where there are 2 or more solutions to the equilibrium problem. In this region there is one solution with a larger radius which corresponds to a stable isothermal sphere, and one or more corresponding to unstable spheres.

Model parameterisation

We can describe a BE sphere fully using three parameters (or two if we refer to a critical BE sphere). Previous studies (e.g. Evans et al. 2001) used the central density, outer radius and gas temperature. We choose to parameterise BE spheres using the temperature, the mass of the sphere, and the external ambient pressure on the sphere. This type of parameterisation is quite useful when examining prestellar cores in the same molecular cloud, in as much as we can presume that they all experience roughly the same external pressure. The sphere is divided into a number of concentric cells (typically 50-100) with equal radial width (Fig. 3.3).

In our study we assume isothermal gas spheres. Generally, dust and gas do not have the same temperature unless the density is quite high, in which case they are thermally coupled (\( n \gtrsim 3 \times 10^4 \text{ cm}^{-3} \), Mathis et al. 1983; Whitworth, Francis & Boffin 1998). However, even non-isothermal models of cores that allow a small gas temperature gradient, give density profiles that are very close to the BE profile (Evans et al. 2001). Thus, our results for isothermal spheres should represent hydrostatic cores reasonably well.
Figure 3.3 Schematic view of Bonnor-Ebert sphere model. Photons are injected from the point \((0, 0, R)\) at such an angle as to imitate an isotropic ambient radiation field.

3.1.2 The illuminating radiation field

Photon injection angle

Because the core is spherically symmetric and the radiation field is isotropic, we can –without loss of generality– inject all photons at the point \((0, 0, R)\), where \(R\) is the radius of the BE sphere (Fig. 3.3). If \(I_0\) is the integrated intensity of the radiation field, then the total luminosity incident on the sphere is

\[
L_{\text{total}} = \pi I_0 4\pi R^2. \tag{3.16}
\]

If we use \(N\) luminosity packets, the luminosity per photon is

\[
\delta L = \frac{\pi I_0 4\pi R^2}{N}. \tag{3.17}
\]

For isotropic intensity the injection angle probability is

\[
p_\theta d\theta = 2\cos(\theta) \sin(\theta) d\theta, \quad \frac{\pi}{2} \leq \theta \leq \pi, \tag{3.18}
\]

(see Appendix C), and the photon injection angle is therefore

\[
\theta = \cos^{-1} \left[ -\mathcal{R}_\theta^{1/2} \right], \quad \mathcal{R}_\theta \in [0, 1]. \tag{3.19}
\]
3.1. RADIATIVE TRANSFER IN PRESTELLAR CORES

Photon frequency

Black (1994) has compiled an average Galactic background spectrum from radio frequencies to the Lyman continuum limit, based both on observations and theoretical modelling (Fig. 3.4). This spectrum consists of an optical component with a peak at around 1 $\mu$m, due to radiation from giant stars and dwarfs; a component due to thermal emission from dust grains with a peak at around 100 $\mu$m; mid-infrared radiation from transiently heated grains in the range 5-100 $\mu$m; and the cosmic background radiation with a peak around 1mm ($T = 2.728 \pm 0.004$ K). This background is similar to that of Mathis et al. (1983) apart from the region from 5 to 400 $\mu$m, where it is stronger on the basis of COBE data. As noted by Black, his estimate only accounts for continuum radiation and does not include strong emission lines, which may have significant power in the far-IR and submillimetre part of the spectrum.

![Graph of photon frequency](image)

**Figure 3.4** Black (1994) Interstellar Radiation Field

The Black (1994) radiation field (hereafter BISRF) seems to be a good approximation to the interstellar radiation field in the solar neighbourhood. However, it is not always an appropriate choice when studying prestellar cores, because many cores are embedded in molecular clouds. Consequently, the radiation field is attenuated at short wavelengths ($< 30 - 40 \mu m$) because the surrounding cloud absorbs a large part of this radiation, and enhanced at long wavelengths ($> 50 \mu m$) due to the thermal emission from the molecular cloud (Mathis et al. 1983). Also the radiation field may be anisotropic. In this work, initially we study cores directly exposed to the
BISRF (like the previous studies of Evans et al. 2001 and Zucconi et al. 2001) but we also extend our study to the more realistic case of cores inside molecular clouds of different sizes.

### 3.1.3 Dust opacities

Typical dust temperatures in prestellar cores are quite low (5 – 20 K) and under these conditions dust grains are expected to coagulate and accrete ice mantles. Following recent studies of prestellar cores (Evans et al. 2001, Zucconi et al. 2001), we use the absorption opacities calculated by Ossenkopf and Henning (1994) (hereafter OH) for a standard MRN (Mathis, Rumpl & Nordsieck 1977) interstellar grain mixture (53% silicate & 47% graphite), with grains that have coagulated and accreted thin ice mantles over a period of $10^5$ years at a density of $10^6$ cm$^{-3}$. We also assume a gas-to-dust mass ratio of 100.

![Image](image)

**Figure 3.5** Ossenkopf & Henning (1994) + MRN (1977) opacities. The solid line represents the absorption opacity and the dashed line the scattering opacity ($\kappa_{\text{abs}} + \kappa_{\text{scat}} = 10.45 \times 10^2$ g cm$^{-2}$ at $\lambda = 0.55$ $\mu$m).

Ossenkopf and Henning only calculated absorption opacities down to 1 $\mu$m, so below this value we use the MRN standard model (grains without ice mantles) with optical constants from Draine & Lee (1984), after scaling to fit the OH absorption opacity at 1 $\mu$m (Fig. 3.5). In any case, the choice of absorption opacities below 1 $\mu$m, does not play an important role in our calculations since at these short wavelengths the core is optically thick and the radiation does not penetrate much inside the core.
3.1. RADIATIVE TRANSFER IN PRESTELLAR CORES

Also, due to lack of data for scattering opacities, we use the MRN scattering opacities after scaling them as before. We should note though that for dust in prestellar cores, scattering is expected to be less by at least a factor of 2 (Ossenkopf; private communication). The choice of scattering opacities does not greatly affect the temperature in the inner regions of the core, since scattering is only important for short wavelength ($\lesssim 20$ $\mu$m) radiation, which, anyway, cannot penetrate deep inside the core. We will discuss the effect of scattering in more detail later.

3.1.4 Code tests

We perform two tests to check the validity of the radiative transfer code in the specific system we study: (i) the “thermodynamic equilibrium test”, in which a Bonnor-Ebert sphere is illuminated by a uniform blackbody radiation field, and (ii) the “pure scattering test” in which the albedo of the dust is set to 1.

**Test 1: Thermodynamic equilibrium**

We perform the thermodynamic equilibrium test (see Section 2.13.3) for an unstable Bonnor-Ebert sphere ($\xi_b=11.8$, $M_{\text{BE}} = 4.5$ $M_\odot$, $T = 11$ $K$, $P_{\text{ext}} = 10^4$ $\text{cm}^{-3}$ $K$). Initially, we perform the test with a blackbody illuminating radiation field having $T = 10$ $K$ and then with a radiation field having $T = 20$ $K$ (using $10^9$ luminosity packets). As seen in Fig. 3.6 the output spectrum is the same as that of the illuminating field and the temperature at any distance from the centre of the core is constant and equal to that of the radiation field. Small variations on the order of 0.1 $K$ are not important and are due to statistical noise.

**Test 2: Pure scattering**

If the radiation field incident on the sphere is isotropic and if the photons just pass through the sphere without interacting, the observed intensity will be the same at each impact parameter $b$, and equal to the intensity of the illuminating field. The same holds if the photons just get scattered, i.e. when the albedo of the grains is set equal to 1. It is easy to understand this when the scattering is isotropic, but the same is also true for non-isotropic scattering. Since the incident field is isotropic, the photons come from all directions and the effect of scattering will simply be to rotate the whole radiation field through an angle $\theta$, so the field will remain isotropic. The same argument holds if a photon undergoes more than one scattering. Thus, if the radiation
just gets scattered in the medium, the emergent spectrum will again be the same as that of the incident radiation.

We perform this test for a stable BE sphere (parameters: $\xi_b = 4.1$, $M_{BE} = 4 \, M_\odot$, $T = 11 \, K$, $P_{ext} = 10^4 \, cm^{-3} \, K$). This time the sphere is illuminated by the BISRF. We do calculations for mean scattering cosine $g = 0$ (isotropic scattering), 0.5 and 1 (using $2 \times 10^7$ luminosity packets). We present our results for the $g = 0.5$ case in Fig. 3.7. The code successfully passed this test too.

### 3.2 Non-embedded prestellar cores

We use the term *non-embedded* to refer to prestellar cores that are directly exposed to the BISRF. We perform simulations for a number of Bonnor-Ebert spheres under different external pressures and for various gas temperatures and masses. In Table 3.1, we list the parameters of our models to show the parameter space investigated. When the ambient pressure is near the maximum value (see Fig. 3.2, left) there are two equilibrium solutions for the same set of $P_{ext}$, $T$ and $M_{BE}$. These two solutions correspond to one subcritical (low central density) and one supercritical sphere (high central density). These can be distinguished by the $\xi_b$ value; if $\xi_b > 6.451$ then the sphere is supercritical. For each model we calculate the temperature profile
of the dust in the core, the core SED and intensity profiles at different wavelengths (90, 170 and 450 \( \mu \text{m} \)).

### 3.2.1 Temperature profiles

The dust temperature inside the core drops from around 17 K at the edge to a minimum at the centre, which may be as low as 7 K, depending on the total optical depth of the sphere. The higher the optical depth to the centre of the core the lower the central temperature and the larger the temperature gradient. In Fig. 3.8b, we plot dust temperature profiles for three representative core models with different density profiles.

Our results are in general agreement with previous similar calculations by Evans et al. (2001) and Zucconi et al. (2001). We compared our results with those of Evans et al. for a system as close as we could get to one of their models. They do not mention what opacities they use for \( \lambda < 1 \mu \text{m} \), they use an ISRF at \( \lambda < 1\mu\text{m} \) different from the BISRF, and some parameters in their model are unclear. We find that the temperature we calculate at the edge of the core is \( \approx 3 \) K higher than their calculation (17 K rather than 14 K). We attribute this difference to different opacities and different ISRF for \( \lambda < 1 \mu \text{m} \). We also find that the temperature is almost
Figure 3.8 Density profiles (a), dust temperature profiles (b), and SEDs (c). Results are shown for models BE2 (solid lines), BE2.2 (dashed lines) and BE7 (dotted lines). Model parameters are given in Table 3.1. Note that BE2 and BE2.2 have the same set of parameters ($P_{\text{ext}}$, $T$, $M_{\text{BE}}$) but BE2 is subcritical and BE2.2 is supercritical. The dash-dot line on the SED graph corresponds to the background SED. The temperature at the centre of more centrally condensed cores is lower and the core emission is shifted towards longer wavelengths.

Figure 3.9 Intensity profiles at 90 (a), 170 (b) and 450 $\mu$m (c), for the models in Fig. 3.8 (BE2: solid lines, BE2.2: dashed lines, BE7: dotted lines). The horizontal solid lines on the profiles correspond to the background intensity at each wavelength. At 90 $\mu$m the intensity increases towards the edge of the core but the emission is just $5-10$ MJy sr$^{-1}$ above the background and, thus, the cores are barely detectable. At 170 $\mu$m the intensity drops towards the edge of the core, or rises by a small amount, if the core is cold enough in the centre. At 450 $\mu$m the intensity drops towards the edge of the core in all cases.
Table 3.1 Non-embedded prestellar cores: Model parameters

<table>
<thead>
<tr>
<th>model</th>
<th>$P_{\text{ext}}$ (K cm$^{-2}$)</th>
<th>T (K)</th>
<th>$M_{\text{BE}}$ (M$_{\odot}$)</th>
<th>$\xi_b$</th>
<th>$\tau_V$</th>
<th>BE sphere kind</th>
</tr>
</thead>
<tbody>
<tr>
<td>BE1</td>
<td>$10^3$</td>
<td>10</td>
<td>2</td>
<td>2.6</td>
<td>4.0</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE2</td>
<td>$10^3$</td>
<td>10</td>
<td>3.5</td>
<td>4.5</td>
<td>8.3</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE2.2</td>
<td>$10^4$</td>
<td>10</td>
<td>3.5</td>
<td>9.9</td>
<td>24.0</td>
<td>supercritical</td>
</tr>
<tr>
<td>BE3</td>
<td>$10^4$</td>
<td>15</td>
<td>2</td>
<td>1.7</td>
<td>2.4</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE4</td>
<td>$10^4$</td>
<td>15</td>
<td>4</td>
<td>2.4</td>
<td>3.6</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE5</td>
<td>$10^4$</td>
<td>15</td>
<td>6</td>
<td>3.2</td>
<td>5.2</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE5.2</td>
<td>$10^4$</td>
<td>15</td>
<td>6</td>
<td>21.6</td>
<td>64.0</td>
<td>supercritical</td>
</tr>
<tr>
<td>BE6</td>
<td>$10^4$</td>
<td>15</td>
<td>1</td>
<td>2.1</td>
<td>9.8</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE7</td>
<td>$10^5$</td>
<td>15</td>
<td>2.6</td>
<td>5.0</td>
<td>30.1</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE7.2</td>
<td>$10^5$</td>
<td>15</td>
<td>2.6</td>
<td>8.5</td>
<td>62.0</td>
<td>supercritical</td>
</tr>
<tr>
<td>BE8</td>
<td>$5 \times 10^4$</td>
<td>15</td>
<td>2</td>
<td>2.6</td>
<td>8.9</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE9</td>
<td>$5 \times 10^4$</td>
<td>15</td>
<td>3.5</td>
<td>4.5</td>
<td>18.2</td>
<td>subcritical</td>
</tr>
<tr>
<td>BE9.2</td>
<td>$5 \times 10^4$</td>
<td>15</td>
<td>3.5</td>
<td>10.1</td>
<td>56.2</td>
<td>supercritical</td>
</tr>
<tr>
<td>BE10</td>
<td>$10^4$</td>
<td>11</td>
<td>4</td>
<td>11.8</td>
<td>30.6</td>
<td>supercritical</td>
</tr>
</tbody>
</table>

$P_{\text{ext}}$ External pressure
T Gas temperature
$M_{\text{BE}}$ Bonnor-Ebert sphere mass
$\xi_b$ $\xi$ parameter (sphere is supercritical if $\xi > 6.451$)
$\tau_V$ Visual optical depth to the centre of the sphere.

1 K lower than reported by Evans et al. at the centre of the core. This may in part be due to slightly different density profiles. Zuconi et al. also reported a higher estimated temperature at the edge ($\approx 16.5$ K) and a lower temperature ($\approx 0.3$ K lower) at the centre of the core, when they compared their model with the Evans et al. calculations. However, these are small differences.

3.2.2 SEDs and intensity profiles

We see from the component version of the SED (Fig. 3.10), where we plot the contribution from scattered, processed and direct photons to the SED for the BE2.2 model, that short wavelength radiation ($\lambda \lesssim 50$ $\mu$m) is absorbed from the core and then is reemitted at longer wavelengths, whereas most of the longer wavelength radiation ($\lambda \gtrsim 50$ $\mu$m) just passes through the core without interacting at all. The UV, optical and NIR radiation that is absorbed is mainly responsible for the heating of the core. A large amount of this radiation will not be available if the core is inside
a molecular cloud, as we discuss later in this chapter. The core emits most of its radiation in the FIR and submm (also see Fig. 3.8c). The peak of the emission is between 110 and 160 $\mu$m (note that this is the peak of $\lambda F_{\lambda}$ not $F_{\lambda}$). At these wavelengths, the core is easily observable against the background. At shorter wavelengths (e.g. 90 $\mu$m) the contrast with the background is not very distinct. Finally, in the optical the core is seen in absorption and appears like a black blob against the bright background.

![Figure 3.10](image) Components of the spectrum for the BE2.2 model. The dotted black line is the SED of the radiation incident on the core, the solid line is the output SED, the dash-dot line is the part of the radiation that passes through the core without interacting, the short-dashed line is the core emission and the long-dashed line is the scattered light.

The radial intensity profile of a core at a specific wavelength $\lambda_{\text{obs}}$ depends on whether this wavelength is shorter or longer than the peak wavelength $\lambda_{\text{peak}}$. If $\lambda_{\text{obs}}$ is much longer than $\lambda_{\text{peak}}$ (e.g. at 450 $\mu$m), then the Rayleigh-Jeans approximation for the Planck function holds, and if the core is optically thin, the intensity is proportional to the product of column density and the temperature. The column density decrease towards the edge of the core is much larger than the corresponding temperature increase, and so the intensity decreases considerably towards the edge (see Fig. 3.9c). If $\lambda_{\text{obs}}$ is much shorter than $\lambda_{\text{peak}}$ (e.g. at 90 $\mu$m) then the Wien approximation holds and the intensity depends on the temperature exponentially, so even a small increase in the temperature can balance the density decrease, and so the intensity increases slightly ($\sim 5$ MJy sr$^{-1}$) towards the edge of the core (Fig. 3.9a). However, the contrast between
core and background radiation is very small ($\sim 5 - 7 \text{ MJy sr}^{-1}$) and non-embedded cores should be barely detectable at 90 $\mu$m. This result is consistent with observations of prestellar cores (Ward-Thompson et al. 2002) which show that cores are usually well defined at 170 and 200 $\mu$m but not always well defined at 90 $\mu$m. Finally if $\lambda$ and $\lambda_{\text{peak}}$ are comparable (e.g. 170 $\mu$m) the intensity either drops from the centre to the edge ($\lambda$ a bit longer than $\lambda_{\text{peak}}$; Fig. 3.9b, models BE2 and BE2.2) or it increases ($\lambda$ a bit smaller than $\lambda_{\text{peak}}$; Fig. 3.9b, model BE7). In general, the contrast with the background is quite large at these intermediate wavelengths.

### 3.2.3 Effects of dust scattering properties

The properties of dust in molecular clouds and prestellar cores are quite uncertain (see André et al. 2000). In this section we examine the effect of different dust scattering properties on the temperature profiles and on the spectra of prestellar cores. We perform radiative transfer calculations using PHAETHON, for a supercritical Bonnor-Ebert sphere (model BE10, see Table 3.1) and different dust properties.

Initially we vary the mean scattering cosine $g$. We see (Fig. 3.11a) that when the scattering is isotropic ($g = 0$, solid line) the dust temperature at a specific radius inside the core is a bit lower ($\sim 0.3 \text{ K}$) than for the case of forward scattering ($g = 1$, dashed line). For the $g = 1$ case at optical wavelengths there is significant intensity only at the very edge of the core where the optical depth through the core is small and radiation can pass straight through (Fig. 3.11b). If photons are scattered forward, they are able to penetrate deeper inside the core and heat it to higher temperatures. As a result more optical photons are absorbed and more FIR photons are emitted. The intensity difference between dust models with different mean scattering cosine is very large in the optical region (Fig. 3.11b) but it is only $\sim 10 - 20\%$ at FIR and submillimetre wavelengths (e.g. 170 and 450 $\mu$m, Fig. 3.11c).

Next, we vary the scattering opacities of the dust (Fig. 3.12). We perform 3 calculations: (a) with MRN scattering opacities $\kappa_{\text{scat}} = \kappa_{\text{scat}}^\text{MRN}$ (solid lines), (b) with $\kappa_{\text{scat}} = \kappa_{\text{scat}}^\text{MRN}/2$ (dotted lines), and (c) with no scattering at all ($\kappa_{\text{scat}} = 0$, dashed lines). The results are similar to the previous case: when there is no scattering more photons are absorbed by the core, heating it to slightly higher temperatures. Scattering provides photons with a quick way out of the core without them being absorbed.
**Figure 3.11** Temperature profiles (a) and intensity profiles at 0.55 μm (b), 170 and 450 μm (c) for a Bonnor-Ebert sphere (model BE10, see Table 3.1) with different dust scattering properties. The dashed line corresponds to mean scattering cosines $g = 1$ (forward scattering), the dotted line to $g = 0.4$ and the solid line to $g = 0$. The dash-dot horizontal lines on the intensity profiles correspond to the background intensity at the wavelength noted on the graph. Different dust mean scattering cosines do not greatly affect the dust temperature profile in the core.

**Figure 3.12** Temperature profiles (a) and intensity profiles at 0.55 μm (b), 170 and 450 μm (c) for a Bonnor-Ebert sphere (model BE10, see Table 3.1) with different dust scattering opacities. The dashed line corresponds to zero scattering opacity, the dotted line to half the MRN scattering opacity and the solid line to the MRN standard model scattering opacity. The dash-dot horizontal lines on the intensity profiles correspond to the background intensity at the wavelength noted on the graph. Different dust scattering opacities do not greatly affect the dust temperature profile in the core.
This study shows that different dust composition, as reflected in different dust scattering opacity and/or different scattering mean cosine, results in only slightly different temperature profiles. The optical intensity profiles are strongly dependent on the dust scattering properties but at FIR and submillimetre wavelengths, where prestellar cores emit most of their radiation, the intensity is not affected significantly. Thus, we conclude that the scattering properties of the dust do not greatly affect the results of our radiative transfer calculations of prestellar cores.

3.3 Prestellar cores embedded in molecular clouds

In many cases prestellar cores are embedded deep inside molecular clouds and the radiation incident on them is different from the interstellar radiation field, and anisotropic (Mathis et al. 1983). The ambient molecular cloud acts like a shield to UV, visual and NIR interstellar radiation, absorbing and re-emitting it in the FIR. It also makes the radiation incident on the core anisotropic because in general the molecular cloud is not homogeneous and it is not spherically symmetric. Even for a spherical core at the centre of a spherical ambient molecular cloud with uniform density, the radiation incident on the core is not isotropic. That is because there will be more radiation incident on a specific point on the embedded core from the radial direction (which is closer to the boundary of the cloud) than from the tangent or any other direction (see Fig. 3.13).

Another factor contributing to the anisotropy of the radiation incident on a prestellar core is the presence of stars or other luminosity sources in the vicinity of the core. For example, according to the Lisèo et al. (1999) model there is a B2V star close to ρ Ophiuchi which increases the UV radiation incident on the cloud from one side. Also the NGC 2068/2071 protoclusters in Orion B (Motte et al. 2001) are in an environment rich in FIR, submm and mm photons, from reprocessed UV radiation from the newly born stars in Orion. In such cases, the BISRF is probably not a very good representation of the radiation field incident on the core.

Previous studies (Evans et al. 2001, Young et al. 2002) have acknowledged that deviations from the BISRF are important and have used a scaled version of the BISRF that is either enhanced at all wavelengths, or selectively in the UV and FIR. This simple approach has a free parameter, the ISRF scaling factor, that is varied arbitrarily to fit the observations, but it is not connected directly to the molecular cloud in which the core is embedded or the transport of radiation inside the cloud, and does not account for the fact that the radiation field incident on an embedded core
is not isotropic. Here, we present more consistent models in which deviation from the BISRF is a direct result of the presence of a molecular cloud that surrounds the core.

![Diagram of a molecular cloud and prestellar core]

**Figure 3.13** Schematic representation of a prestellar core embedded in a molecular cloud (not in scale). The radiation incident on the core is not isotropic because \( \tau_i > \tau_r = \tau_{\text{cloud}} \).

### 3.3.1 Model description

We examine a simple model of a spherical prestellar core which is at the centre of a spherical molecular cloud (see Fig. 3.13). We try to mimic the conditions in \( \rho \) Ophiuchi, where condensations have masses in the range 0.05–3 M\(_{\odot}\) and dimensions 1 – 6 \( \times 10^3 \) AU (\( \sim 7 – 42 \) arcsec). The thermal pressure at the edge of the cloud is \( \sim 10^6 \) cm\(^{-3}\) K and the estimated particle density is \( \sim 2 \times 10^4 \) cm\(^{-3}\) (Liseau et al. 1999). In our study we examine cores with dimensions 4 – 8 \( \times 10^3 \) AU and masses 0.4 – 1.2 M\(_{\odot}\). We assume that the molecular cloud outside the core has constant particle density \( n(H_2) = 0.77 \times 10^4 \) cm\(^{-3}\) (corresponding to \( n_{\text{rot}} = 0.96 \times 10^4 \) cm\(^{-3}\) for a gas with mean molecular weight \( \mu = 2.3 \) and hydrogen abundance by mass \( X = 0.7 \)). We also assume that the dust in the molecular cloud has the same composition as the dust in the core and, therefore, the same opacities. As in the study of non-embedded cores we use the Ossenkopf and Henning (1994) opacities (see Section 3.1.3). We use a BE sphere density profile for the prestellar cores, with fixed ambient pressure at \( \sim 10^6 \) cm\(^{-3}\) K. Thus, the free parameters defining the BE profile are the mass of the sphere and the gas temperature. Because \( n(H_2) \) is specified, the visual optical depth \( \tau_{\text{cloud}} \) is the only free parameter for the ambient cloud. \( \tau_{\text{cloud}} \) also determines the extent
of the cloud. Motte et al. (1998) calculate $A_V \sim 10$ mag for ρ Ophiuchus, but depending on the position of the core in the cloud, the extinction could be up to $\sim 40$ mag. We use visual optical depths 5, 10 and 20. The detailed parameters of our models are listed in Table 3.2.

### Table 3.2 Embedded pre-stellar cores: Model parameters

<table>
<thead>
<tr>
<th>model</th>
<th>$M_{BE}(M_\odot)$</th>
<th>$T$(K)</th>
<th>$\xi_b$</th>
<th>$n_c$(cm$^{-3}$)</th>
<th>$n_b$(cm$^{-3}$)</th>
<th>$\tau_V$</th>
<th>$R_{BE}$(AU)</th>
<th>$\tau_{cloud}$</th>
<th>$R_{cloud}$(AU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EM1</td>
<td>0.8</td>
<td>15</td>
<td>4.7</td>
<td>$4.5 \times 10^5$</td>
<td>$6.7 \times 10^4$</td>
<td>87</td>
<td>$6.1 \times 10^3$</td>
<td>0</td>
<td>$6.1 \times 10^3$</td>
</tr>
<tr>
<td>EM1.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM1.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM1.20</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM2</td>
<td>0.8</td>
<td>15</td>
<td>9.4</td>
<td>$2.4 \times 10^6$</td>
<td>$6.7 \times 10^4$</td>
<td>227</td>
<td>$5.2 \times 10^3$</td>
<td>0</td>
<td>$5.2 \times 10^3$</td>
</tr>
<tr>
<td>EM2.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM2.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM2.20</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM3</td>
<td>0.4</td>
<td>15</td>
<td>2.4</td>
<td>$1.4 \times 10^5$</td>
<td>$6.7 \times 10^4$</td>
<td>36</td>
<td>$5.4 \times 10^3$</td>
<td>0</td>
<td>$5.4 \times 10^3$</td>
</tr>
<tr>
<td>EM3.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM3.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM3.20</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM4</td>
<td>1.2</td>
<td>20</td>
<td>3.6</td>
<td>$1.9 \times 10^5$</td>
<td>$5.0 \times 10^4$</td>
<td>61</td>
<td>$8.1 \times 10^3$</td>
<td>0</td>
<td>$8.1 \times 10^3$</td>
</tr>
<tr>
<td>EM4.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM4.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM4.20</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM5</td>
<td>1.2</td>
<td>20</td>
<td>15.4</td>
<td>$6.1 \times 10^6$</td>
<td>$5.0 \times 10^4$</td>
<td>430</td>
<td>$6.2 \times 10^3$</td>
<td>0</td>
<td>$6.2 \times 10^3$</td>
</tr>
<tr>
<td>EM5.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM5.10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EM5.20</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Embedded core properties: $M_{BE}$: mass, $T$: gas temperature, $\xi_b$: $\xi$ parameter of the BE sphere $(\xi > 6.451$ for supercritical spheres), $n_c$: central density, $n_b$: boundary density, $\tau_V$: visual optical depth to the centre of the sphere, $R_{BE}$: radius of the sphere.

- Ambient cloud properties: $\tau_{cloud}$: visual optical depth of the cloud (see Fig. 3.13), $R_{cloud}$: cloud radius.

#### 3.3.2 Temperature profiles and mass estimates

The dust temperature profile inside the core depends on the optical depth of the molecular cloud in which the core is embedded, and the density profile of the core. (Additionally, the dust opacities are important, but we will not study their influence here.) The presence of even a moderately thick cloud of $\tau_{cloud} = 5$ around the core, shields the core from UV and NIR radiation, resulting in a less steep temperature profile inside the core than in the case of a core that is directly
Figure 3.14  Density profiles (a), dust temperature profiles (b) and SEDs (c), for BE spheres at \( T=15 \) K with mass 0.8 \( \text{M}_\odot \), under external pressure \( P_{\text{ext}} = 10^6 \text{cm}^{-3}\text{K}, \) surrounded by a spherical ambient cloud with visual optical depth 20 (model EM1.20, solid lines), 5 (model EM1.05, dotted lines) and 0 (model EM1, dashed lines; no surrounding cloud). The dash-dot line on the SED graph corresponds to the background SED. The deeper the core is embedded, the lower the dust temperature inside the core. The dust temperature is lower than 12 K even when the core is embedded in a relatively thin molecular cloud with visual extinction 5 mag.

Figure 3.15  Intensity profiles at 90 (a), 170 (b), 450 and 850 \( \mu \text{m} \) (c), for the models in Fig. 3.14 (EM1.20: solid lines, EM1.05: dotted lines, EM1: dashed lines). The horizontal solid lines on the profiles correspond to the background intensity at the wavelength marked on the graph. At 90 \( \mu \text{m} \) the core is seen in absorption against the background but the core is not easily distinguishable. At 170 \( \mu \text{m} \) the intensity increases towards the edge of the core only if the core is not very deeply embedded. However, very sensitive observations are needed to detect this feature. At 450 and 850 \( \mu \text{m} \) the intensity drops towards the edge of the core.
exposed to the interstellar radiation field. When there is no surrounding cloud the temperature drops from 16 K at the edge of the core to around 6-7 K in the centre ($\Delta T \approx 9 - 10$ K, depending on the core density), whereas with a $\tau_{\text{cloud}} = 5$ surrounding cloud the temperature drops from around 11 K to 7 K ($\Delta T \approx 4$ K), as seen in Figs. 3.14b and 3.16b. A deeply embedded core ($\tau_{\text{cloud}} = 20$) is almost isothermal at around 7-8 K, with $\Delta T \lesssim 1.5$ K for a not very centrally condensed core (Fig. 3.14b), and $\Delta T \approx 3$ K for a supercritical core (Fig. 3.16b). Our studies show that temperatures are probably lower than 12 K in cores surrounded by even a relatively thin cloud (visual $\tau_{\text{cloud}} = 5$), which seems to be the case for many of the prestellar cores in $\rho$ Ophiuchi. Previous studies (Motte et al. 1998, Johnstone et al. 2000) of prestellar cores in $\rho$ Oph assumed isothermal dust at temperatures from 12 to 20 K, when calculating core masses from mm observations. At these wavelengths the dust emission is optically thin, and consequently the observed flux is

$$F_\lambda = B_\lambda(T_{\text{dust}}) \tau_\lambda \Delta \Omega = B_\lambda(T_{\text{dust}}) \kappa_\lambda N(H_2) \mu m_H \Delta \Omega. \tag{3.20}$$

Hence, the inferred column density is

$$N(H_2) = \frac{F_\lambda}{\mu m_H \Delta \Omega \kappa_\lambda B_\lambda(T_{\text{dust}})}. \tag{3.21}$$

$\Delta \Omega$ is the solid angle of the telescope beam for a resolved source, or the solid angle of the source if unresolved, $N(H_2)$ is the hydrogen column density, $\kappa_\lambda$ is the mm dust opacity per unit mass, and $B_\lambda$ is the Planck function. At mm wavelengths and temperatures < 20 K the Rayleigh-Jeans approximation holds, so $B_\lambda(T_{\text{dust}}) \propto T_{\text{dust}}$. Therefore, the estimated column density, and consequently the mass, depends on the observed mm flux, and the dust opacity and temperature,

$$N(H_2) \propto \frac{F_\lambda}{\kappa_\lambda T_{\text{dust}}}. \tag{3.22}$$

Thus, the masses of the prestellar condensations calculated by Motte et al. and Johnstone et al., using mm continuum observations, may be underestimated by up to a factor of 2, which will affect their evaluation of the core mass function in the $\rho$ Oph protocluster, and the inferred stability or instability of the observed cores. Detailed modelling for each of the prestellar cores, taking into account their environment (i.e. surrounding cloud and nearby luminosity sources), is needed to calculate their masses with better accuracy. Also, as Motte et al. point out, the dust opacity and also the dust-to-gas ratio, introduce additional uncertainties in mass calculations.
3.3.3 SEDs and intensity profiles

In the UV and optical (0.01-1 $\mu$m), the radiation coming from the system is scattered light and direct background radiation (mainly coming from the edge of the cloud where the optical depth is small). In the NIR and MIR (1-50 $\mu$m) most of the radiation is direct background radiation that just passes through the outer, optically thin parts of the cloud. This depends on the assumed background radiation field, the optical depth of the cloud (and hence the dust properties) and the extent of the cloud. The FIR, submm, mm range (60-1300 $\mu$m) is the most interesting range since the core emits most of its radiation at these wavelengths. Many terrestrial and space-borne observatories cover (or have covered) this range: ISOPHOT/ISO (90, 170 and 200 $\mu$m), SCUBA/JMCT (350-1300 $\mu$m), IRAM (1300 $\mu$m) and finally the upcoming SIRTF (3.6-160 $\mu$m, to be launched in 2003) and Herschel (75-500 $\mu$m, to be launched in 2007).

At 90 microns the core is seen in absorption against the background (Figs. 3.15a and 3.17a). The intensity depends on the temperature exponentially, so the relatively small increase in temperature towards the edge of the core can compensate for the rapid decrease in the column density, and the intensity increases towards the edge of the core. For a very centrally-condensed core (e.g. models EM2x, Fig. 3.17a) the decrease towards the centre is around $\sim 8-10$ MJy sr$^{-1}$ (depending on how deep the core is embedded in the cloud; for more deeply embedded cores the intensity decrease is smaller), and this would be very difficult to detect. For less centrally-condensed cores (e.g. EM1x, Fig. 3.15a) the decrease is even smaller ($\sim 4-6$ MJy sr$^{-1}$). Thus, very sensitive (say $\sim 1 - 3$ MJy sr$^{-1}$) observations are needed to detect cores in absorption. This sensitivity is very close to the limits of current instruments, so it is very difficult to observe embedded prestellar cores at 90 $\mu$m.

At wavelengths near the peak of the emission (150-250 $\mu$m) the intensity increases by a small amount ($\sim 5 - 20$ MJy sr$^{-1}$ above the background) towards the edge of the cloud and then decreases to the background intensity (Figs. 3.15b and 3.17b). If the temperature increase towards the edge of the core is big enough to compensate for the decrease in column density, the outer parts of the core are just visible (e.g. models with visual optical depth $\tau_{\text{cloud}} = 5$). On the other hand, if the increase of the temperature is not high enough, as happens when the core is deeply embedded ($\tau_{\text{cloud}} = 20$), then the core cannot be distinguished from the background. Thus, our models indicate that cores can be observed at 150-250 $\mu$m only if they are surrounded by a cloud with a relatively small visual optical depth $\tau_{\text{cloud}} \sim 5$, in which case the intensity increase is $\sim 10$ MJy sr$^{-1}$. Cores could in principle be observed even if they are deeply embedded, provided
there were accurate observations of $\sim 1$ MJy sr$^{-1}$ at 150-250 $\mu$m. This result agrees with the fact that ISO did not detect the prestellar condensations in $\rho$ Oph (André et al. 2000).

Finally, at submillimetre and millimetre wavelengths (400-1300 $\mu$m) the Rayleigh-Jeans approximation for the Planck function holds, and the observed intensity is proportional to the product of the core column density and temperature. Thus, at the edge of the core the intensity drops considerably because the temperature increase cannot compensate for the column density decrease. The core can easily be observed at 400-500 $\mu$m, where the contrast with the background is quite large ($\sim 50-150$ MJy sr$^{-1}$). At wavelengths longer than $\sim 600$ $\mu$m the background radiation becomes important and the core emission is not much larger than the background emission. For example at 850 $\mu$m (Figs. 3.15 and 3.17c) the core emission is only $\sim 20-50$ MJy sr$^{-1}$ above the background, depending on the density profile of the core and how deeply the core is embedded inside the molecular cloud. High accuracy observations are needed to observe cores at mm wavelengths, but they are available. For example, the sensitivity of IRAM is around $\sim 1$ MJy sr$^{-1}$. The peak luminosities at 1300 $\mu$m that we compute with our models are comparable with the observed luminosities of Motte et al. (1998).

To check if our results are affected by the extent of the ambient cloud, we study a core with the same parameters as the EM2.05 model but embedded in a more extended, less dense cloud. In both models the optical depth of the cloud is the same. As seen in Fig. 3.18, the temperature and intensity profiles at 90, 170 and 450 $\mu$m of the two models are almost identical inside the core. This result indicates that the only parameter of the ambient cloud that is important in determining the dust temperature and the SED of a core embedded in the centre of a molecular cloud, is the optical depth of the molecular cloud.

3.3.4 Diagnostics

In Table 3.3, we list the peak intensities (maximum intensity above or below the background) at wavelengths 90, 170, 450, 850, 1300 $\mu$m, for cores embedded in molecular clouds with visual optical depths 5 and 20. The lower intensity values correspond to less condensed cores (subcritical) and the higher intensity values to more condensed cores (supercritical). This table indicates that embedded cores are most easily distinguished from the background radiation around 450 $\mu$m. The peak emission from embedded cores could be as low as $\sim 10$ MJy sr$^{-1}$ above the background at 1300 $\mu$m, but it is at least $\sim 40$ MJy sr$^{-1}$ at 450 $\mu$m. The wavelength range between 400 and 500 $\mu$m seems favourable for observing embedded cores but the atmospheric transmission is not
Figure 3.16 The same as in Fig. 3.14, but for a supercritical BE sphere with the same parameters (EM2x models): Density profiles (a), dust temperature profiles (b) and SEDs (c), for BE spheres at 15 K, with mass 0.8 M_☉, under external pressure P_{ext} = 10^6 cm\(^{-3}\) K, surrounded by a spherical ambient cloud with visual optical depth 20 (model EM2.20, solid lines), 5 (model EM2.05, dotted lines) and 0 (model EM2, dashed lines; no surrounding cloud). The dash-dot line on the SED graph corresponds to the background SED.

Figure 3.17 Intensity profiles at 90 (a), 170 (b), 450 and 850 μm (c), for the models in Fig. 3.16 (EM2.20: solid lines, EM2.05: dotted lines, EM2: dashed lines). The horizontal solid lines on the profiles correspond to the background intensity at the wavelength marked on the graph. In this case (more centrally condensed core than that in Fig. 3.15), the intensity at the centre of the core at 90 μm is lower and, thus, the core is relatively more easily observed in absorption than a less centrally condensed core. In addition, the increase of the intensity towards the edge of the core at 170 μm, is larger in this case and thus easier to observe.
3.3. PRESTELLAR CORES EMBEDDED IN MOLECULAR CLOUDS

![Graphs showing density, temperature, and intensity profiles](image)

**Figure 3.18** Density profiles (a), dust temperature profiles (b) and intensity profiles (c) at 90, 170 and 450 μm, for a supercritical BE sphere at 15 K, with mass 0.8 M☉, under external pressure $P_{\text{ext}} = 10^6 \text{cm}^{-3} \text{K}$, surrounded by a spherical ambient cloud with visual optical depth 5 and $n_{\text{crit}} = 0.96 \times 10^4 \text{ cm}^{-3}$ (model EM2.05, solid lines) and $n_{\text{crit}} = 0.45 \times 10^4 \text{ cm}^{-3}$ (same optical depth as before but more extended cloud, dotted lines). The horizontal solid lines on the profiles correspond to the background intensity at 170, 90 and 450 μm, from top to bottom. The dust temperature and the intensity profiles are almost identical inside the core for the two models examined, indicating that these profiles are determined mainly by the optical depth of the core rather than its physical extent.

![Graphs showing density, temperature, and intensity profiles](image)

**Figure 3.19** Comparison of a subcritical (model EM1.05, dotted lines) with a supercritical (model EM2.05, solid lines) BE sphere, embedded in a molecular cloud with visual optical depth 5. Density profiles (a), dust temperature profiles (b) and intensity profiles (c) at 90, 170 and 450 μm. The horizontal solid lines on the profiles correspond to the background intensity at 170, 90 and 450 μm, from top to bottom. The dust temperature inside a more centrally condensed core is lower than for a less centrally condensed core. The core emission is shifted towards longer wavelengths and, thus, a supercritical core will emit more radiation at submm wavelengths than a subcritical core.
Table 3.3  Typical peak* intensities for embedded cores

<table>
<thead>
<tr>
<th>$\lambda$ ((\mu m))</th>
<th>$I_\lambda^a$ (MJy sr(^{-1}))</th>
<th>$\tau_{\text{cloud}} = 5$</th>
<th>$\tau_{\text{cloud}} = 20$</th>
</tr>
</thead>
<tbody>
<tr>
<td>90(^b)</td>
<td>5-15</td>
<td>$\sim 3$</td>
<td></td>
</tr>
<tr>
<td>170</td>
<td>10-15</td>
<td>$\sim 3$</td>
<td></td>
</tr>
<tr>
<td>450</td>
<td>55-160</td>
<td>40-130</td>
<td></td>
</tr>
<tr>
<td>850</td>
<td>20-80</td>
<td>15-70</td>
<td></td>
</tr>
<tr>
<td>1300</td>
<td>10-40</td>
<td>10-25</td>
<td></td>
</tr>
</tbody>
</table>

* The term peak refers to the maximum intensity above or below the background (as noted) at a specific wavelength.

\(^a\) These are typical approximate peak intensities for a core embedded in a cloud with visual optical depth $\tau_{\text{cloud}} = 5$ and $\tau_{\text{cloud}} = 20$. The deeper the core is embedded, the less distinct from the background it is. The lower value corresponds to a subcritical core and the higher value to a supercritical core.

\(^b\) At 90 \(\mu m\) the core is seen in absorption against the background.

good in this range and space observations are needed. The upcoming Herschel space telescope will be operating in this range.

Continuum intensity observations at different submm wavelengths can be used to determine if a core is subcritical or supercritical, assuming cores can be described as BE spheres. If the core is supercritical, it is more condensed in the centre and the optical depth to the centre of the core is larger than a subcritical, less condensed core. This means that the dust temperature at the centre of the core is less for a supercritical core, and the resultant spectrum is shifted towards longer wavelengths. Thus, a supercritical core emits more radiation at longer wavelengths (e.g. 450 \(\mu m\); see Fig. 3.19) than a subcritical core. We can exploit the fact that the intensity at 170-200 \(\mu m\) varies little for different cores in the same environment, and use the colour index $CI = m(450 \, \mu m) - m(170 \, \mu m)$ to distinguish between subcritical and supercritical cores, eliminating in this way any uncertainties in the distances to the observed cores. CI will be larger for supercritical cores. This result can be used to determine whether a core is subcritical or supercritical when the core cannot be resolved and the usual density criterion ($\rho_{\text{centre}}/\rho_{\text{edge}} > 14.1$ for supercritical spheres) is not useful.

Our models can also be used to estimate the visual extinction of the ambient cloud surrounding an embedded core. The outer parts of even deeply embedded cores ($\tau_{\text{cloud}} \sim 20 - 30$) are expected
to be just visible in emission at 170-200 \( \mu \text{m} \) (\( \sim 3 \text{ MJy sr}^{-1} \) above the background), whereas cores embedded in a moderately thick cloud \( (\tau_{\text{cloud}} \lesssim 5 - 7) \) will be more visible (\( \sim 10 \text{ MJy sr}^{-1} \) above the background), as seen in Figs. 3.15b and 3.17b. The higher the increase in the intensity near the core boundary, the less embedded is the core. Thus, very sensitive observations of embedded prestellar cores at 170-200 \( \mu \text{m} \) (\( \sim 1 - 3 \text{ MJy sr}^{-1} \)), might allow us to determine the extinction of the cloud surrounding the core, and thus to estimate roughly the position of the core inside the molecular cloud.

### 3.4 Summary

We study cores that are directly exposed to the ISRF and find similar results (temperature and intensity profiles) with Evans et al. (2001), using a different radiative transfer method. We extend our study to cores that are embedded inside spherical molecular clouds. We assume that the ambient cloud has uniform density, and that the dust composition is the same as that in the embedded core. In this case, the radiation incident on the embedded core is not isotropic and cannot be represented by the Black (1994) approximation, since the ambient cloud shields the core from UV, optical and NIR photons and enhances the FIR and mm part of the spectrum. We find that, in this case, the temperature is generally less than 12 K, even for cores in ambient clouds with low visual extinction (\( \sim 5 \text{ mag} \)). The temperature gradients inside embedded cores are smaller than in the case of non-embedded cores; deeply embedded cores are almost isothermal. Recent studies (André et al. 2003) using a different approach, in which they estimate the effective radiation field incident on an embedded core from observations, also find that the temperature inside embedded cores is lower than in non-embedded cores. Previous mass estimates using mm fluxes have assumed isothermal cores at temperatures 12-20 K and, consequently, they may have underestimated the masses of the cores by up to a factor of 2. However, more detailed modelling is needed for each specific core for more accurate mass estimates.

Our models provide a view of cores at a wide range of wavelengths. We find that embedded cores can be observed at 400-500 \( \mu \text{m} \), where the core is easily distinguished from the background. Embedded cores can also be observed at 600-1300 \( \mu \text{m} \). The contrast of the core radiation against the background radiation is not large but very sensitive observations are available in this range. In addition, most of the background radiation is the CMB, which can be substracted easily. At shorter wavelengths the cores are just visible in emission (170-200 \( \mu \text{m} \)) or in absorption against
the background. We also find that very sensitive observations at 170-200 μm can be used to estimate the visual extinction of the cloud surrounding a core, and thus to get a rough idea of where the core lies in the environment of the protocluster. The upcoming Herschel satellite will be observing in the 60-700 μm range with high sensitivity and high angular resolution (André 2002), and will test our models. Sensitive intensity observations in this range will also reveal very low-mass condensations present in embedded protoclusters, that were previously undetected or marginally detected. These observations combined with theoretical models will enable us to estimate with great accuracy the temperature profiles of resolved prestellar cores. In addition, mm observations from the ground will provide accurate mass estimates for the cores, and they will constrain the dust opacity.

Theoretical modelling should be done for each core individually, taking into account the core surroundings (ambient cloud, local luminosity sources). The Monte Carlo approach for radiative transfer is inherently 3D and can treat such asymmetric systems. In the next chapter we extend our study to asymmetric models of prestellar cores.
Chapter 4

Asymmetric Models of Prestellar Cores

Previous continuum radiative transfer models of prestellar cores have examined non-embedded cores (Evans et al. 2001), embedded cores (André et al. 2003) and non-embedded flattened cores (Zucconi, Walmsley, & Galli 2001). The above studies have focused on spherical Bonnor-Ebert (BE) cores, apart from Zucconi et al. who use a semi-analytical approximate radiative transfer method to study magnetically flattened cores. In this chapter, we present radiative transfer models of asymmetric non-embedded and embedded cores, with density profiles different from the BE profile but consistent with what observations suggest (i.e. a density profile that falls as $r^{-2}$ at large distances from the centre of the core but is flat near the centre). In Section 4.1 we describe how we adapt PHAETHON to study asymmetric cores. In Section 4.2 we present simulations of flattened prestellar cores (non-embedded and embedded in molecular clouds), and in Section 4.3 we examine asymmetric cores that are denser on one side. Finally, in Section 4.5, we summarise our results.

4.1 Initial system setup

PHAETHON (see Chapter 2) is adapted for the study of cores with spherical shape but with a non-symmetric density distribution. The core itself is divided into a number of cells by spherical and conical surfaces. The spherical surfaces are evenly spaced in radius, and there are typically 50-100 of them. The conical surfaces are evenly spaced in polar angle, and there are typically
Figure 4.1  L-packet injection into the core: The packet is injected from a random point $(\theta, \phi)$ on the surface of the sphere at such an angle $\theta_{\text{in}}, \phi_{\text{in}}$ as to imitate an isotropic radiation field. The frequency of the injected packet is chosen from the Black (1994) radiation field.

10-20 of them. Hence the core is divided into 500-2000 cells. The specific number of cells used is chosen so that the density and temperature differences between adjacent cells are small.

The $L$-packets are injected from the outside of the core with such a direction as to mimic an isotropic radiation field incident on the core (see Fig. 4.1). To do that we first define (using random numbers $\mathcal{R}_i \in [0,1]$, $i = 1, 2, \ldots$), the $L$-packet injection point on the surface of the core,

$$\theta = \cos^{-1}(1 - 2\mathcal{R}_1) , \quad (4.1)$$

$$\phi = 2\pi\mathcal{R}_2 , \quad (4.2)$$

and then the direction of the ingoing packet ($L$-packet injection vector, Fig. 4.1),

$$\theta_{\text{in}} = \cos^{-1} \left( \mathcal{R}^{1/2}_3 \right) , \quad (4.3)$$

$$\phi_{\text{in}} = 2\pi\mathcal{R}_4 , \quad (4.4)$$

where $\theta_{\text{in}}$ is the angle between the normal vector to the tangent plane at the point of entry and the packet injection vector, and $\phi_{\text{in}}$ is the polar angle defined on the tangent plane.

We further assume that the radiation field incident on the core is the Black (1994) interstellar radiation field (hereafter BISRF), which consists of radiation from giant stars and dwarfs, thermal emission from dust grains, mid-infrared emission from transiently heated small grains, and the
4.2. FLATTENED PRESTELLAR CORES (DISK-LIKE ASYMMETRY)

Our cosmic background radiation. This is a good approximation to the radiation field in the solar
neighbourhood but it is not always a good choice when studying prestellar cores, since in many
cases the core environment plays an important role in determining the radiation field incident
on the core. Here, we simulate the effect of the core environment by embedding the core in a
molecular cloud which modulates the radiation field incident on the core. Another option is to
estimate the effective radiation field incident on an embedded core by observing it directly (André
et al. 2003).

The dust composition (and therefore the dust opacity) in prestellar cores is uncertain, but in
such cold and dense conditions, dust particles are expected to coagulate and accrete ice. As in
our previous study of prestellar cores (see Chapter 3), we use the Ossenkopf & Henning (1994)
opacities for a standard MRN interstellar grain mixture (53% silicate and 47% graphite) that has
coagulated and accreted thin ice mantles over a period of $10^5$ yr at a density of $10^6$ cm$^{-3}$.

4.2 Flattened prestellar cores (disk-like asymmetry)

4.2.1 Non-embedded cores: the model

Core collapse models predict that an initially spherical core will flatten as the collapse evolves
due to the effect of a dipolar magnetic field and the process of ambipolar diffusion (e.g. Ciolek
& Mouschovias 1994). Observations of magnetic field geometry on the plane of the sky, using
polarisation directions (Ward-Thompson et al. 2000), indeed indicate a uniform magnetic field in
prestellar cores. However, the observed magnetic fields are not perpendicular to the long axes of
the cores, and, therefore, the question of how the presence of a magnetic field affects core collapse
remains open. The flattening of a core could also be due to rotation. Observations suggest
that cores rotate uniformly with a typical ratio of rotational to gravitational energy $\beta \sim 0.02$
(Goodman et al. 1993).

In our models, we assume that the core is spherical in shape, but the density distribution is
not spherically symmetric. More specifically, we assume a flattened core, i.e. a core that is denser
on the equatorial plane. The goal of this study is to discover distinctive features in the SED
and/or on the isophotal maps that could be indicative of the density and temperature structure
of the core and its evolutionary stage.
We choose a core density profile that depends both on the radial distance $r$ and the polar angle $\theta$:

$$n(r, \theta) = n_c \frac{1 + A \left( \frac{r}{r_0} \right)^2 \sin^p(\theta)}{\left[ 1 + \left( \frac{r}{r_0} \right)^2 \right]^2}. \quad \text{(4.5)}$$

$n_c$ is the density at the centre of the core, and $r_0$ the scale length. $A$ is a factor that determines the equatorial-to-polar optical depth ratio $e$ (i.e. the optical depth from the centre to the surface of the core at $\theta = 90^\circ$ divided by the optical depth from the centre to the surface of the core at $\theta = 0^\circ$). The exponent $p$ determines how fast the optical depth rises from the pole to the equator. This density profile is similar to the BE sphere density profile, similar to density profiles predicted by amibipolar diffusion models (Ciolek & Basu 2000), and consistent with observations of prestellar cores (i.e. it drops as $r^{-2}$ at large distance from the centre of the core and is flatter near the centre).

We examine cores with central density $n_c = 10^6 \text{ cm}^{-3}$, scale length $r_0 = 2 \times 10^3 \text{ AU}$, outer radius $R_{\text{core}} = 2 \times 10^4 \text{ AU}$, and different $p$ and $e$ values (see core density profiles on the $y - z$ plane in Fig. 4.2). The parameters of our models are listed in Table 4.1.

### 4.2.2 Results: core temperatures, SEDs and images

In non-embedded cores, the dust temperature drops from around 17 K at the edge of the core to 7 K at the centre of the core, as previous studies indicate (Zucconi et al. 2001; Evans et al. 2001; Stamatellos & Whitworth 2003). We also find that the dust temperature inside flattened prestellar cores is $\theta$ dependent (see Figs. 4.3), similar to the results of Zucconi et al. (2001). As

<table>
<thead>
<tr>
<th>model ID</th>
<th>asymmetry type</th>
<th>$e$</th>
<th>$p$</th>
<th>$M (M_\odot)$</th>
<th>$\tau_V(\theta = 0^\circ)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>disk-like</td>
<td>1.5</td>
<td>4</td>
<td>2.0</td>
<td>94</td>
</tr>
<tr>
<td>1.2</td>
<td>disk-like</td>
<td>2.5</td>
<td>4</td>
<td>5.1</td>
<td>94</td>
</tr>
<tr>
<td>1.3</td>
<td>disk-like</td>
<td>1.5</td>
<td>1</td>
<td>5.0</td>
<td>94</td>
</tr>
<tr>
<td>1.4</td>
<td>disk-like</td>
<td>2.5</td>
<td>1</td>
<td>7.3</td>
<td>94</td>
</tr>
</tbody>
</table>

$e$: Equatorial-to-polar optical depth ratio

$M$: Core mass

$\tau_V$: Visual optical depth from the centre to the surface of the core along the pole ($\theta = 0^\circ$).
expected, the equator of the core is colder than the poles. The difference in temperature between two points with the same distance \( r \) from the centre of the core but with different polar angles \( \theta \), is larger for the more flattened (less symmetric) cores (those with \( e = 2.5 \); Figs. 4.3b,d). The difference is also larger for the \( p = 4 \) models than for the \( p = 1 \) models. For example, at half the radius of the core (\( 1 \times 10^4 \) AU) the temperature difference between the point at \( \theta = 0^\circ \) (core pole) and the point at \( \theta = 90^\circ \) (core equator), is 5 – 6 K for the \( p = 4 \) models (Figs. 4.3a, 4.3b) but only \( \sim 2 \) K for the \( p = 1 \) models (Figs. 4.3c, 4.3d). This temperature difference will affect the appearance of the core at wavelengths shorter than or near the core peak emission, where the Planck function is strongly (exponentially) dependent on the temperature.

The SED (Fig. 4.4) of a specific core, for the model parameters we examine, is the same at any viewing angle, because the core is optically thin to the radiation it emits (FIR and longer wavelengths). Thus, it is not possible to distinguish between flattened and spherical cores, using SED observations, unless the core is extremely flattened, so that it is optically thick on the equator at FIR and longer wavelengths. If we assume a polar visual optical depth of 94 (as in the models discussed here), then in order to see a difference in the SED when viewing the core edge on, the optical depth in this direction should be at least 1, at FIR and longer wavelengths. If, for example, the optical depth at \( 200 \) \( \mu \)m \( \tau_{200\mu m} = 1 \) then the visual optical depth would be \( \tau_V = \tau_{200\mu m} \times (\kappa_V / \kappa_{200\mu m}) \approx 5 \times 10^3 \) (using the Ossenkopf & Henning (1994) opacities), and thus the equatorial-to-polar optical depth ratio would be \( e \approx 50 \), i.e. much more flattened than the cores we examine here.

In contrast, the isophotal maps of a core do depend on the observer’s viewing angle. Additionally, they depend on the wavelength of observation. Our code calculates images at any wavelength, and it provides an ideal tool for direct comparison with observations, e.g. at mid-infrared (ISO/ISOCAM), far-infrared (ISO/ISOPHOT) and submm/mm (SCUBA, IRAM) wavelengths. We distinguish two wavelength regions on which we focus: (i) the region near the peak of the core emission (150-250 \( \mu \)m; we choose 200 \( \mu \)m as a representative wavelength), and (ii) at wavelengths much longer than the peak (submm and mm region; we choose 850 \( \mu \)m as a representative wavelength). In each of the above regions the isophotal maps have similar general characteristics.

At 200 \( \mu \)m the core appearance depends both on its temperature and its column density in the observer’s direction. It is seen in Figs. 4.6-4.9, that the cores appear spherical when viewed pole-on and flattened when viewed edge-on. The outer parts of a core can be more or less luminous than the centre parts, depending on the core temperature and the observer’s viewing angle. For
Figure 4.2  Density distribution on the $y-z$ plane (a) for a flattened asymmetric core with equatorial-to-polar optical depth ratio $e = 1.5$ and $p = 4$ (model 1.1), (b) for a more flattened asymmetric core, with $e = 2.5$ and $p = 4$ (model 1.2), (c) for a core with $e = 1.5$ and $p = 1$ (model 1.3), and (d) for a more flattened core, with $e = 2.5$ and $p = 1$ (model 1.4). We plot iso-density contours every $10^{0.5}\text{cm}^{-3}$. The central contour corresponds to $n = 10^{5.5}\text{cm}^{-3}$.
Figure 4.3 Temperature distribution on the $y-z$ plane, for the models presented in Fig. 4.2. We plot iso-temperature contours from 8 to 18 K, every 2 K.
Figure 4.4  SED for the core models in Figs. 4.2, 4.3; model 1.1 ($e = 1.5, p = 4$; short-dashed line), model 1.2 ($e = 2.5, p = 4$; solid line), model 1.3 ($e = 1.5, p = 1$; long-dashed line) and model 1.4 ($e = 2.5, p = 1$; dash-dot line). The SED of each core is independent of the observer’s viewing angle. The dotted line on the graph corresponds to the incident/background SED.

example, at close to pole-on viewing angles the outer parts of the core are more luminous than the inner parts of the core (limb brightening; e.g. Figs. 4.6-4.9, $\theta = 0^\circ$). This happens because the temperature is higher in the outer parts and this compensates for the lower column density (since at wavelengths near the peak of the core emission and shorter, the Planck intensity $B_{\nu}(T)$ depends on temperature as $B_{\nu}(T) \propto e^{-\alpha/T}$, $\alpha =$ const). At other viewing angles the appearance of the core is determined by a combination of temperature and column density effects (Figs. 4.6-4.9, $\theta = 30^\circ, 60^\circ, 90^\circ$). This interplay between core temperature and column density along the line of sight results in characteristic features on the images of the cores. Such features include (i) the two intensity minima at almost symmetric positions relative to the centre of the core, on the image at $30^\circ$ (Fig. 4.7-4.9), and (ii) the two intensity maxima, again at symmetric positions relative to the centre of the core, on the images at $90^\circ$ (Figs. 4.6-4.7). (It is also worth mentioning that although the characteristic features appear in symmetric positions relative to both axes of density-symmetry, we should expect deviations from symmetry to arise if the radiation field incident on the core is not isotropic).

We conclude that isophotal maps at 200 \( \mu \)m contain useful information, and sensitive, high resolution observations at 200 \( \mu \)m, could be helpful in determining the core density and temperature structure and the orientation of the core with respect to the observer. In Fig. 4.5, we present
a perpendicular cut through the centre of the core images presented in Fig. 4.7. We also plot the beam size of the ISOPHOT C-200 camera (90″, or 9000 AU for a core at 100 pc) and the beam size of the upcoming (2007) Herschel (13″, or 1300 AU, for the 170 μm band of PACS or 17″~1700 AU for the 250 μm band of SPIRE). ISOPHOT’s resolution may not be good enough to detect the features mentioned above. Indeed, a search in the Kirk et al. (2003) sample of ISO/ISOPHOT observations (also see Ward-Thompson et. al 2002) does not reveal any cores with such distinctive features. However, Herschel should, in principle, be able to detect such features in the future.

![Graph](image)

**Figure 4.5** A perpendicular cut through the centre of the core images presented in Fig. 4.7 for model 1.2 (also including the background radiation field). We also plot the beam size of ISO/ISOPHOT at 200 μm (90″ ~ 9000 AU, for a core at 100 pc) and the beam size of the upcoming (2007) Herschel (13″ ~ 1300 AU for the 170 μm band of PACS or 17″ ~ 1700 AU for the 250 μm band of SPIRE). ISO’s resolution may not be good enough to detect any of the features on the graph, but Herschel will have a much better resolution and should be able to detect such features in the future.

In the second wavelength region (submm and mm wavelengths) the core emission is in effect regulated by the column density alone (e.g. at 850 μm, Figs. 4.10-4.13). Thus, the intensity is larger at the centre, where the column density is also larger. For the same reason the core appears flattened when the observer looks at it from any direction other than pole-on. It is also evident that the peak intensity of the core is much larger when the core is viewed edge-on. Therefore, flattened cores are more prominent when viewed edge-on. This introduces a possible observational selection effect which should be taken into account when studying the shape statistics of prestellar
Figure 4.6 Isophotal maps at 200 μm at viewing angles 0°, 30°, 60° and 90°, for a flattened core with equatorial-to-polar optical depth ratio $c = 1.5$ and $p = 4$ (model 1.1). We plot an isophotal contour at 5 MJy sr$^{-1}$ and then from 60 to 110 MJy sr$^{-1}$, every 5 MJy sr$^{-1}$. There are characteristic symmetric features due to core temperature and orientation with respect to the observer. We note that in these isophotal maps, and in all subsequent isophotal maps, the axes $(x, y)$ refer to the plane of sky as seen by the observer.
Figure 4.7 Same as Fig. 4.6, but for a more flattened core, with equatorial-to-polar optical depth ratio $e = 2.5$ and $p = 4$ (model 1.2).
**Figure 4.8** Same as Fig. 4.6, but for a core with equatorial-to-polar optical depth ratio $e = 1.5$ and $p = 1$ (model 1.3).
Figure 4.9  Same as Fig. 4.6, but for a core with equatorial-to-polar optical depth ratio $e = 2.5$ and $p = 1$ (model 1.4).
Figure 4.10 Isophotal maps at 850 μm at viewing angles 0°, 30°, 60° and 90°, for a flattened core with equatorial-to-polar optical depth ratio $e = 1.5$ and $p = 4$ (model 1.2). We plot an isophotal contour at 1 MJy sr$^{-1}$ and then from 5 to 50 MJy sr$^{-1}$, every 5 MJy sr$^{-1}$. The core appears elongated when viewed at an angle other than $\theta = 0°$. 
Figure 4.11  Same as Fig. 4.10, but for a more flattened core, with equatorial-to-polar optical depth ratio $e = 2.5$ and $p = 4$ (model 1.2).
Figure 4.12  Same as Fig. 4.10, but for a core with equatorial-to-polar optical depth ratio $e = 1.5$ and $p = 1$ (model 1.3).
Figure 4.13  Same as Fig. 4.10, but for a core with equatorial-to-polar optical depth ratio $e = 2.5$ and $p = 1$ (model 1.4).
cores. Low-mass flattened cores are more likely to be detected if they are edge-on. This is true for optically thin mm and submm continuum observations, and also for optically thin molecular line observations. For example, when comparing the projected shapes of condensations from hydrodynamic simulations with the observed shapes using solely optically thin continuum or molecular line observations, one should expect a lower number of observed near-spherical cores than indicated by the simulations. This may be the reason for the small excess of high axis ratio cores in the simulations by Gammie et al. (2003) (see their Fig. 9).

4.2.3 Embedded prestellar cores

In the previous section, we studied cores that are directly exposed to the interstellar radiation field (as approximated by the BISRF). However, cores are generally embedded in molecular clouds, with visual optical depths ranging from 2-10 (e.g. in Taurus) up to 40 (e.g. in ρ Ophiuchi). The ambient cloud absorbs the energetic UV and optical photons and re-emits them in the FIR and submm (because the ambient cloud is generally cold, $T_{\text{cloud}} \sim 20-100$ K). Therefore, the radiation incident on a core that is embedded in a cloud is reduced in the UV and optical, and enhanced in the FIR and submm (Mathis et al. 1983). Previous radiative transfer calculations of spherical cores embedded at the centre of an ambient cloud (Stamatellos & Whitworth 2003), have shown that embedded cores are colder ($T < 12$ K) and that the temperature gradients inside these cores are smaller than in non-embedded cores. André et al. (2003) also found that the temperatures inside embedded cores are lower than in non-embedded cores (assuming that they are heated by the same ISRF), using a different approach, in which they estimated the effective radiation field incident on an embedded core from observations.

Here, we examine the more general case of embedded flattened cores. We model a core with the same set of parameters as model 1.2 (p=4, e=2.5) but embedded in a uniform density ambient cloud with different visual extinctions $A_V$ ($A_V = 1.086 \tau_V$). The ambient cloud is illuminated by the BISRF. In Fig. 4.14, we present the temperature profiles at $\theta = 0^\circ$ (core pole; upper curves) and $\theta = 90^\circ$ (core equator; lower curves), (i) for a non-embedded core (dashed lines; model 1.2), (ii) for the same core embedded at the centre of an ambient cloud with $A_V = 4$ (dotted lines), and (iii) for the same core embedded at the centre of an ambient cloud with $A_V = 13$.

A core embedded in an ambient cloud with $A_V = 4$ that is illuminated by the same ISRF as the non-embedded core (i.e. the BISRF) is colder, and the temperature gradient inside the core is lower, than in the case of a non-embedded core (see the temperature profile in Fig. 4.15
4.2. FLATTENED PRESTELLAR CORES (DISK-LIKE ASYMMETRY)

Figure 4.14 The effect of the parent cloud on cores. Temperature profiles of a non-embedded core (model 1.2; dashed lines), and of a core at the centre of a cloud with visual extinction $A_V = 4$ (dotted lines), and $A_V = 13$ (solid lines). The upper curve of each set of lines corresponds to the direction towards the pole of the core ($\theta = 0^\circ$), and the bottom curve to the direction towards the core equator ($\theta = 90^\circ$). The core is colder when it resides inside a thicker parent cloud (i.e. when it is illuminated by a radiation field that is weakened at short ($< 10 \mu$m) wavelengths), and the temperature differences between different parts of the core are smaller. Thus, the characteristic features in the isophotal maps at wavelengths near the peak of the core SED are weakened.

Figure 4.15 Temperature distribution on the $y-z$ plane, for the same model presented in Figs. 4.2b and 4.3b ($e = 2.5$, $p = 4$, model 1.2), but embedded in the centre of an ambient molecular cloud of visual extinction $A_V = 4$. We plot iso-temperature contours from 8 to 13 K, every 1 K. The core is colder than the non-embedded core (Fig. 4.3b) and the temperature gradient inside the core is smaller.
**Figure 4.16** Same as Fig. 4.5, i.e. model 1.2, but for a flattened core embedded in a uniform molecular cloud with visual extinction $A_V = 4$. The features at different angles are weaker than in the case of a non-embedded core.

**Figure 4.17** Same as Fig. 4.5, i.e. model 1.2, but for a flattened core embedded in a uniform molecular cloud with visual extinction $A_V = 13$. The features at 30° no longer exist, but there are two characteristic intensity minima at symmetric positions at 60° and 90°.
and compare with the profile in Fig. 4.3b). The isophotal maps are similar to those of the non-embedded core model (Figs. 4.7 and 4.11) but the characteristic features discussed in the previous section are less prominent. This is because the temperature gradient inside the core is smaller when the core is embedded (see Fig. 4.14). For example, at half the radius of the core \( r = 1 \times 10^4 \) AU the temperature difference between the point at \( \theta = 0^\circ \) and the point at \( \theta = 90^\circ \), is \( 5 - 6 \) K for the non-embedded core but only \( \sim 1.5 \) K for the same core embedded in an \( A_V = 4 \) ambient cloud. In Fig. 4.16 we present a perpendicular cut through the centre of the embedded core image at viewing angle 30°. It is evident that the features are quite weak, but they have the same size as in the non-embedded core (Fig. 4.5), and they may be detectable with Herschel, given an estimated rms sensitivity better than \( \sim 1 - 3 \) MJy sr\(^{-1} \) at 170-250 \( \mu \)m for clouds outside the Galactic plane (dependent on cirrus confusion).

For a core embedded in an ambient cloud with \( A_V = 13 \), the temperature differences between different parts of the core are even smaller (\( \lesssim 1 \) K at \( r = 1 \times 10^4 \) AU, see Fig. 4.14), but characteristic features continue to exist (e.g. two symmetric intensity minima at 60° and 90°, see Fig. 4.17).

Thus, continuum observations near the peak of the core emission, could be used to obtain information about the core density and temperature structure and orientation, even if the core is very embedded (\( A_V \sim 10 - 20 \)).

### 4.2.4 The effect of a UV-enhanced ISRF on embedded cores

We now examine the effect that a UV-enhanced ISRF has on the temperature profiles and isophotal maps of deeply embedded cores. We consider an ISRF that consists of the BISRF, plus an additional component of diluted blackbody flux from a star with \( T_* = 6000 \) K or \( T_* = 10000 \) K, that isotropically illuminates the molecular cloud in which the core resides. We use a dilution parameter \( \omega_* = 10^{-13} \), so that the total additional luminosity illuminating the cloud is

\[
L = \omega_* 4\pi R_{\text{cloud}}^2 \sigma T_*^4, \tag{4.6}
\]

where \( \sigma \) is the Stefan-Boltzmann constant. This additional radiation enhances the radiation incident on the cloud by a factor of \( \sim 3 \) (for \( T_* = 6000 \) K) to \( \sim 30 \) (for \( T_* = 10000 \) K), at \( \lambda = 0.4 \ \mu \)m, compared with the standard BISRF.
Figure 4.18 The effect of an UV-enhanced ISRF on embedded cores. Temperature profiles of a core with the same set of parameters as model 1.2 (p=4, e=2.5), embedded in a uniform density cloud with visual extinction $A_V = 13$, that is illuminated by the BISRF (solid lines), by the BISRF plus a diluted blackbody of $T_*=6000$ K (dotted lines) and by the BISRF plus a diluted blackbody of $T_*=10000$ K (dashed lines). The upper curve of each set of lines corresponds to the direction towards the pole of the core ($\theta = 0^\circ$), and the bottom curve to the direction towards the core equator ($\theta = 90^\circ$). The core is hotter when the illuminating radiation field is enhanced at UV wavelengths but the temperature differences between different parts of the core are not significantly enhanced.

In Fig. 4.18, we present the temperature profiles at $\theta = 0^\circ$ (core pole; upper curves) and $\theta = 90^\circ$ (core equator; lower curves) for a core with the same set of parameters as model 1.2 (p=4, e=2.5), embedded in a uniform density cloud with visual extinction $A_V = 13$, illuminated by different ISRFs. The bottom pair of curves corresponds to illumination by the standard BISRF, and the upper two sets of curves to illumination enhanced by a diluted blackbody with $T_*=6000$ K and $T_*=10000$ K. The core is hotter when the ambient cloud is illuminated by a more energetic UV field, by $1 - 2$ K for the models we examine. We expect that this difference should be larger for more energetic ISRFs. The temperature differences between different parts of the core seem also to increase, but only by a small amount (< 0.5 K). This means that the characteristic features on the isophotal maps at wavelengths near the peak of the core emission are not significantly changed.
However, for a more energetic illuminating field the enhancement may be larger. For example, the external UV radiation field incident on $\rho$ Ophiuchi is estimated to be $\sim 10 - 100$ times stronger than the BISRF, due to the presence of a nearby B2V star (Liseau et al. 1999). In this case, we expect that the core is hotter and that the temperature differences may be sufficiently large ($\sim 2$ K) to produce detectable features on the isophotal maps at $200 \mu$m. Other luminosity sources, such as newly-born stars that are near the core (within visual optical depth $\tau_V \approx 10 - 15$), may provide the additional UV, optical and NIR heating, needed to produce the temperature gradients within the core which are required for the appearance of the characteristic features on the $150 - 250 \mu$m isophotal maps.

Thus, continuum observations near the peak of the core emission may reveal features characteristic of the core structure even if the core is more deeply embedded ($A_V > 20$), provided that the radiation field incident on the core is sufficiently intense.

### 4.3 “South-pole” asymmetric cores

#### 4.3.1 The model

We consider non-embedded cores with a “south-pole” asymmetry, i.e. the core is denser towards the south pole (see Fig. 4.19):

$$n(r, \theta) = n_c \frac{1 + A \left( \frac{r}{r_0} \right)^2 \left[ \sin(\theta/2) \right]^p}{\left[ 1 + \left( \frac{r}{r_0} \right)^2 \right]^2}, \quad (4.7)$$

where the parameters are the same as defined in Eq. (4.5). Such cores might arise (transiently or even quasi-statically), as a result of complex dynamical interactions during the collapse of magnetised, turbulent giant molecular clouds (Ballesteros-Paredes et al. 2003). Cores denser on one side have also been indicated by $850 \mu$m SCUBA observations (e.g. L1521F, L63; Kirk 2002), although strictly these observations are indicative only of the column density along the line of sight.

In this section, we examine cores with central density $n_c = 10^6$ cm$^{-3}$, scale length $r_0 = 2 \times 10^3$ AU, outer radius $R_{\text{core}} = 2 \times 10^4$ AU, and different $p$ indices and $e$ values, where $e$ is now the south-to-north pole optical depth ratio (i.e. the optical depth from the centre to the surface
of the core at $\theta = 180^\circ$ divided by the optical depth from the centre to the surface of the core at $\theta = 0^\circ$).

<table>
<thead>
<tr>
<th>model ID</th>
<th>asymmetry type</th>
<th>$e$</th>
<th>$p$</th>
<th>$M$ (M$_{\odot}$)</th>
<th>$\tau_V(\theta = 0^\circ)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>south-pole</td>
<td>1.5</td>
<td>4</td>
<td>1.4</td>
<td>94</td>
</tr>
<tr>
<td>2.2</td>
<td>south-pole</td>
<td>2.5</td>
<td>4</td>
<td>3.4</td>
<td>94</td>
</tr>
<tr>
<td>2.3</td>
<td>south-pole</td>
<td>1.5</td>
<td>1</td>
<td>2.4</td>
<td>94</td>
</tr>
<tr>
<td>2.4</td>
<td>south-pole</td>
<td>2.5</td>
<td>1</td>
<td>6.3</td>
<td>94</td>
</tr>
</tbody>
</table>

$e$: South-to-north pole optical depth ratio

$M$: Core mass

$\tau_V$: Visual optical depth from the centre to the surface of the core along the north pole ($\theta = 0^\circ$).

### 4.3.2 Results: core temperatures, SEDs and images

In Fig. 4.19, we present the core density profile on the $y-z$ plane for model 2.2 ($p = 4$, $e = 2.5$), and in Fig. 4.20 the corresponding temperature profile. The temperature drops from $\sim 18$ K at the edge of the core to $\sim 7$ K at the centre of the core, and the denser “southern” parts of the core are colder. The difference between regions of the core with the same $r$ but different $\theta$ is larger for the $p = 4$ models than for the $p = 1$ models, and also larger for the more asymmetric models ($e = 2.5$) than for the less asymmetric models ($e = 1.5$). For example, at half the radius of the core ($1 \times 10^4$ AU) the temperature difference between the point at $\theta = 0^\circ$ (core north pole) and the point at $\theta = 180^\circ$ (core south pole) is $\sim 7$ K for the $p = 4$, $e = 2.5$ model, $\sim 5$ K for the $p = 4$, $e = 1.5$ model, $\sim 4$ K for the $p = 1$, $e = 2.5$ model and $\sim 3$ K for the $p = 1$, $e = 1.5$ model.

As in the case of flattened cores, these temperature differences result in characteristic features on isophotal maps at wavelengths near the peak of the core emission. In Fig. 4.21, we present 200 $\mu$m images at different viewing angles. The core appears spherically symmetric when viewed pole-on, but the effects of a denser “southern” part start to show when we look at the core at different viewing angles. Comparing with the images at 200 $\mu$m for disk-like cores (Fig. 4.6-4.9), we see that in this case there is only one axis of symmetry. Thus, just the degree of symmetry of such features could be indicative of the core density structure. These features contain information about the core density, temperature and orientation with respect to the observer, and therefore...
4.3. "SOUTH-POLE" ASYMMETRIC CORES

Figure 4.19  Density distribution on the $y-z$ plane for a "south-pole" asymmetric core with south-to-north pole optical depth ratio $e = 2.5$ and $p = 4$ (model 2.2). We plot iso-density contours every $10^{0.8}\text{cm}^{-3}$. The central contour corresponds to $n = 10^{5.5}\text{cm}^{-3}$.

Figure 4.20  Temperature distribution on the $y-z$ plane, for the model presented in Fig. 4.19 ($e = 2.5$, $p = 4$, model 2.2). We plot iso-temperature contours from 8 to 18 K, every 2 K. The denser, southern parts of the core are colder.
Figure 4.21 Isophotal maps at 200 \( \mu \text{m} \) at viewing angles 0°, 30°, 60° and 90°, for a flattened core with south-to-north pole optical depth ratio \( e = 2.5 \) and \( p = 4 \) (model 2.2). We plot an isophotal contour at 5 MJy sr\(^{-1} \) and then from 60 to 110 MJy sr\(^{-1} \), every 5 MJy sr\(^{-1} \).
Figure 4.22 Isophotal maps at 850 μm at viewing angles 0°, 30°, 60° and 90°, for a flattened core with south-to-north pole optical depth ratio $e = 2.5$ and $p = 4$ (model 2.2). We plot an isophotal contour at 1 MJy sr$^{-1}$ and then from 5 to 50 MJy sr$^{-1}$, every 5 MJy sr$^{-1}$. The core appears elongated when viewed at an angle other than $\theta = 0°$. 
observations near the peak of the core emission are important. ISO/ISOPHOT resolution was not high enough to detect such features.

The 850 μm images (Fig. 4.22) map the column density of the core along the line of sight. We point out the similarities between the maps in Fig. 4.22, and SCUBA observations of L1521F, L1544, L1582A, L1517B, L63 and B133 (see Kirk 2002). Further modelling for each specific core is required to make more detailed comparisons.

As in the case of flattened cores (Section 4.2), the SEDs of the slightly asymmetric cores we examine are independent of the observer’s viewing angle, because they are optically thin at long wavelengths.

### 4.4 Comparison with observations

We use PHAETHON to model L1544 with a disk-like density profile (Eq. 4.5), and L1517B, L63 and B133 with south-pole asymmetric density profiles (Eq. 4.7). The parameters of our models are listed in Table 4.3. We fit the SED and the SCUBA 850 μm images, and we calculate the temperature profile of each core. To fit the observational data we first assume the kind of core asymmetry (disk-like or south-pole) and the asymmetry parameter ε, based on the 850 μm image of the core. Then we vary the mass of the core (by adjusting the central core density and the core flattening radius), so as to fit the submm and mm SED data. Finally, we vary the extinction through the ambient cloud in order to fit the FIR SED data.

The results are presented in Figs. 4.23-4.30. We plot the temperature profile of each core and the immediate ambient cloud in different directions (Figs. 4.23a, 4.25a, 4.27a, 4.29a), the fitted SED and the observed SED data for each core (Figs. 4.23b, 4.25b, 4.27b, 4.29b), the 850 μm isophotal map of our models (Figs. 4.24a, 4.26a, 4.28a, 4.30a), and the SCUBA 850 μm images (Figs. 4.24b, 4.26b, 4.28b, 4.30b). Our models reproduce reasonably well the inner regions of the cores. However, they do not reproduce the asymmetries in the outer regions of the cores. These asymmetries may be due to anisotropic illumination of the core and/or due to anisotropies in the surrounding ambient cloud. For example, if the core is near the edge of the ambient molecular cloud, the radiation incident on the part of the core that is closer to the edge of the cloud will be larger.
4.4. COMPARISON WITH OBSERVATIONS

The dust temperatures in the cores we model are from $\sim 7$ to $\sim 11$ K. The temperature gradients are relatively small and they depend on how deep each core is embedded in the ambient cloud; more embedded cores are almost isothermal (e.g. L1517B, Fig. 4.25a). The dust temperatures we calculate with our models are lower than the temperatures estimated by Kirk (2002) (see Table 4.3). Kirk (2002) calculated the dust temperature of each core using FIR (90, 170 and 200 $\mu$m) ISO/ISOPHOT observations. However, ISO observations have difficulty distinguishing the core from the ambient cloud, and thus the larger temperature may be due to the presence of the hotter ambient cloud in the observing beam.

As a result of overestimating the dust temperature, the core masses calculated by Kirk (2002) are underestimated. This is because the estimated mass of each core is approximately inversely proportional to the assumed dust temperature (see Section 3.3.2). More accurately, using Eq. (3.21), we have

$$M_\lambda(T) \propto F_\lambda \frac{e^{\alpha_\lambda/T} - 1}{\kappa_\lambda},$$

(4.8)

where

$$\alpha_\lambda = \frac{hc}{k\lambda},$$

(4.9)

and $F_\lambda$ the flux emitted by the core, and $\kappa_\lambda$ is the assumed dust opacity per unit mass. Substituting for $h,c$ and $k$, we find that $\alpha_{850\mu m} = 16.9$ K and $\alpha_{1.3mm} = 11.05$ K. Now suppose that the correct temperature at the centre of a core is $T = 7$ K. If an isothermal core having $T = 9$ K is assumed, then using the 850 $\mu$m flux the mass is underestimated by a factor of $f = (e^{\alpha_{850\mu m}/(7K)} - 1)/(e^{\alpha_{850\mu m}/(9K)} - 1) = 1.9$ ($f = 1.6$ using the 1.3 mm flux). If the temperature assumed is even larger than the correct temperature, the mass is further underestimated, e.g. for $T = 12$ K the mass is underestimated by a factor of 3.3 using the 850 $\mu$m flux ($f = 2.5$ using the 1.3 mm flux). Thus, even small overestimates in core temperatures (on the order of 2 – 3 K) could lead to underestimating core masses by a factor of 2 to 3.

From Table 4.3 we see that the masses estimated by Kirk (2002) are similar to the masses we calculate. However, Kirk uses a dust opacity $\kappa_{850\mu m} = 0.01$ cm$^2$g$^{-1}$, which is smaller by a factor of 2 than the dust opacity we use ($\kappa_{850\mu m} = 0.02$ cm$^2$g$^{-1}$). Thus to compare mass estimates we need to divide the Kirk (2002) values by 2. By doing this we find that indeed core masses are underestimated by a factor of $\sim 2$. Our findings indicate that the errors in calculating core masses from submm and mm observations are on the order of 2-3 (including the error introduced by the uncertainties in the dust opacity).
Table 4.3  Asymmetric models of prestellar cores: comparison with observations

<table>
<thead>
<tr>
<th></th>
<th>L1544</th>
<th>L1517B</th>
<th>L63</th>
<th>B133</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>asymmetry</td>
<td>disk-like</td>
<td>south pole</td>
<td>south pole</td>
</tr>
<tr>
<td>$n_c$ (cm$^{-3}$)</td>
<td>2.4 $\times$ 10$^5$</td>
<td>2.7 $\times$ 10$^5$</td>
<td>2.7 $\times$ 10$^5$</td>
<td>2.7 $\times$ 10$^5$</td>
</tr>
<tr>
<td>$r_0$ (pc)</td>
<td>0.015</td>
<td>0.018</td>
<td>0.015</td>
<td>0.018</td>
</tr>
<tr>
<td>$R_{\text{core}}$ (pc)</td>
<td>0.075</td>
<td>0.075</td>
<td>0.075</td>
<td>0.1</td>
</tr>
<tr>
<td>$e$</td>
<td>2</td>
<td>1.5</td>
<td>2.2</td>
<td>1.5</td>
</tr>
<tr>
<td>$p$</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>$A_V^{\text{cloud}}$</td>
<td>23.7</td>
<td>38.8</td>
<td>18.4</td>
<td>8.6</td>
</tr>
<tr>
<td>$D$ (pc)</td>
<td>140</td>
<td>140</td>
<td>130</td>
<td>200</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>$\theta_{\text{obs}}$ ($^\circ$)</th>
<th>$T_{\text{edge}}$ (K)</th>
<th>$T_{\text{centre}}$ (K)</th>
<th>$L_{\text{core}}$ (L$_\odot$)</th>
<th>$M$ (M$_\odot$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>60</td>
<td>8.7</td>
<td>7.5</td>
<td>0.10</td>
<td>2.5</td>
</tr>
<tr>
<td>b</td>
<td>60</td>
<td>8.0</td>
<td>7.3</td>
<td>0.05</td>
<td>1.6</td>
</tr>
<tr>
<td>c</td>
<td>75</td>
<td>9.3</td>
<td>7.5</td>
<td>0.09</td>
<td>1.9</td>
</tr>
<tr>
<td></td>
<td>90</td>
<td>11</td>
<td>7.8</td>
<td>0.2</td>
<td>1.8</td>
</tr>
</tbody>
</table>

(a) Model parameters. $n_c$: central number density; $r_0$: the scale length of the core density profile; $R_{\text{core}}$: outer radius of the core; $e$: asymmetry parameter, i.e. the equatorial-to-polar optical depth ratio for disk-like asymmetry (L1544) or the south-to-north pole optical depth ratio for south-pole asymmetry (L1517B, L63, B133); $p$: sine power index of the density profile (see Eqs. 4.5 and 4.7); $A_V^{\text{cloud}}$: visual extinction of the ambient cloud; $D$: distance of the core from the Earth.

(b) Fitting results. $\theta_{\text{obs}}$: core orientation angle; $T_{\text{edge}}$: dust temperature at the edge of the core; $T_{\text{centre}}$: dust temperature at the centre of the core; $L_{\text{core}}$: total luminosity emitted by the core; $M$: estimated core mass.

(c) Previous estimates. $T_{\text{iso}}$: isothermal core temperature calculated by Kirk (2002) using FIR (90, 170 and 200 $\mu$m) ISO/ISOPHOT observations; $M_{\text{iso}}^{850\mu\text{m}}$: submillimetre mass calculated using $T_{\text{iso}}$. Note that this is based on the assumption that the dust opacity is $\kappa_{850\mu\text{m}} = 0.01$ cm$^2$g$^{-1}$, i.e. smaller than the dust opacity we assume, $\kappa_{850\mu\text{m}} = 0.02$ cm$^2$g$^{-1}$, thus to compare mass estimates we need to divide the Kirk (2002) values by 2.
4.4. COMPARISON WITH OBSERVATIONS

Figure 4.23  L1544 model (parameters listed in Table 4.3). (a) Dust temperature profile of the core and the immediate ambient cloud. Different lines correspond to different directions (from $\theta = 0^\circ$, upper line, to $\theta = 90^\circ$, bottom line). (b) SED of the core. The line corresponds to our model, and the points to the observed SED (data taken from Kirk 2002).

Figure 4.24  (a) L1544 850 $\mu$m isophotal map of our model. The core is viewed at an angle $\theta = 60^\circ$. The image has to be rotated anticlockwise by $\sim 60^\circ$ on the observer’s plane to fit the SCUBA image. (b) 850 $\mu$m SCUBA image of L1544 (from Kirk 2002).
Figure 4.25  L1517B model (parameters listed in Table 4.3).  (a) Dust temperature profile of the core and the immediate ambient cloud. Different lines correspond to different directions (from $\theta = 0^\circ$, upper line, to $\theta = 180^\circ$, bottom line).  (b) SED of the core. The line corresponds to our model, and the points to the observed SED (data taken from Kirk 2002).

Figure 4.26  (a) L1517B 850 $\mu$m isophotal map of our model. The core is viewed at an angle $\theta = 60^\circ$. The image has to be rotated anticlockwise by $\sim 30^\circ$ on the observer's plane to fit the SCUBA image. (b) 850 $\mu$m SCUBA image of L1517B (from Kirk 2002).
4.4. COMPARISON WITH OBSERVATIONS

Figure 4.27  L63 model (parameters listed in Table 4.3). (a) Dust temperature profile of the core and the immediate ambient cloud. Different lines correspond to different directions (from $\theta = 0^\circ$, upper line, to $\theta = 180^\circ$, bottom line). (b) SED of the core. The line corresponds to our model, and the points to the observed SED (data taken from Kirk 2002).

Figure 4.28  (a) L63 850 $\mu$m isophotal map of our model. The core is viewed at an angle $\theta = 75^\circ$. The image has to be rotated clockwise by $\sim 90^\circ$ on the observer's plane to fit the SCUBA image. (b) 850 $\mu$m SCUBA image of L63 (from Kirk 2002).
**Figure 4.29** B133 model (parameters listed in Table 4.3). (a) Dust temperature profile of the core and the immediate ambient cloud. Different lines correspond to different directions (from $\theta = 0^\circ$, upper line, to $\theta = 180^\circ$, bottom line). (b) SED of the core. The line corresponds to our model, and the points to the observed SED (data taken from Kirk 2002).

**Figure 4.30** (a) B133 850 $\mu$m isophotal map of our model. The core is viewed at an angle $\theta = 90^\circ$. (b) 850 $\mu$m SCUBA image of LB133 (from Kirk 2002).
4.5 Discussion

We have performed accurate two-dimensional continuum radiative transfer calculations for non-spherical prestellar cores, which are probably more realistic than the BE sphere model. Our models illustrate the importance of performing non-spherically symmetric radiative transfer calculations and observing cores around the peak of their SED, by showing the effect that even small asymmetries have on the temperature profile and isophotal maps of starless and prestellar cores. Our main results are:

- For the cores treated here, which are optically thin at the long wavelengths where most of the emission occurs, the SED is essentially the same at any viewing angle. Thus, for the case of flattened cores, observations cannot distinguish between edge-on and face-on cores using solely SEDs.

- Isophotal maps at submm wavelengths (e.g. at 850 μm) are column density tracers, whereas maps at wavelengths around the peak of the core emission (e.g. 200 μm) depend strongly both on the column density and the temperature along the line of sight. Continuum images of cores at such wavelengths should contain characteristic features indicative of the core structure and orientation. Therefore, sensitive, high-resolution observations at 170-250 μm (Herschel) combined with long-wavelength observations (e.g. 850 μm or 1.3 mm) can be used to infer information about the temperature structure and orientation of the core.

- Cores embedded in ambient molecular clouds are colder than cores directly exposed to the ISRF and have lower temperature gradients within them (provided that all cores are heated by the same ISRF). As a result, the characteristic features in the 200 μm isophotal maps are weaker (for cores embedded in ambient clouds with visual extinction less than $A_V \sim 10$), and may even disappear completely (for more deeply embedded cores, e.g. $A_V > 20$). However, our models predict that if the ISRF incident on the ambient molecular cloud is enhanced in the UV region, then the embedded cores are hotter and the temperature gradients inside them may be sufficient to produce detectable characteristic features even in very embedded cores.

- The shapes of asymmetric cores depend strongly on the observer’s viewing angle. For example, disk-like cores appear more flattened when viewed edge-on. Our models also indicate that edge-on cores should be easier to detect than pole-on cores. This may introduce
a selection effect that should be taken into account when studying the statistics of the shapes of cores, using solely optically thin continuum or optically thin molecular line observations.

- The characteristic features at 200 µm are symmetric with respect to two axes for flattened cores, and with respect to one axis for the south-pole asymmetric cores. Thus, just the degree of symmetry of these features, could be indicative of the core density structure. Triaxial cores may show no symmetry at all. However, the lack of symmetry in the features could also indicate that the radiation field incident on the core is anisotropic.
Chapter 5

Monte Carlo Radiative Transfer & SPH

Hydrodynamic simulations are in most cases the only way to study the details of star formation. For a non-magnetic system, the hydrodynamic equations are:

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho = -\rho \nabla \cdot \mathbf{v}, \quad (5.1)$$

Momentum Equation:

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{\nabla P}{\rho} - \nabla \phi + \mathbf{F}_{\text{viscous}}, \quad (5.2)$$

Energy Equation:

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = -\frac{P}{\rho} \nabla \cdot \mathbf{v} + \frac{\Gamma - \Lambda}{\rho}, \quad (5.3)$$

where $\rho$ is the density, $\mathbf{v}$ is the velocity, $P$ the pressure, $\phi$ the gravitational potential, $\mathbf{F}_{\text{viscous}}$ the viscous force per unit mass, $u$ the thermal energy per unit mass, and $\Gamma$ and $\Lambda$ the heating and cooling functions of the fluid, respectively.

Smoothed Particle Hydrodynamics (SPH) is a Lagrangian computational method that uses a large number of particles to describe a fluid, by assigning properties such as mass, position, velocity and temperature to each particle and calculating derivatives using local averages. The main advantage of this method is that there are no limitations on the geometry of the system or
how far it may evolve from the initial conditions. However, SPH cannot resolve boundaries and shocks well, although some techniques exist for minimising these difficulties. Recent developments include the use of sinks in regions of very high density (Bate, Bonnell, & Price 1995), the use of a barotropic equation of state, that changes from isothermal to adiabatic in high-density, opaque regions (Bonnell 1994), a switch to reduce viscosity (Morris & Monaghan 1997), SPH with magnetic fields, where the ions and neutrals are treated independently (Hosking & Whitworth 2003), Godunov-type SPH (Inutsuka 1994; Cha & Whitworth 2003a), where a Riemann solver is used to integrate the equations of motion, and SPH with particle splitting (Kitsionas & Whitworth 2002), where more particles are generated in regions of interest, to increase the resolution of the simulation.

Radiative transfer is generally not included in SPH, mainly due to the large computational cost incurred when radiation transfer is treated fully in three dimensions. Radiative transfer simulations alone are very computationally demanding. The Monte Carlo approach for equilibrium radiative transfer with frequency distribution adjustment, provides a way to study systems with arbitrary geometries in an efficient way.

In this chapter, we present a method to use Monte Carlo radiative transfer with frequency distribution adjustment, to calculate the temperature, SED and isophotal maps of SPH simulation results. This is useful for comparing numerical results directly with observations, and even though the radiative transfer is not treated consistently within the hydrodynamic simulation, it is formulated so that it may be extended in this direction in the future.

Initially, we describe the basics of SPH with emphasis on the building of the SPH tree, which is used to calculate efficiently the gravity forces in an SPH simulation. We then present a method to perform Monte Carlo radiative transfer calculations on a single SPH snapshot, using the SPH tree to construct the radiative transfer cells with which the photons interact. The method is similar to the tree-structured adaptive grid used by Kurosawa & Hillier (2001), but it is implemented using the SPH tree structure developed by Barnes & Hut (1986), in order to minimize the computational burden that will be added to the hydrodynamic simulations when the two methods are combined. We then describe a technique to account for the large temperature gradients that are expected very close to stars, by using an additional spherical grid around each star, in parallel to the Cartesian SPH tree grid. Finally, we discuss the potential of the method for implementation in an efficient, self-consistent SPH-RT scheme.
5.1 Smoothed Particle Hydrodynamics (SPH)

SPH was first introduced by Lucy (1977) and Gingold & Monaghan (1977) (see Benz 1990, Benz 1991, Monaghan 1992 for reviews). This method represents the fluid by a large number of particles that move under their mutual interaction (gravity, pressure forces and viscosity) and the action of any external forces. The properties of the fluid at any point are calculated by taking a weighted average of those properties over the local neighbourhood. Thus, SPH is, in effect, a sophisticated interpolation method that allows any quantity to be expressed in terms of its values at specific points, i.e. the particles that constitute the system.

For example, consider a quantity $f$. We can calculate a smoothed value of this quantity at any point $\mathbf{r}$ in the system, from the value of $f$ in the neighbourhood of $\mathbf{r}$,

$$
\langle f(\mathbf{r}) \rangle = \int W(\mathbf{r} - \mathbf{r}', h) f(\mathbf{r}') d\mathbf{r}',
$$

(5.4)

where $W$ is an interpolating function, called the smoothing kernel, and $h$ is the smoothing length, a quantity that measures the extent of the kernel. The kernel $W$ satisfies a normalisation condition,

$$
\int W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' = 1,
$$

(5.5)

and

$$
\lim_{h \to 0} W(\mathbf{r} - \mathbf{r}', h) = \delta(\mathbf{r} - \mathbf{r}').
$$

(5.6)

From the above it follows that $\langle f(\mathbf{r}) \rangle \to f(\mathbf{r})$, when $h \to 0$, as expected.

Suppose that the fluid is represented by $N$ particles that are distributed in space according to a number density distribution

$$
n(\mathbf{r}) = \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j).
$$

(5.7)

Given that

$$
n(\mathbf{r}_j) = \frac{\rho(\mathbf{r}_j)}{m_j},
$$

(5.8)

where $m_j$ is the mass of each particle, then from Eq. (5.4), for $f(\mathbf{r}) = \rho(\mathbf{r})$, we obtain

$$
\langle \rho(\mathbf{r}) \rangle = \sum_{j} m_j W(|\mathbf{r} - \mathbf{r}_j|, h).
$$

(5.9)
This equation can be interpreted as if every particle were smoothed over space according to the kernel $W$ (the name of the method comes from this interpretation). Another way to look at the above equation is just as an interpolation scheme (Benz 1991), where the particles have no physical meaning but are only interpolation points that are co-moving with the fluid.

### 5.1.1 SPH smoothing kernel

The smoothing kernel that is widely used (Monaghan & Lattanzio 1985) is a polynomial of 3rd order,

$$W(r, h) = \frac{\sigma}{f(r/h)} \begin{cases} 1 - \frac{3}{2}s^2 + \frac{3}{4}s^3, & \text{if } 0 \leq s < 1 \\ \frac{1}{4}(2 - s)^3, & \text{if } 1 \leq s < 2 \\ 0, & \text{otherwise} \end{cases}$$

(5.10)

where $s = r/h$, $D$ is the number of dimensions and $\sigma$ is a normalisation factor with values $2/3$, $10/7\pi$ and $1/\pi$ in one, two and three dimensions, respectively. The smoothing kernel is zero for $r > 2h$. Thus, to determine a physical quantity at the position of a given particle $i$, only the particles that are within distance $2h$ contribute to the weighted mean. To retain a specified resolution, the smoothing length $h$ is varied, so that the number of particles that contribute to the mean remains constant. Thus, each particle has its own smoothing length, which in 3-dimensional calculations is chosen so that a sphere with radius $2h$ centred at the specific particle contains $N_{\text{neigh}} = 50 \pm 5$ other particles.

### 5.1.2 SPH fluid equations

To solve the fluid equations, we have to express them in SPH terms, using an appropriate smoothing kernel and summing over all the particles. In the next sections we discuss the specifics of a basic SPH implementation.

**Continuity Equation**

The continuity equation is just Eq. (5.9),

$$\rho_i = \sum_j m_jW(|\mathbf{r}_i - \mathbf{r}_j|, h_i).$$

(5.11)

This gives the density $\rho_i$ at the position $\mathbf{r}_i$ of particle $i$. 
5.1. SMOOTHED PARTICLE HYDRODYNAMICS (SPH)

Momentum equation

The momentum equation should be symmetric in \( i \) and \( j \), so that it conserves linear and angular momentum. This is satisfied by setting

\[
\frac{d\mathbf{v}_i}{dt} = \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i W(r_{ij}, h_{ij}) - \nabla \phi_i
\]  

(5.12)

where \( P_i, P_j \) are the pressures and \( \rho_i, \rho_j \) the densities at the particles \( i \) and \( j \), respectively. The term, \( \sum_j m_j (P_i/\rho_i^2 + P_j/\rho_j^2) \nabla_i W(r_{ij}, h_{ij}) \), is the pressure acceleration acting on particle \( i \), the term \( \sum_j m_j \Pi_{ij} \nabla_i W(r_{ij}, h_{ij}) \) the viscous acceleration, and the term \( -\nabla \phi_i \) the gravitational acceleration. The viscosity parameter \( \Pi_{ij} \) is

\[
\Pi_{ij} = \frac{(-\alpha c_{ij} \mu_{ij} + \beta \mu_{ij}^2)}{\rho_{ij}},
\]

(5.13)

where

\[
\mu_{ij} = \begin{cases} 
\frac{h_{ij} v_{ij} \cdot r_{ij}}{(r_{ij}^2 + 0.1 h_{ij}^2)} & \text{if } \mathbf{v}_{ij} \cdot \mathbf{r}_{ij} < 0 \\
0 & \text{if } \mathbf{v}_{ij} \cdot \mathbf{r}_{ij} \geq 0 
\end{cases}
\]

(5.14)

and \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j, r_{ij} = |\mathbf{r}_{ij}|, \rho_{ij} = (\rho_i + \rho_j)/2, h_{ij} = (h_i + h_j)/2, c_{ij} = (c_i + c_j)/2 \), and \( \alpha, \beta \) are the viscosity parameters. The linear term \( (-\alpha c_{ij} \mu_{ij}) \) introduces a bulk viscosity and the quadratic term \( (\beta \mu_{ij}^2) \) is to prevent colliding particle streams from inter-penetrating; it is similar to the Von Neumann-Richtmyer viscosity used in finite difference methods. A shortcoming of this term is that it introduces a considerable amount of shear viscosity.

Thermal energy equation

If the fluid does not remain isothermal, we have to use the thermal energy equation, which can be written as

\[
\frac{du_i}{dt} = \frac{1}{2} \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \mathbf{v}_{ij} \cdot \nabla_i W(r_{ij}, h) + \frac{\Gamma_i - \Lambda_i}{\rho_i},
\]

(5.15)

where \( \Gamma_i \) and \( \Lambda_i \) are the heating and cooling functions, respectively.
5.1.3 Integration scheme & time step setting

Numerical integration in SPH can be performed using the a standard integration scheme such as the leapfrog, the predictor-corrector or the Runge-Kutta method. The time step of the integration is determined taking into account the velocity of the given particle, the velocity gradient, the forces acting on the particle, the viscous diffusion term and the Courant condition, according to which the time step should be larger than the physical interaction time between particles. The maximum possible time step is chosen for each particle using the following condition:

\[ \Delta t_{\text{max}}^i = \gamma \min (\Delta t_v^i, \Delta t_{v_v}^i, \Delta t_a^i, \Delta t_{cv}^i), \]  

(5.16)

where \( \gamma \) is a proportionality constant (\( \gamma \sim 0.3 \)). The first term,

\[ \Delta t_v^i = \frac{h_i}{|v_i|}, \]  

(5.17)

ensures that during a single timestep changes in the particle positions are smaller than \( h \) (which is on the order of the separation between nearest neighbour particles). The second term,

\[ \Delta t_{v_v}^i = \frac{1}{|\nabla \cdot v_i|}, \]  

(5.18)

ensures that during a single timestep the fractional change in the local density is small. The third term,

\[ \Delta t_a^i = \left( \frac{h_i}{R_i} \right)^{1/2}, \]  

(5.19)

ensures that during a single timestep changes in the relative velocities of the particles are small. The last term is

\[ \Delta t_{cv}^i = \frac{h_i}{c_i + \zeta (\alpha c_i + \beta \max_j \{\mu_{ij}\})}, \]  

(5.20)

where \( \zeta \) is a parameter usually taken to be \( \sim 1.2 \) and \( \alpha, \beta \) are the viscosity parameters. This term combines the Courant and the viscous time step controls (Monaghan 1992).

The timestep could be chosen to be the same for all particles of the system and set to the minimum timestep calculated by Eq. (5.16). However, in order to speed up the simulation a minimum timestep \( \Delta t_0 \) is defined, plus a set of larger timesteps \( \Delta t_n = 2^n \Delta t_0 \) \( (n = 0, 1, 2, 3, \ldots) \). Then each particle is assigned the largest timestep \( \Delta t_n \) consistent with the condition \( \Delta t_n < \Delta t_{\text{max}}^i \).
5.1. SMOOTHED PARTICLE HYDRODYNAMICS (SPH)

5.1.4 The SPH tree

The calculation of the gravitational forces acting on the particles is generally the most computationally expensive part of an SPH simulation. Consider a system represented by \( N \) particles. To determine the gravitational force \( a_i^{\text{grav}} \) on particle \( i \), the contributions of all the other \( N - 1 \) particles should be summed,

\[
a_i^{\text{grav}} = - \sum_{j \neq i} \frac{m_j}{r_{ij}^2} \mathbf{r}_{ij}.
\] (5.21)

Thus, \( N(N - 1) \) calculations must be performed and the time needed will be proportional to \( \sim N^2 \).

A more efficient way, is to use a recursive spatial tessellation octal tree, as developed by Barnes and Hut (1986) and implemented within the SPH context by Hernquist & Katz (1989). The whole distribution of particles is contained within a virtual cubic cell, the root cell, which is divided into eight virtual cubic subcells of equal size. If one of these subcells contains more than one particle, it is also subdivided into eight subcells. The same procedure continues until every cell contains just one particle or no particles at all. This ensemble of virtual cells and subcells constitutes the SPH tree.

After the tree is constructed the code walks the tree to calculate the gravity forces. To find the gravitational force acting on a given particle, we start by calculating the distance between the particle and the centre of the eight subcells of the root cell. If a cell’s centre of mass is close to the particle then this cell is opened to its subcells. If a cell’s centre of mass is far from the particle then it is not opened and the gravitational force on the particle is computed as if all the mass of the cell was concentrated at its centre of mass. In practice, this means that particles, which are very far away from the particle being considered, do not contribute individually to the sum of Eq. (5.21), but collectively through the cell in which they are contained. The condition for opening a cell is \( l/D < \theta \), where \( l \) is the edge length of the cell under consideration, \( D \) the distance between the particle and the cell’s centre of mass, and \( \theta \) the tolerance angle (\( \theta < 0.577 \); Salmon & Warren 1994). The advantage of this method is that the amount of calculations, and thus the time needed, scales as \( N \log N \). Therefore, this method is much more efficient than calculating the gravity forces by summing the contributions from all particles individually, at least for \( N \gtrsim 4000 \).

There are other ways to construct an SPH tree, such as the isomass binary tessellation tree (e.g. Cha 2002), in which parent cells are split so that the two resulting child cells contain the same number of particles (plus or minus one) and the split is made normal to the axis along which
the particles in the parent cell have the largest second moment. This tree is more expensive to build but less expensive to walk, and handles filamentary structures better than the Barnes & Hut (1986) tree. Another option is the nearest neighbour tree (Press 1986; Benz et al. 1990) which is a binary tree that is built from the bottom to the top: starting from the actual SPH particles, mutual neighbours are replaced with one particle, then, on the next level, mutual neighbours are replaced with one particle, and so on. This procedure stops when there is only one particle left. Thus, closest neighbours are contained in the same cell within the binary tree.

Once the tree is constructed, it is also used to calculate the hydrodynamic forces acting on the particles. For a given particle $i$ with smoothing length $h_i$, only its neighbours, i.e. particles within distance $2h_i$, contribute to the pressure and viscous forces. The initial smoothing length of each particle is calculated from the number of neighbours, $N_{\text{neigh}}$, that each particle should have ($N_{\text{neigh}} = 50 \pm 5$). If $\rho_i$ is the density at the particle, then on average

$$\rho_i = \frac{N_{\text{neigh}} m_i}{3 \pi (2h_i)^3}.$$  \hspace{1cm} (5.22)

Solving the above for $h_i$, we obtain

$$h_i = \left[ \frac{3N_{\text{neigh}} m_i}{32 \pi \rho_i} \right]^{1/3}. \hspace{1cm} (5.23)$$

After the smoothing length $h_i$ of a particle is computed, the tree is used to find its neighbours. Initially, a cube with edge $4h_i$ is constructed, centred on this particle, and then the cells which this cube overlaps are found, starting from the root cell (Hernquist & Katz 1989). Each overlapped cell is opened and then it is examined to determine whether its subcells overlap the cube centred on the particle. This procedure of opening cells continues until we reach an actual particle, that is then a neighbour of the particle examined. This method considerably reduces the time needed to find neighbours, as compared with examining all the particles one by one.

In summary, the construction of an hierarchical tree structure is an integral part of any SPH code, and is used to increase the efficiency of force calculation and neighbour identification.

### 5.1.5 SPH: The algorithm

An SPH simulation starts by setting up the initial conditions for the system under study, i.e. the particle positions to reflect the system’s density profile, the particle velocities and the boundary conditions. Then the tree is built and walked to calculate the gravitational forces. The
tree is walked one more time to find neighbours and calculate the hydrodynamic forces. Then the
system is advanced for a half time-step (needed from the integration method), the tree is built
and walked again, and the system is advanced for a full time-step. This procedure continues until
the system has been evolved for a specified time.

5.2 Radiative transfer in hydrodynamic simulations

The Monte Carlo radiative transfer method with frequency distribution adjustment is fast
compared to the traditional iterative Monte Carlo methods. However, even without iteration, it
is computationally expensive, because it requires a large number of $L$-packets to be simulated to
reduce the inherent statistical noise of the method. Hydrodynamic simulations are also com-
putationally expensive, and thus the inclusion of radiative transfer in hydrodynamic simulations, in
an efficient way, is computationally very challenging. In this first approach to this problem, we
concentrate on doing radiative transfer (RT) on single snapshots of SPH simulations.

5.2.1 Construction of radiative transfer cells

The radiative transfer cells (hereafter RT cells) absorb, scatter and reemit $L$-packets. These
cells are constructed so that their linear size is less than, or on the order of, the local directional
temperature and the density scale-heights (see Section 2.6). This ensures that the temperature
and density do not vary significantly between two adjacent cells. The construction of the cells
depends on the specific system under study, and, thus, in a hydrodynamic simulation, where
the system changes from step to step, the RT cells would need to be constructed at every step.
Therefore, a robust algorithm for the construction of RT cells is needed.

To construct RT cells in an SPH simulation it not straightforward because the density dis-
tribution is not known a priori but should be derived from the SPH particles that represent the
system under study. We take advantage of the fact that SPH uses an octal tree structure (Barnes
& Hut 1986) to group particles together when calculating gravity forces. When the SPH tree is
being built, we give identity numbers to each of the cells created at every level of the tree. We
also record information about the size of each cell and the number of SPH particles it contains.
These cells serve as potential RT cells. The mass and the density of each potential RT cell, to be
used in the radiative transfer calculation, are determined from the mass of the SPH particles in
the cell and the size of the cell,
\[ M_{\text{cell}} = N_{\text{cell}}^{\text{sph}} m_{\text{sph}} \]  
(5.24)
and
\[ \rho_{\text{cell}} = \frac{N_{\text{cell}}^{\text{sph}} m_{\text{sph}}}{S_{\text{cell}}^3} \]  
(5.25)
where \( N_{\text{cell}}^{\text{sph}} \) is the number of SPH particles within the given cell, \( m_{\text{sph}} \) the mass of each particle and \( S_{\text{cell}} \) the linear size of the cell.

We must then choose which of these cells will be the actual active RT cells. We can do that either by choosing a maximum allowable RT cell size, \( S_{\text{max}} \),
\[ S_{\text{cell}} \lesssim S_{\text{max}}, \]  
(5.26)
or a maximum number, \( N_{\text{max}} \), of SPH particles that should be contained in each RT cell.
\[ N_{\text{cell}}^{\text{sph}} \lesssim N_{\text{max}}. \]  
(5.27)
Each one of the above conditions leads to a unique subgroup of SPH cells that constitute the active RT cells. The first way has the disadvantage that \( S_{\text{max}} \) must be set at the beginning of the simulation. We may then have big cells in high-density regions, that would not be resolved adequately, or small cells in very low-density regions that would be below the SPH resolution limit and, therefore, not suitable for RT cells. The second way is adaptive, since if \( N_{\text{max}} \) is chosen to be close to \( N_{\text{neigh}} \) (the mean number of SPH neighbours), then the size of the cell will be adjusted automatically to be on the order of the smoothing length \( h \), i.e. the resolution of the SPH simulation. In order to avoid RT cells that contain only a few SPH particles, we choose \( N_{\text{max}} \sim 70 - 100 \), i.e. somewhat larger than \( N_{\text{neigh}} \).

5.2.2 L-packet propagation and interaction

The propagation of \( L \)-packets in the computational domain is performed in small steps, \( \delta S \), that gradually decrease the optical depth \( \tau \) of the \( L \)-packet until \( \tau = 0 \), whereupon the \( L \)-packet reaches an interaction point. This is generally the most computationally expensive aspect of a Monte Carlo radiative transfer code (see Section 2.12). The computational time for propagating \( L \)-packets is even larger for radiative transfer calculations within SPH, because, in this case, there is no analytical expression for the density along the path of the \( L \)-packet (needed for calculating
the optical depth decrements until the \( L \)-packet interacts with the medium. The density must instead be calculated through the cell where the \( L \)-packet resides at each step of the calculation. This means that we need to find the RT cell of the \( L \)-packet after each step \( \delta S_i \). This adds a considerable amount to the code running time. Therefore, it is even more critical in this case to choose an appropriate step \( \delta S_i \).

Similarly to our previous calculations (see Section 2.7), we choose the propagation step \( \delta S_i \) using the following condition:

\[
\delta S_i = \text{MIN} \{ \eta_k S_c, \eta_l (\tau_l + \epsilon) l, \eta_r |r| \},
\]

(5.28)

where \( S_c \) is the size of the cell where the \( L \)-packet is, \( l = (\kappa \lambda \rho_l)^{-1} \), and \( \eta_k, \eta_l, \eta_r \) are constants that determine the accuracy we demand (typical values 0.1 to 1). The physical meaning of each of the terms in the above equation is described in Section 2.7. The only difference is the addition of the term \( \eta_k S_c \) in place of the directional density scale-height term \( \eta_r h_{\rho} \). This term ensures that the \( L \)-packet does not travel a distance that it is too large in comparison to the size of the local cell. The method by which the RT cells are constructed, with the condition that each cell should contain \( \sim 50 \) SPH particles, means that the size of each cell is on the order of \( 4h \).

As an \( L \)-packet propagates through the computational domain, we use the SPH tree to find which cell the \( L \)-packet is in. The search starts from the root cell and continues to the lower level cells, until an active RT cell is reached. A more efficient way would be to perform the search upwards, starting from the cell where the \( L \)-packet was before the last step.

5.2.3 Remark

The method we use to construct RT cells, is implemented relatively easily within SPH and exploits information about the tree already calculated and needed for SPH. Thus, it does not add much to the code running time. This algorithm is also an efficient method to find which RT cell the \( L \)-packet is in, that is critical for the efficiency of the code, because as the \( L \)-packet propagates through the computational domain, this procedure is done many times for each packet.

5.3 Tests

We consider a uniform sphere with density \( n = 8.6 \times 10^4 \text{cm}^{-3} \), mass \( M = 100 M_\odot \) and radius \( R = 3.5 \times 10^4 \text{AU} \). We represent this sphere within the SPH context, using \( N = 20,000 \) particles,
each one with mass $m = M/N = 5 \times 10^{-3} \, M_\odot$. These particles are distributed in space in a pseudo-random way so as to reproduce an approximately uniform density sphere. To do this we use spherical polar coordinates $(r, \theta, \phi)$ and put

$$M(r)/M(R) = \mathcal{R}_r,$$  \hfill (5.29)

where $M(r)$ is the mass interior to $r$, and $\mathcal{R}_r$ a random number $\in [0, 1]$. From the above we obtain, using $M(r) = 4/3\pi r^3 \rho$,

$$r = \mathcal{R}_r^{1/3} R.$$  \hfill (5.30)

We also choose random azimuthal and polar angles using two random numbers $\mathcal{R}_\phi, \mathcal{R}_\theta \in [0, 1]$,

$$\phi = 2\pi \mathcal{R}_\phi,$$  \hfill (5.31)

$$\theta = \cos^{-1}(1 - 2\mathcal{R}_\theta).$$ \hfill (5.32)

Then the cartesian coordinates $(x, y, z)$ for each particle are calculated using

$$x = r \sin(\theta) \cos(\phi),$$
$$y = r \sin(\theta) \sin(\phi),$$
$$z = r \cos(\theta).$$ \hfill (5.33)

We test the method of constructing RT cells within SPH, and propagating $L$-packets through these cells, (i) using the thermodynamic equilibrium test, where the sphere is embedded in an isotropic blackbody radiation field with a given temperature, (ii) illuminating the sphere by the Black (1994) interstellar radiation field (BISRF) and comparing our results with the results obtained using a previously tested grid of concentric radial cells (see Chapter 3), and (iii) embedding a small luminosity source in the centre of the sphere and comparing the results with those obtained using concentric radial cells. We present the results in the following subsections.

### 5.3.1 Sphere embedded in an isotropic blackbody radiation field

We illuminate the sphere with an isotropic blackbody radiation field having $T = 15$ K. We inject $L$-packets at random positions $(R, \theta, \phi)$ on the surface of the sphere and with random injection angles $\theta_{in}$ and $\phi_{in}$ so as to imitate an isotropic radiation field. The sphere should then adopt the temperature of the illuminating radiation field, i.e. 15 K.
5.3. TESTS

We present the results of a simulation using $10^8$ $L$-packets, constructing RT cells containing a maximum of 60 SPH particles. This leads to cells containing typically 15-35 particles (Fig. 5.2). This number is smaller than we want (we want around 55 particles per cell), but it does not affect this test.

We plot the density of the active RT cells (i.e. cells where $L$-packets have been absorbed or scattered) as a function of radius (Fig. 5.2a). We see that the density of the RT cells is close to the expected density of the uniform sphere, with some statistical variations, as expected for randomly distributed particles. Each cell contains around $N = 20$ particles, so the statistical variance in the number of SPH particles contained in each cell is $\Delta N = \sqrt{20} = 4.5$, i.e. a fractional variation of $\sim 22\%$.

There is also a number of cells that appear to be outside the radius of the sphere. In fact, these are cells that have a small part inside the sphere, but their centre is outside the sphere, and, therefore they contain a very small number of particles (see Fig. 5.1). The density in these irregular cells is much less than the actual density. These cells are a side effect of representing a sphere with an ensemble of cubic cells.

![Diagram showing irregular RT cells](image)

**Figure 5.1** Irregular RT cells. We present the region near the edge of the sphere. The particles (black dots) represent the spherical density distribution and the squares the constructed RT cells. Some cells (shaded regions) have only a small part within the sphere and contain only a small number of particles. The density in these cells is not calculated correctly.
**Figure 5.2** Thermodynamic equilibrium test: a uniform density sphere, represented by 20,000 particles within the SPH context, illuminated by an isotropic blackbody radiation field with $T = 15$ K, using $10^6$ L-packets. We construct RT cells using the SPH tree, with the condition that each cell contain less than $N_{\text{max}} = 60$ particles. This procedure creates $N_{\text{cells}} = 1,484$ cells. We plot: (a) the density of the RT cells (triangles), the real value of density (middle dotted horizontal line), and the boundary of the sphere (solid perpendicular line). Note the existence of irregular cells, whose centre is outside the sphere. (b) the temperature of the RT cells, and (c) the relative error (%) in temperature. The temperature is calculated with good accuracy within the sphere radius.

**Figure 5.3** Same as in Fig. 5.2, but using $10^7$ L-packets, and RT cells that contain less than $N_{\text{max}} = 200$ particles. The automated procedure that uses the SPH tree, creates $N_{\text{cells}} = 282$ cells. Thus, the statistical errors in density (a), and temperature (b), are very small. However, the resolution of the RT cells is not very good (i.e. the linear size of the cells is larger).
5.3. TESTS

The temperature that we calculate is very close to the expected temperature (15 K), with the error being less than 3% (Fig. 5.2b). The error is higher near and outside the edge of the sphere, because of the presence of the irregular cells.

We also present a simulation using $10^7 L$-packets, constructing RT cells containing a maximum of 200 SPH particles, that leads to cells with a typical number of 80-120 particles (Fig. 5.3). In this case the density is calculated much more accurately (Fig. 5.3a), apart from the region near the edge of the sphere. The same is true for the temperature calculation (Fig. 5.3b), where the error is now $\sim 1\%$, because even though we use a smaller number of packets, they are distributed among a smaller number of cells.

To minimise the errors in calculating the density (and therefore the temperature) when constructing RT cells from SPH virtual cells, we should choose $N_{\text{max}} \sim 100$, in order to have cells with an adequate number of SPH particles. If we want better resolution in the RT simulation, then a larger number of SPH particles should be used in the hydrodynamics simulation.

5.3.2 Sphere embedded in the ISRF

In this test, the sphere is illuminated by the Black (1994) interstellar radiation field (BISRF). The advantage of this test is that the BISRF includes $L$-packets in a wide wavelength range (UV to mm wavelengths), including regions where scattering dominates (UV and optical) and regions where absorption/emission dominates (IR and submm). Therefore, we can test the validity of the method for a wide range of wavelengths. As previously, we use 20,000 SPH particles to represent the sphere. We build the SPH tree in the usual manner. Then we descend the tree until we reach the highest cells containing less than $N_{\text{max}} = 100$ SPH particles, and these are identified as RT cells.

We present the results in Fig. 5.4, and compare them with calculations performed for the same sphere outside the SPH context, i.e. using a continuous density distribution and concentric radial cells (see Chapter 3). The temperature we calculate using the RT-SPH scheme is in good agreement with the expected temperature (Fig. 5.4a), apart from the region near the edge of the sphere, where the temperature gradient is large and the RT cells are not small enough to capture this steep profile.

The presence of irregular cells near the edge of the sphere affects the SED of the system. The $L$-packets that would otherwise leave the system after scattering, are stopped by the irregular cells and then may get scattered back into the sphere. This is evident in the SED of the system.
Figure 5.4 A uniform density sphere, represented by 20,000 particles, illuminated by the BISRF radiation field, using $10^7$ $L$-packets. We construct RT cells using the SPH tree, with the condition that each cell contain less than $N_{\text{max}} = 100$ particles. This procedure creates $N_{\text{cells}} = 723$ cells. We plot (a) the temperature of the RT cells (triangles) and the expected temperature (solid line), and (b) the SED of the system (solid line), the expected value (dashed line) and the illuminating field (dotted line). The temperature is calculated relatively well. It is slightly overestimated near the edge of the core, because its gradient is too large to be captured by the RT cells. The SED is considerably underestimated at UV and optical wavelengths due to the presence of the irregular cells (see text).

Figure 5.5 Uniform density sphere illuminated by the BISRF. Same as in Fig. 5.4, but with a special routine that discards outgoing $L$-packets when $r > R_{\text{sphere}}$ to avoid back-scattering by the irregular cells. The SED at UV and optical wavelengths is calculated with better accuracy than in Fig. 5.4.
Figure 5.6 Uniform density sphere illuminated by the BISRF. Same as in Fig. 5.5, but for a sphere represented by 200,000 particles using $10^8$ $L$-packets (better resolution run). We construct RT cells using the SPH tree, with the condition that each cell contain less than $N_{\text{max}} = 100$ particles. This procedure creates $N_{\text{cells}} = 11,862$ cells. The temperature and SED are calculated with better accuracy than before.

(Fig. 5.4b), where the scattered radiation escaping from the system (UV and optical) is $\sim 10$ times lower than expected. A quick way to solve this problem is to disregard $L$-packets that are outside the radius of the sphere (previously these packets were followed until they were outside the root SPH cell). We see (Fig. 5.5), that the optical and UV parts of the SED are calculated more accurately with this method.

To have better resolution in regions where the temperature gradient is high, we must increase the number of SPH particles used in the hydrodynamics simulation. This increases the resolution of SPH and in turn the resolution provided by the RT cells. We performed an RT simulation for a sphere with the same characteristics, but represented by 200,000 particles. The resolution obtained by the RT cells is now better and the temperature profile, and SED, of the system are closer to the expected values (Fig. 5.6).

Another way to improve the resolution in regions where the temperature gradient is large, is to continue subdividing each RT cell into smaller RT cells, locally. For these small RT cells that contain a number of SPH particles much lower than the maximum one ($N \ll N_{\text{max}}$), the density should be calculated from the density of the parent cell with a number of SPH particles of order $N_{\text{max}}$. In other words, we divide an RT cell with size on the order of the SPH resolution, into a number of equal mass smaller RT cells, with the same density as the parent RT cell. This
should increase the resolution of the RT simulations, but we will need to simulate more luminosity packets in order have good statistics for these smaller RT cells.

5.3.3 Low-temperature source surrounded by a spherical envelope

We assume a uniform density sphere (with the same characteristics as in the previous sections), and a low-temperature source ($T_{BB} = 30$ K, $L = 7L_{\odot}$) at the centre of the sphere. We use 200,000 SPH particles to represent the sphere, and $10^8$ $L$-packets for the radiative transfer simulation. We build the SPH tree in the usual manner. Then we descend the tree until we reach the highest cells containing less than $N_{\text{max}} = 100$ SPH particles, and these are identified as RT cells.

![Figure 5.7](image)

Figure 5.7 Uniform density sphere illuminated by a central luminosity source. The sphere is represented by 20,000 particles, and the central source using $10^8$ $L$-packets. We construct RT cells using the SPH tree, with the condition that each cell contain less than $N_{\text{max}} = 60$ particles. This procedure creates $N_{\text{cells}} = 13,050$ cells. We plot (a) the temperature of the cells (triangles) and the expected value (solid line), (b) the SED of the reprocessed radiation (solid line) and the expected SED (dashed line), and (c) the relative error (%) in calculating the SED. The temperature is calculated with good accuracy, with some deviations very close to the centre of the sphere and near the edge of the sphere. The SED is computed well with some small deviations at short wavelengths (see text for discussion).

In Fig. 5.7, we present the results for the temperature (Fig. 5.7a) and the emitted SED (Fig. 5.7b) of the sphere, compared with the temperature and the SED calculated using the accurate method of dividing the sphere into concentric spherical cells. The temperature we calculate is very close to the expected temperature. There is a small deviation ($\lesssim 2.5$ K) near the centre of the sphere, where the size of the RT cells is not small enough to capture the
relatively steep temperature gradient. This problem is expected to be very prominent near a high-temperature luminosity source, e.g., for a star. The temperature gradient near the star is very large and very small cells are needed to capture this rapid change (we address this problem in the next section). There is an additional problem in calculating the temperature near the edge of the sphere, due to the presence of irregular RT cells.

These small temperature differences affect the SED of the system. There is a deficiency of radiation at short wavelengths ($< 130 \, \mu m$), because the temperature is underestimated very close to the central source. There are also some small differences of a statistical nature at long wavelengths ($> 2000 \, \mu m$), where fewer $L$-packets are emitted from the system.

## 5.4 Stars in SPH-RT simulations

The presence of stars in SPH-RT simulations requires special treatment. The temperature very close to the star is expected to be high and the dust close to the star will be destroyed by sublimation and chemical sputtering (e.g. Lenzuni et al. 1995). The dust destruction temperature is thought to be between $1200 \, K$ and $2100 \, K$ (Lenzuni et al. 1995; Duschl et al. 1996) and it depends on the assumed dust composition and the dust destruction processes considered. We do not examine the details of dust destruction. We just assume that dust destruction occurs at a given temperature $T_{\text{dest}}$. If $r_d$ is the radius of a dust grain then the dust heating rate, $\mathcal{G}$, is

$$
\mathcal{G} = \pi r_d^2 \int_0^{\infty} Q_\nu \left( \frac{R_*}{r} \right)^2 B_\nu(T_*) \, d\nu.
$$

(5.34)

where $Q_\nu$ is the dust absorption efficiency. On the other hand, the dust cooling is

$$
\mathcal{L} = 4\pi r_d^2 \int_0^{\infty} Q_\nu B_\nu(T_{\text{dust}}) \, d\nu
$$

(5.35)

Assuming that the dust is in thermodynamic equilibrium, the heating rate should equal the cooling rate, $\mathcal{G} = \mathcal{L}$. Combining Eqs. (5.34)-(5.35), and putting $Q_\nu \propto \nu^\beta$ ($1 \leq \beta \leq 2$), we obtain

$$
T_{\text{dust}} = \left( \frac{R_*}{2r} \right)^{2/(4+\beta)} T_*.
$$

(5.36)
At the dust destruction radius, \( r = R_{\text{dust}} \), the dust temperature is \( T_{\text{dust}} = T_{\text{dest}} \). Thus, from the previous equation, we calculate \( R_{\text{dust}} \) for a given \( T_{\text{dest}} \):

\[
R_{\text{dust}} = R_\ast \left( \frac{T_\ast}{T_{\text{dest}}} \right)^{(4+\beta)/2}.
\] (5.37)

This radius defines a spherical volume around the star devoid of dust. The region just outside this volume is characterised by large temperature gradients.

### 5.4.1 Definition of the problem

In our basic model, the RT cells, constructed from the SPH tree cells, can capture density and temperature variations down to the resolution limit of SPH (\( \sim h \)). However, the resolution of the RT cells very close to the star should be on the order of, or less than, the dust destruction radius, \( R_{\text{dust}} \), which is much smaller than \( h \), unless a large number of SPH particles are used in the simulation. The density and temperature gradients close to the star are large and smaller size cells are needed in this region.

In Fig. 5.8, we present schematically the region around a star. We plot (a) the star and the RT (SPH) cells around it, and (b) the temperature profile in this region. The solid curve on Fig. 5.8b represents the real value of the temperature, and the horizontal dashed lines, the temperature computed using the RT cells. The temperature is constant within each of the RT cells. The temperature gradient within each cell is very large and the temperature computed is an incorrect “weighted” average of the real temperature. Thus, very close to the star the temperature is underestimated and farther away from the star it is overestimated (the temperature is calculated correctly only a few RT cells away from the star, but for simplicity, in Fig. 5.8 we assume that the temperature is calculated correctly at the second RT cell). This affects the transfer of radiation in the medium, because \( L \)-packets that are absorbed very close to the star are reemitted from a wavelength distribution corresponding to a lower temperature than the true one, thus at longer wavelengths. Therefore, they are able to propagate farther away from the star or even escape from the system. Thus, smaller cells are needed very close to the star.
Figure 5.8 Stars in SPH-RT simulations. (a) The region around the star: RT cells (squares) constructed from the SPH tree, and the additional star grid proposed (shaded region). (b) The temperature profile of the region around the star. We plot the temperature calculated using the RT-SPH cells (dashed horizontal lines) and the temperature computed with the star grid (solid curves, correct value). The small spherical cells of the additional grid are able to capture the rapid change in temperature near the star ($T_{\text{sub}} \equiv T_{\text{dest}}$ is the dust destruction temperature).
5.4.2 Solution Method

To solve the problem that arises when calculating the temperature very close to a star, we propose the construction of a spherical grid around the star, hereafter referred to as the star grid (see Fig. 5.8 for a schematic representation), with the following parameters:

- The dust destruction radius, $R_{\text{dust}}$, which is determined by the temperature $T_*$ and the radius $R_*$ of the star, or equivalently, the luminosity of the star. For simplicity we will put

$$L_* = L_\odot \left( \frac{M_*}{M_\odot} \right)^3 + \frac{G M_* \dot{M}_*}{R_*} = 4\pi R_*^2 \sigma T_*^4,$$

where $M_*$ is the mass the star and $\dot{M}_*$ the accretion rate onto the star. The first term in Eq. (5.38) is the intrinsic luminosity of the star, and the second term the luminosity released due to accretion of material onto the star. For a PMS star we can assume $R_* = 3R_\odot$.

- The outer radius $R_{\text{eg}}$, of the spherical grid around the star, which should be on the order of the SPH resolution in the specified region, or, equivalently, on the order of the size of the RT cells in the neighbourhood of the star.

- The density profile close to the star ($r < R_{\text{eg}}$). The size of this region is smaller than the resolution limit of SPH, and thus the RT cells do not capture density variations on this scale. We may assume that

$$\rho = \rho_0 \left( \frac{R_{\text{dust}}}{r} \right)^p, \quad R_{\text{dust}} < r < R_{\text{eg}},$$

where the index $p = 0 - 2$. We then need to estimate $\rho_0$, i.e. the density at $r = R_{\text{dust}}$. If the density for $r < R_{\text{eg}}$ is equal to the SPH density $\rho_{\text{ph}}$ (which is constant within $R_{\text{eg}}$), then the mass contained within this radius is

$$M = \frac{4}{3} \pi R_{\text{eg}}^3 \rho_{\text{ph}}.$$

Assuming instead the density profile given by Eq. (5.39) the mass contained between $R_{\text{dust}}$ and $R_{\text{eg}}$, is

$$M = \frac{4\pi \rho_0 R_{\text{dust}}^p (R_{\text{eg}}^{3-p} - R_{\text{dust}}^{3-p})}{3 - p}.$$

The masses calculated with the different density profiles are set to be the same. Therefore, equating Eq. (5.40) and Eq. (5.41), we obtain

$$
\rho_0 = \frac{(3 - p)R_{\text{eg}}^3}{3R_{\text{dust}}^p (R_{\text{eg}}^3 - R_{\text{dust}}^3 - p)} \rho_{\text{ sph}}. \tag{5.42}
$$

Once all the above parameters are specified, the region around the star is divided into a number of concentric cells (typically \(\sim 20\) cells) from \(r = R_{\text{dust}}\) to \(r = R_{\text{eg}}\), with equal logarithmic width. This procedure must be followed for every star in an SPH simulation, and it ensures that the temperature very close to the star is computed properly. The complication that this introduces into an RT calculation is minimal; we only have to take special care when propagating \(L\)-packets for \(r < R_{\text{eg}}\).

In Fig. 5.8, we present schematically the star grid that is used in addition to the RT cells constructed via the SPH tree. The \(L\)-packets that are inside \(r < R_{\text{eg}}\) interact with cells of the star grid rather than the RT-SPH cells. There is some overlapping between the two sets of cells but this is minimal and does not create any major problems with the radiative transfer calculation, as our tests indicate (see next section). The star grid accounts for the dust destruction calculation around the star, and the radial spherical cells are small enough to capture the steep temperature gradient so that the temperature is calculated correctly close to the star.

### 5.4.3 Tests

We test the above method for including stars in radiative transfer calculations within SPH, using the Ivezić et al. (1997) test for a star \((T_\ast = 2500\ \text{K})\) surrounded by a spherical envelope with a density profile

$$
\rho = \rho_0 \left( \frac{R_{\text{dust}}}{r} \right)^2, \quad r > R_{\text{dust}}, \tag{5.43}
$$

where

$$
\rho_0 = \frac{\tau_V}{(\kappa_{1\mu m} + \alpha_{1\mu m}) [1 - (R_{\text{dust}}/R_{\text{sphere}})]} \frac{1}{R_{\text{dust}}}. \tag{5.44}
$$

\(\tau_V\) is the optical depth from the centre to the edge of the envelope at \(\lambda = 1\ \mu\text{m}\). The dust opacities are the same as in Section 2.13.1. We perform the test for envelopes with visual optical depths \(\tau_V = 1\) and \(\tau_V = 100\), and compare the results with calculations using a grid of concentric cells (see Section 2.13.1).
We represent the envelope using 20,000 SPH particles, which are distributed randomly, with azimuthal and polar angles calculated from Eqs. (5.31) and (5.32), and radii calculated from Eq. (5.29). The mass between \( R_{\text{dust}} \) and \( r \) is

\[
M(r) = \int_{R_{\text{dust}}}^{r} 4\pi r^2 \rho d r = 4\pi \rho_0 R_{\text{dust}}^2 (r - R_{\text{dust}}),
\]

(5.45)

hence, substituting in Eq. (5.29), we obtain

\[
\frac{M(r)}{M(R)} = \frac{r - R_{\text{dust}}}{R - R_{\text{dust}}} = \mathcal{R}_r.
\]

(5.46)

Thus, the radial distance \( r \) of the particle is

\[
r = R_{\text{dust}} + \mathcal{R}_r (R - R_{\text{dust}}).
\]

(5.47)

We use the SPH tree to construct radiative transfer cells that contain fewer than \( N_{\text{max}} = 55 \) particles. Near the star we construct the proposed star grid, i.e. a spherical grid with 30 concentric cells with equal logarithmic widths. In accordance with the guidelines of the previous section, we define:

- The dust destruction radius \( R_{\text{dust}} \).

We set \( R_{\text{dust}} = 9.11 R_\odot \) for \( \tau_\nu = 1 \) and \( R_{\text{dust}} = 17.67 R_\odot \) for \( \tau_\nu = 100 \), in accordance with Ivezic et al. (1997).

- The outer radius \( R_{\text{eg}} \).

This should be on the order of the cell size close to the star, which is \( \sim 1 \) AU \( \approx 200 R_\odot \). For both of our models we set \( R_{\text{eg}} = 20 R_{\text{dust}} \).

- The density profile close to the star, and the density at \( r = R_{\text{dust}} \).

We use Eq. (5.39), we assume \( p = 2 \), and use as \( \rho_0 \) the actual density at \( r = R_{\text{dust}} \) (given by Eq. (5.44)). This is not very different from what we would get from analysing the RT cells close to the star. For example, for the \( \tau_\nu = 100 \) model, the density of the cells near the star is \( \rho_{\text{sph}} \sim 6 - 9 \times 10^{-13} \text{ cm}^{-3} \), and using Eq. (5.42) we find that \( \rho_0 \sim 4 - 7 \times 10^{-11} \text{ cm}^{-3} \), which is close to the real value, \( \rho_0 \sim 8 \times 10^{-11} \text{ cm}^{-3} \), as calculated by Eq. (5.44).
5.4. STARS IN SPH-RT SIMULATIONS

Test I: $\tau_V = 1$.

We present the results of RT calculations using $5 \times 10^7$ $L$-packets, for an envelope with visual optical depth $\tau_V = 1$, without (Fig. 5.9) and with (Fig. 5.10) the star grid. It is seen (Fig. 5.9a) that, without using the additional star grid, the temperature is underestimated very close to the star ($r < 7R_{\text{dust}}$), overestimated for $7R_{\text{dust}} < r < 100R_{\text{dust}}$ and then underestimated near the edge of the envelope ($r > 600R_{\text{dust}}$). Very close to the star the size of the RT cells is $\sim 10R_{\text{dust}}$, and, therefore, any temperature variations on scales smaller than this cannot be captured. At $r < 10R_{\text{dust}}$ the temperature is the same as the temperature at $r = 10R_{\text{dust}}$ (the temperature is constant within the cell), and thus the temperature is underestimated close to the star.

This incorrect temperature affects the radiation transfer in the envelope; $L$-packets that are absorbed very close to the star, are reemitted from a spectrum with temperature lower than the correct one, and thus at longer wavelengths. They are then able to penetrate deeper into the envelope or even escape. This explains the lower than expected temperature near the edge of the envelope.

In the SED of the system (Fig. 5.9b) there is an excess of radiation at short wavelengths (0.5–2 $\mu$m), and a deficiency of radiation between 3 and 20 $\mu$m, both because of the overestimated temperature at $10R_{\text{dust}} < r < 100R_{\text{dust}}$.

In Fig. 5.10, we present the results using an additional grid around the central star. The cells close to the star have very small size ($\Delta r_{\text{cell}} \ll 10R_{\text{dust}}$) and they are able to capture the steep temperature decrease near the star (Fig. 5.10a). The temperature is calculated accurately and small variations relative to the benchmark calculation (solid line) are due to statistical noise. The SED is also calculated accurately (Fig. 5.10b), with only small statistical noise at short ($< 0.3$ $\mu$m) and long ($> 100$ $\mu$m) wavelengths.

Test II: $\tau_V = 100$.

We also perform the same test for for an envelope with visual optical depth $\tau_V = 100$, using $10^7$ $L$-packets. In Fig. 5.11, we present the results obtained without using a special grid around the star. The temperature is calculated relatively well, apart from the region close to star (Fig. 5.11a); this leads to an excess of radiation at short wavelengths ($< 5$ $\mu$m) as seen on the SED of the system (Fig. 5.11b). However, when we use the special grid around the star, both the temperature and the SED are estimated accurately (Fig. 5.12).
Figure 5.9 Radiative transfer calculation, using $5 \times 10^7$ $L$-packets, in a spherically symmetric envelope ($\tau_V = 1$) surrounding a star. The envelope is represented by 20,000 particles within the SPH context. We use RT cells constructed from the SPH tree (1,276 RT cells) but we do not use an additional grid around the star. (a) Temperature profile: the solid line corresponds to the benchmark calculation and the triangles to the calculation with RT cells constructed using the SPH tree. The temperature is not calculated correctly because the temperature gradient near the star is very large and smaller cells are needed to capture it. (b) System SED: the dotted line corresponds to the benchmark calculation and the solid line to the calculation with RT cells constructed using the SPH tree. (c) Relative difference between the calculated ($F_\lambda$) and the benchmark ($F_\lambda^0$) flux.

Figure 5.10 Same as in Fig. 5.9 but using an additional grid around the star, that includes a volume devoid of matter ($r < R_{\text{dust}}$), and concentric spherical cells (30 additional cells) of equal logarithmic width, up to $r = 20R_{\text{dust}}$. The temperature is calculated with good accuracy, even very close to the dust destruction radius. Small differences relative to temperature and SED of the benchmark calculation, are due to statistical noise.
Figure 5.11  Radiative transfer calculation, using $10^7$ $L$-packets, in a spherically symmetric envelope ($\tau_V = 100$) surrounding a star (same as in Fig. 5.9 but for a more massive envelope). This calculation is performed without using a special grid around the star. RT cells were constructed using the SPH tree (1,310 cells). (a) Temperature profile: the solid line corresponds to the benchmark calculation and the triangles to the calculation with RT cells constructed using the SPH tree. (b) System SED: the dotted line corresponds to the benchmark calculation and the solid line to the calculation with RT cells constructed using the SPH tree. (c) Relative difference between the calculated ($F_\lambda$) and the benchmark ($F_\lambda^0$) flux.

Figure 5.12  Same as in Fig. 5.11 but using an additional grid around the star (30 additional cells), that includes a volume devoid of matter ($r < R_{\text{dust}}$), and concentric spherical cells of equal logarithmic width, up to $r = 20R_{\text{dust}}$. Both the temperature and the SED are calculated with good accuracy.
5.5 Summary

In this chapter, we implement a method for performing radiative transfer simulations in arbitrary structures resulting from SPH simulations.

SPH is a Lagrangian method that uses a large number of particles to represent the fluid. The particles interact with each other through gravity and hydrodynamic forces (pressure and viscosity forces). Properties of the fluid at a given point are calculated as weighted averages over the local neighbourhood. SPH also uses a hierarchical tree structure to calculate the gravity forces acting on each particle, so that distant particles contribute collectively rather than individually in calculating these forces. This procedure is much more efficient than calculating the individual contributions from all the particles that represent the system.

We use the SPH tree to construct radiative transfer (RT) cells. RT cells are constructed so that each cell contains a number of SPH particles close to the number of neighbours that each particle must have in SPH. This method naturally creates radiative transfer cells with size on the order of the local SPH smoothing length. In addition, it uses the SPH tree structure already built within SPH, hence it can be implemented within an SPH simulation without greatly increasing the computational time.

We test the method using the thermodynamic equilibrium test for a uniform density sphere, in which the sphere is embedded in a blackbody radiation field. The method performs well with this test; the RT cells that represent the sphere acquire the same temperature as the illuminating field. The temperature is slightly underestimated near the edge of the sphere due to the presence of cells that contain only a few SPH particles (irregular cells).

We also illuminate the sphere with the BISRF, and show that the irregular cells back-scatter radiation that would otherwise escape from the system. This problem is eliminated with an adjusted propagation routine for the $L$-packets.

We then examine a system comprising a low-temperature luminosity source embedded at the centre of a uniform density sphere. The temperature and the SED are calculated with good accuracy. Very close to the luminosity source the temperature is slightly underestimated due to the fact that the temperature gradient near the source is relatively large. This also slightly affects the SED of the system at short wavelengths. The problem is more pronounced when a star is included in the RT simulation. The region very close to the star is characterised by a large temperature gradient which cannot be captured by the normal RT cells, because these cells are on the order of the smoothing length near the star, i.e. too large. To solve this problem we
propose the use of an additional grid of concentric spherical cells around the star (star grid). We test this new method using the benchmark calculations of Ivezic et al. (1997), and show that it performs very well.

The radiative transfer simulations applied to SPH density fields produce dust temperature distributions, SEDs and intensity maps at different wavelengths. Hence, they can be used for comparing the results of hydrodynamic simulations directly with observations. However, we do not treat the radiative transfer consistently within SPH simulations, in the sense that we do not combine it with an energy equation. Hence, we do not capture the full effect of radiation transfer on the evolution of the system. This may be important in some systems (e.g. a fragmenting protostellar disk).
Chapter 6

Radiative Transfer in Disks

Disks are very common around young stars. Dust continuum observations have shown that at least 50% of PMS stars are surrounded by disks of dust and gas (e.g. Strom et al. 1989, André et al. 1990) and it is believed that most stars start off with disks around them. Disks have masses from $10^{-3}$ to $10^{-1}$ M$_\odot$, radii from 10 to 1000 AU, and lifetimes up to a few Myrs. They are responsible for most of the infrared radiation that is observed in the spectra of PMS stars. Disk material slowly circles inwards and finally accretes onto the central star producing UV radiation. The evolution of a protostellar disk around an isolated star is determined by the combined effects of the star's gravity and irradiation, and the angular momentum transport processes in the disk. If the star/disk system is in a cluster then gravitational forces due to passing stars, and radiation from hot neighbouring stars also affect the disk evolution.

In this chapter, we perform SPH hydrodynamic simulations of axisymmetric disks and non-axisymmetric perturbed disks, and also radiative transfer simulations on snapshots during the evolution of the disks. Disks can be perturbed by passing stars, by irradiation from nearby hot stars or by planets forming within the disk. Disks are dynamically evolved using SPH, and the radiation transfer calculations are performed using PHAETHON. The radiation transfer is not treated consistently within SPH since we do not combine it with an SPH energy equation, and hence it does not affect the evolution of the disk. However, the goal of this work is to test the adaptability of PHAETHON to treat arbitrary geometries within SPH, rather than to study the details of disk evolution. In the future we plan to combine the two methods into a consistent SPH-RT scheme.
6.1 Disk initial conditions

We set the initial disk density, temperature and rotational velocity using information from theoretical models and observations. In this section we describe the initial conditions in detail.

6.1.1 Disk surface density

Steady disk theory (e.g. Natta 1993) suggests that the surface density of an accretion disk follows a power law of the form \( \Sigma(R) \propto R^{-3/4} \alpha^{-1} \), where \( R \) is the distance from the central star on the disk mid-plane, and \( \alpha \) is the viscosity parameter in the Shakura-Sunyaev prescription for viscosity (Shakura & Sunyaev 1973). Semi-analytical theoretical studies of cloud collapse and subsequent disk creation (Lin and Pringle 1990) indicate that \( \Sigma(R) \sim R^{-p} \), where \( p \) is between 1 and 3/2. The same model also predicts a much steeper density profile near the edge of the disk. In this study we assume a surface density profile

\[
\Sigma(R) = \Sigma_0 \left( \frac{R_0^2}{R_0^2 + R^2} \right)^{p/2},
\]

where \( \Sigma_0 \) is the surface density at \( R = 0 \), \( R_0 \) is the softening radius, which is used to prevent the surface density from getting nonphysically large near the star, and \( R \) denotes the distance from the star on the disk mid-plane. If \( x - y \) is the disk mid-plane then \( R = \sqrt{x^2 + y^2} \). (We note that in this chapter \( R \) is used to denote the distance from the star on the disk mid-plane and \( r = \sqrt{x^2 + y^2 + z^2} \) to denote the distance from star in three dimensions). For the models presented in this chapter we use \( p = 1 \).

We can calculate the disk mass interior to radius \( R \) by integrating the surface density:

\[
M(R) = \int_0^R \Sigma(R) 2\pi R dR.
\]

Substituting for \( \Sigma(R) \) and calculating the integral, we obtain

\[
M(R) = \pi R^2 \Sigma_0 \left[ \left( \frac{R_0^2 + R^2}{R_0^2} \right)^{1-p/2} - 1 \right].
\]

The total mass of the disk is obtained from the above formula by setting \( R = R_{\text{disk}} \):

\[
M_{\text{disk}} = \pi R^2 \Sigma_0 \left[ \left( \frac{R_0^2 + R_{\text{disk}}^2}{R_0^2} \right)^{1-p/2} - 1 \right].
\]
6.1. DISK INITIAL CONDITIONS

6.1.2 Disk temperature

The two major physical processes that heat the disk are irradiation from the central star and energy generated by viscous dissipation within the disk. In the case of a fully reprocessing (or passive) disk, i.e. a disk that just absorbs and reemits radiation from the central star, the flux of stellar radiation at distance $R$ from the star, scales as $1/R^2$ and the incident angle of the radiation on the surface of the disk scales as $1/R$ (assuming a geometrically thin disk). Thus, the total radiation incident on unit area of the disk scales as $1/R^3$ (see Hartmann 1998):

$$F_{\text{incident}} \propto \sigma T^4_* \left( \frac{R}{R_*} \right)^{-3}, \quad (6.5)$$

where $\sigma$ is the Stefan-Boltzmann constant, $T_*$ and $R_*$ the temperature and radius of the star, respectively. Assuming that the disk radiates like a blackbody, then

$$F_{\text{emitted}} \propto \sigma T^4_d(R), \quad (6.6)$$

where $T_d(R)$ is the temperature of the disk at distance $R$. By equating the absorbed and the emitted radiation, we obtain

$$T_d(R) \propto T_* \left( \frac{R}{R_*} \right)^{-3/4}. \quad (6.7)$$

In the case of an active accretion disk, i.e. a disk that is heated by energy produced by viscous dissipation within the disk, the heating depends on how angular momentum is transferred between parts of the disk that rotate with different angular velocities. If half of the gravitational potential energy released by matter in-spiralling through an annulus between $R + \Delta R$ and $R$ is radiated away as blackbody radiation, then

$$\frac{GM_* \dot{M}}{2R} \Delta R \frac{\Delta R}{R} \simeq 2 \times 2\pi R \Delta R \sigma T^4_d(R), \quad (6.8)$$

where $\dot{M}$ is the accretion rate, $R$ is the distance from the central star and $T_d(R)$ is the disk temperature at distance $R$. From the above, we obtain

$$T_d(R) \simeq \left( \frac{GM_* \dot{M}}{8\pi \sigma R^3} \right)^{1/4}. \quad (6.9)$$
We notice that in both passive and active accretion disks the temperature in the disk is expected to vary as \( R^{-3/4} \). The difference is that for active accretion disks the proportionality constant is determined by the mass accretion rate \( \dot{M} \) and the mass of the central star, whereas for passive disks it is determined by the luminosity of the central star \( L_* \).

It can be shown (see Hartmann 1998) that for \( T_d(R) \propto R^{-3/4} \) the SED varies with the wavelength \( \lambda \) as \( \lambda F_\lambda \propto \lambda^{-4/3} \). However, observations show that \( \lambda F_\lambda \propto \lambda^{-2/3} \), which suggests that \( T_d(R) \propto R^{-3/5} \). Furthermore, SEDs of many systems are almost flat, suggesting even hotter disks. This problem could be solved if disks are flared rather than flat (Kenyon & Hartmann 1987), i.e. the thickness of the disk increases as the distance from the star increases. In this case the disk temperature decreases less rapidly, depending on the degree of flaring. The problem could also be solved by a thin envelope surrounding the star, in addition to the disk. Natta (1993) pointed out that even a small amount of dust distributed above the disk will scatter a considerable amount of radiation back towards the disk mid-plane, heating the disk. Chiang and Goldreich (1997) proposed a more refined disk model in which the outer parts of the disk are optically thin, forming a “disk atmosphere”. In this model, dust grains that are in the disk atmosphere absorb unattenuated radiation from the star and become hotter, creating a superheated region in the outer regions of the disk.

We choose to parametrise the disk temperature using a general profile

\[
T_d(R) = \left[ T_0^2 \left( \frac{R^2 + R_0^2}{A U^2} \right)^{-q} + T_\infty^2 \right]^{1/2},
\]

(6.10)

where \( R_0 \) is a softening radius that prevents the temperature from being infinitely large close to the centre of the star, \( T_0 \) is the temperature at \( R = 1AU \) (provided that \( R_0 \ll 1AU \), which is generally true) and \( T_\infty \) is the temperature far away from the star. Beckwith et al. (1990) and Osterloh & Beckwith (1995) observed a large number of PMS stars in the Tau-Aur dark cloud and found temperature power law indices \( q \) from 0.35 up to 0.8. In the models presented here we assume \( q = 0.5 \), hence we do not examine the effects of different temperature profiles on the disk structure.

### 6.1.3 Disk thickness

We calculate the thickness \( z_0 \) of the disk by balancing the vertical component of the gravitational force of the star and the gravitational force of the underlying disk, against the pressure
6.1. DISK INITIAL CONDITIONS

force due to the disk temperature (disk thermal pressure):

\[
\frac{GM_* z_0(R)}{R^2} + \pi G \Sigma(R) \approx \frac{c_s^2(R)}{z_0(R)},
\]

(6.11)

where \(c_s^2(R) = kT(R)/(\mu m_p)\) is the local sound speed. The above equation can be written as

\[
\frac{GM_*}{R^3} z_0^2(R) + \pi G \Sigma(R) z_0(R) - c_s^2(R) = 0,
\]

(6.12)

which is a simple quadratic equation with a positive root

\[
z_0(R) = -\frac{\pi \Sigma(R) R^3}{2M_*} + \left[ \left( \frac{\pi \Sigma(R) R^3}{2M_*} \right)^2 + \frac{R^3}{GM_* c_s^2(R)} \right]^{1/2}
\]

(6.13)

The disk thickness depends on the assumed temperature and density profile, and also on the mass of the central star. In Fig. 6.1 we plot the disk thickness for a low-mass \((M_{\text{disk}}=0.01 \, M_\odot)\), Fig. 6.1a) and a high-mass disk \((M_{\text{disk}}=0.5 \, M_\odot\) Fig. 6.1b). The more massive disk is less flared.

**Figure 6.1** (a) Thickness \(z\) against \(x\) for a system with \(M_{\text{disk}}=0.01 \, M_\odot\), \(R_{\text{disk}}=1000 \, \text{AU}\), \(M_*=1 \, M_\odot\), \(p = 1\), \(q = 0.5\), \(T_0=300 \, \text{K}\), \(T_\infty=10 \, \text{K}\), \(R_0=0.25 \, \text{AU}\). The disk is flared. (b) Same as (a) but for a more massive disk \((M_{\text{disk}} = 0.5 \, M_\odot)\). The more massive disk is less flared.
6.1.4 Disk volume density

Theoretical studies of steady accretion disks (e.g. Frank, King & Raine 1992) suggest that the
density of the disk drops with the distance from the disk mid-plane following a gaussian profile.
Here, we assume a simple sinusoidal profile

\[
\rho(R, z) = \rho(R, 0) \cos \left[ \frac{\pi z}{2z_0(R)} \right], \quad |z| < z_0(R).
\]  

(6.14)

We can calculate \( \rho(R, 0) \) using the fact that the surface density is given by

\[
\Sigma(R) = \int_{-z_0(R)}^{z_0(R)} \rho(R, z) dz,
\]

(6.15)

where \( z_0(R) \) is the thickness of the disk at distance \( R \) from the star (see Eq. 6.13). Substituting
for \( \rho(R, z) \) and integrating, we obtain

\[
\Sigma(R) = \frac{4z_0(R)}{\pi} \rho(R, 0).
\]

(6.16)

Then, we solve for \( \rho(R, 0) \), using Eq. (6.1):

\[
\rho(R, 0) = \frac{\pi \Sigma_0}{4z_0(R)} \left( \frac{R_0^2}{R_0^2 + R^2} \right)^{p/2}.
\]

(6.17)

Hence, finally the disk volume density profile is

\[
\rho(R, z) = \frac{\pi \Sigma_0}{4z_0(R)} \left( \frac{R_0^2}{R_0^2 + R^2} \right)^{p/2} \cos \left[ \frac{\pi z}{2z_0(R)} \right].
\]

(6.18)

6.1.5 Disk rotation

We assume that all parts of the disk at distance \( R \) from the central axis rotate with the same
velocity \( v \), independently of the distance \( z \) from the disk mid-plane. (This is not necessarily true
as the velocity may be smaller at higher \( z \), leading to vertical momentum transfer and possibly
turbulence). We calculate the initial velocity of the disk at distance \( R \) from the star by assuming
that the centrifugal force is the sum of the gravitational forces of the star and the disk, on the
mid-plane of the disk. We assume that there are no vertical motions in the disk i.e. \( v_{z,i} = 0 \),
where \( i \) runs over all SPH particles. The gravitational acceleration \( g_i \) acting on a given SPH
particle \( i \) on the \( x-y \) plane is calculated using the SPH tree code gravity (see Section 5.1.4). We
then calculate the modulus $v_i$ of the rotatational velocity of the particle $i$

$$v_i = \sqrt{R_i |\mathbf{g}_i|} ,$$  \hspace{1cm} (6.19)

where $|\mathbf{g}_i| = \sqrt{g_{x,i}^2 + g_{y,i}^2}$ is the gravitational acceleration of the particle on the $x - y$ plane (i.e. the disk mid-plane), $R_i$ its the distance from the star, and $v_i = \sqrt{v_{x,i}^2 + v_{y,i}^2}$. Assuming that the disk rotates counterclockwise we have

$$v_{x,i} = -v_i \frac{y_i}{R_i} ,$$ \hspace{1cm} (6.20)

$$v_{y,i} = v_i \frac{x_i}{R_i} .$$ \hspace{1cm} (6.21)

In Fig. 6.2, we present the disk velocity profile for a low-mass disk ($M_{\text{disk}}=0.01 \, M_\odot$, Fig. 6.2a) and a high-mass disk ($M_{\text{disk}}=0.5 \, M_\odot$ Fig. 6.2b). The less massive disk rotates with keplerian velocity, because the self-gravity of the disk is not important compared to the gravity of the star. The more massive disk rotates faster than a keplerian disk due to the effect of its self-gravity.

**Figure 6.2** (a) Velocity profile for a representative low-mass disk ($M_{\text{disk}}=0.01 \, M_\odot$, $R_{\text{disk}}=1,000 \, \text{AU}$, $M_* = 1 \, M_\odot$, $p = 1$, $q = 0.5$, $T_0=300 \, \text{K}$, $T_{\infty}=10 \, \text{K}$, $R_0=0.25 \, \text{AU}$, $N=10,000$). The solid line is the velocity of the particles if we ignore the disk self gravity (keplerian rotation). The disk rotates with the keplerian velocity. (b) Same as (a) but for a more massive disk ($M_{\text{disk}} = 0.5 \, M_\odot$). The disk rotates faster than a keplerian disk, due to its self-gravity.
6.2 SPH disk setup

To construct an SPH disk, we distribute the SPH particles randomly, using a Monte Carlo approach, to reproduce the disk properties as described in the previous section. We also set the mass of each particle and its smoothing length, and impose a perturbation on the disk.

6.2.1 Position, mass and initial smoothing length of SPH particles

We use three uniformly distributed random numbers \( \mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3 \) to distribute the SPH particles so as to approximately reproduce the disk’s initial density profile (see Appendix D). The distance \( R \) of the particle from the rotation axis is

\[
R = R_0 \omega^{1/2},
\]

where

\[
\omega = \left(1 + \mathcal{R}_1 \frac{M_{\text{disk}}}{\pi R_0^2 \Sigma_0}\right)^{2/(2-p)} - 1.
\]

The \( x \) and \( y \) coordinates of the SPH particle are

\[
x = R \cos(2\pi \mathcal{R}_2),
\]

\[
y = R \sin(2\pi \mathcal{R}_2).
\]

Finally, the \( z \) coordinate of the particle is

\[
z = z_0(R) \frac{2}{\pi} \sin^{-1}(2\mathcal{R}_3 - 1),
\]

where \( z_0(R) \) is calculated from Eq. (6.13).

The particle mass is calculated from the total disk mass, \( M_{\text{disk}} \), by assuming that all particles have the same masses, hence

\[
m_i = \frac{M_{\text{disk}}}{N},
\]

where \( N \) is the total number of SPH particles used in the simulation.

The initial smoothing length of each particle is calculated from the mean number of neighbours \( N_{\text{neigh}} \) that each particle must have (\( N_{\text{neigh}} \approx 50 \pm 5 \)). If \( h_i \) is the smoothing length of particle \( i \),
then the density inside a sphere of radius $2h_i$ centred on the particle is

$$\rho(R_i, z_i) = \frac{N_{\text{neigh}} m_i}{\frac{4}{3} \pi (2h_i)^3}. \quad (6.28)$$

Solving the above for $h_i$, we obtain

$$h_i = \left[ \frac{3N_{\text{neigh}} m_i}{32\pi \rho(R_i, z_i)} \right]^{1/3}. \quad (6.29)$$

### 6.2.2 Azimuthal density perturbations

Azimuthal density perturbations are imposed on the disk by moving the particles along $\phi$, keeping their distance from the centre constant. Consider a ring of radius $r$ with $N$ particles on it. Suppose that $\mu(\phi)$ is the line particle density (particles per unit length). Then for an unperturbed disk we have that

$$\mu(\phi) = \frac{N}{2\pi r}. \quad (6.30)$$

After imposing a perturbation, we want the new line density $\mu^*$ to very with the new azimuthal angle $\phi^*$, as

$$\mu^*(\phi^*) = \frac{N}{2\pi r} [1 + A \cos(m\phi^*)], \quad (6.31)$$

where $m$ is the mode and $A$ is the amplitude of the perturbation. According to the above equation, the line density is larger at specific azimuthal angles and lower at other azimuthal angles, depending on the mode $m$ of the simulation. We can find the relationship between the old and the new azimuthal angle, using the fact that the total number of particles on the ring from 0 to $\phi$ before the perturbation is the same as the number of particles from 0 to $\phi^*$ after the perturbation. Before the perturbation the number of particles from 0 to $\phi$ is

$$N(\phi) = \int_0^\phi \mu(\phi) r \, d\phi = \int_0^\phi \frac{N}{2\pi r} r \, d\phi = \frac{N\phi}{2\pi}. \quad (6.32)$$

After the perturbation the number of SPH particles from 0 to $\phi^*$ is

$$N^*(\phi^*) = \int_0^{\phi^*} \mu^*(\phi^*) r \, d\phi^* = \int_0^{\phi^*} \frac{N}{2\pi r} [1 + A \cos(m\phi^*)] r \, d\phi^* = \frac{N}{2\pi} [\phi^* + \frac{A \sin(m\phi^*)}{m}]. \quad (6.33)$$

Hence, since $N^*(\phi) = N(\phi)$,

$$\phi = \phi^* + \frac{A}{m} \sin(m\phi^*). \quad (6.34)$$
6.3 Models of protostellar disks: GM Aurigae

GM Aurigae is a classical T Tauri star ($M_* = 0.85 M_\odot$) surrounded by a disk, as evidenced by the infrared excess in the SED of the system and NICMOS NIR observations (see Schneider et al. 2003). The size of the disk is estimated to be $\sim 300$ AU and its mass $\sim 0.047 M_\odot$. Previous studies (Rice et al. 2003) have shown that the SED of the GM Aurigae system is consistent with the presence of a gap around the central star. This gap may be induced by a planet orbiting close to the star.

We model GM Aurigae using SPH and perform radiative transfer simulations using PHAETHON. The parameters of our model are listed in Table 6.1. The SPH particles ($10^5$ particles) that represent the disk are initially distributed in space as described in Section 6.1. We assume a disk density profile with $\rho \propto R^{-1}$ and a disk temperature profile with $T \propto R^{-0.5}$. First, we study an axisymmetric disk and then a disk with an azimuthal perturbation (see Section 6.2.2), having mode $m = 1$ (one-arm spiral) and amplitude $A = 0.5$. According to Eq. (6.31) this means that the surface density at $\phi = 0$ is 3 times higher than the surface density at $\phi = \pi$. In both cases the disk is truncated at a radius of $R_{\text{gap}} = 5$ AU.

<table>
<thead>
<tr>
<th>$M_*$</th>
<th>0.85 $M_\odot$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_*$</td>
<td>4000 K</td>
</tr>
<tr>
<td>$R_*$</td>
<td>1.75 $R_\odot$</td>
</tr>
<tr>
<td>$M_{\text{disk}}$</td>
<td>0.047 $M_\odot$</td>
</tr>
<tr>
<td>$R_{\text{gap}}$</td>
<td>5 AU</td>
</tr>
<tr>
<td>$R_{\text{disk}}$</td>
<td>300 AU</td>
</tr>
<tr>
<td>$D$</td>
<td>140 pc</td>
</tr>
</tbody>
</table>

$M_*, T_*, R_*$: Mass, temperature and radius of the central star.

$M_{\text{disk}}, R_{\text{disk}}, R_{\text{gap}}$: Disk mass, disk radius and disk inner gap size.

$D$: Distance of GM Aurigae from the Earth.

We perform radiative transfer simulations on both axisymmetric and perturbed disks, using PHAETHON. We use the SPH tree to construct the radiative transfer cells, as described in Section 5.2.1. We construct RT cells that contain a maximum of $N_{\text{max}} = 12$ SPH particles. In the method we described in the previous chapter, the density of each cell is calculated by dividing the mass contained within each cell by the volume of the cell. Here we have chosen a very low $N_{\text{max}}$.
in order to have small volume RT cells, and thus better resolution for the radiative transfer simulation. The number of SPH particles per cell is very small and the statistical error in calculating the density would be very large, if we were to use the previous method. In this case, we assume that the density of a cell containing \( N < N_{\text{max}} \) SPH particles is the same as the density of the smallest higher level SPH cell that contains more than \( N = 50 \) SPH particles. Using this method, the density of each cell is calculated more accurately. To capture the steep temperature gradient very close to the star we use an additional grid around the star (see Section 5.4). We construct a 2-dimensional grid using spherical and conical surfaces. We use 32 spherical surfaces and 9 conical surfaces, and thus there are 288 cells. The inner radius of this grid is set at \( R_{\text{gap}} = 5 \) AU and the outer radius at \( R_{\text{eg}} = 2.44 R_{\text{gap}} \) (the size of the star grid is on the order of the surrounding RT cells constructed using the SPH tree).

![Graph](image)

**Figure 6.3** Dust properties used for the radiative transfer simulations of the GM Aurigae disk. (a) Dust absorption opacity (solid line) and scattering opacity (dashed line). (b) Dust albedo. The size of the dust grains of this model is larger than the size of the grains of a standard interstellar medium mixture.

We use the same dust opacity that Wood et al. \( (2002a) \) used to fit the HH30 observations (see also Wood et al. \( 2002b) \). The absorption and scattering opacity, and the dust albedo are shown in Fig. 6.3. The dust size distribution of this model is

\[
n(a)da = C_i a^{-p} e^{-(a/a_c)^p} da
\]  
\( (6.35) \)
where $p = 3.5$, $q = 0.6$, $a_c = 50$ $\mu$m, with minimum size $a_{\text{min}} = 0.01$ $\mu$m and maximum size $a_{\text{max}} = 1000$ $\mu$m. The assumed dust mixture comprises larger dust grains than a standard interstellar medium mixture (e.g. the standard MRN mixture; Mathis, Rumpl, & Nordsieck 1977). This is consistent with the idea of grain growth within protoplanetary disks. As a result, the dust opacity of the adopted model is smaller than the corresponding MRN opacity for wavelengths $\lambda \lesssim 3$ $\mu$m, and larger for $\lambda \gtrsim 10$ $\mu$m.

### 6.3.1 Model I: Axisymmetric disk

The disk is constructed using the procedure described in Section 6.1 and is evolved using SPH, so that it relaxes to its equilibrium state. In Fig. 6.4 we present a top view and side view of the disk. As the disk evolves angular momentum is redistributed within the disk by viscous forces. Particles that are near the star accrete onto the star, whereas particles in the outer region of the disk move outwards (see Lynden-Bell & Pringle 1974).

![Figure 6.4](image)

**Figure 6.4** SPH simulation of an axisymmetric disk model representing GM Aurigae (see parameters in Table 6.1). (a) Top view of the disk. (b) Side view of the disk.

Using PHAETHON we perform radiative transfer simulations on the disk. $L$-packets are emitted isotropically from the central star into the computational domain. We use the SPH tree to construct the radiative transfer cells. We construct RT cells that contain a maximum of $N_{\text{max}} = 12$ SPH particles, and we use an additional 2-dimensional grid around the central star. In Figs. 6.5-6.6, we present the results of the radiative transfer simulation. We plot the disk density and
Figure 6.5  Radiative transfer simulations of an axisymmetric disk model representing GM Aurigae. (a) Disk density profile on the \(x - y\) plane (disk mid-plane). (b) Disk temperature profile on the \(x - y\) plane. (c) Disk density profile on the \(x - z\) plane. (d) Disk temperature profile on the \(x - z\) plane. The disk is heated axisymmetrically. Small asymmetries are due to statistical noise.
temperature on the $x - y$ plane (Figs. 6.5a,b), on the $x - z$ plane (Figs. 6.5c,d), and the SED of the system at different viewing angles (Fig. 6.6).

The disk is heated axisymmetrically (within the statistical uncertainties) and the disk temperature falls off approximately as $\sim R^{-0.5}$ (see Figs. 6.5b,d). It is evident (Fig. 6.5d) that the disk mid-plane is colder than the surface of the disk. The resolution in the $z$ direction (i.e. perpendicular to the disk mid-plane) is just good enough to capture the rapid increase of temperature near the surface of the disk.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{sed.png}
\caption{SED of an axisymmetric disk model for GM Aurigae, at different viewing polar angles ($\theta_{\text{obs}} = 0^\circ, 20^\circ, 50^\circ, 70^\circ$ and $90^\circ$, from top to bottom). The SED at $\theta_{\text{obs}} = 50^\circ$ is plotted in red colour, and the SEDs at $\theta_{\text{obs}} = 0^\circ$ and $20^\circ$ are almost indistinguishable. The dotted line corresponds to the intrinsic SED of the central star (i.e. a blackbody distribution having $T_\star = 4000$ K). The green squares correspond to the observational data (see Schneider et al. 2003). The SED at $\theta_{\text{obs}} = 50^\circ$ (red line) fits the data best.}
\end{figure}

In Fig. 6.6 we present the spectral energy distribution of the star/disk at different viewing angles. To calculate the SEDs we count $L$-packets that escape within a tolerance angle of $10^\circ$ from the specified direction of the observer $\theta_{\text{obs}}$. We calculate the SED for viewing polar angles $\theta_{\text{obs}} = 0^\circ, 20^\circ, 50^\circ, 70^\circ$ and $90^\circ$. The SED of the system is essentially indistinguishable for $\theta_{\text{obs}} = 0^\circ$ and $20^\circ$ (nearly face-on disk). At small polar viewing angles direct starlight dominates the SED at optical wavelengths, and emission from the disk dominates the SED at IR wavelengths. As the observing angle increases towards $90^\circ$ (i.e. the disk is observed nearly edge-on) less direct
starlight is able to escape through the optically thick disk mid-plane. The SED at viewing angle $\theta_{\text{obs}} = 50^\circ$ (red line in Fig. 6.6) fits the data best, as previous studies have suggested (Rice et al. 2003).

6.3.2 Model II: Perturbed disk

We perform a simulation similar to the one in Section 6.3.1 but for a perturbed disk. The presence of a planet orbiting around the central star is likely to induce density waves in the disk. Here, we do not examine the details of the planet-disk interaction but artificially impose an $m=1$, $A=0.5$ azimuthal perturbation, as described in Section 6.2.2.

![SPH simulation of a perturbed disk model representing GM Aurigae (see parameters in Table 6.1). (a) Top view of the disk. (b) Side view of the disk. The disk is non-axisymmetric.](image)

In Fig. 6.7 we present a top view and side view of the disk at $t = 480$ yrs after the start of the simulation. The presence of a single-arm spiral density wave, is evident in the $x-y$ plot. Using the method described by Sleath & Alexander (1996), we decompose the structure of the disk into a sum of Fourier components corresponding to different modes (see Appendix E). We present the results of this analysis in Fig. 6.8. The only significant mode in the disk is the $m = 1$ mode, i.e. the mode corresponding to a single-arm spiral. Using the fact that the maximum strength $F$ occurs at $\zeta = -2.8$ (see Fig. 6.8), we calculate that the pitch angle of the density wave in Fig. 6.7a is $\beta \approx 20^\circ$. 
Figure 6.8  Fourier analysis of the disk structure in Fig. 6.7a. $F$ denotes the strength of a specific mode $m$, and the parameter $\zeta = -m/\tan(\beta)$ determines the pitch angle $\beta$ of the spiral (see Appendix E). On this graph we plot only the strength of the $m = 1$ mode (the strengths of the other modes are close to zero). From the graph, we see that the maximum $F$ occurs at $\zeta \approx -2.8$, hence the pitch angle of the spiral arm in Fig. 6.7a is $\beta \approx 20^\circ$.

We again use PHAETHON to perform radiative transfer simulations on the disk. We use the SPH tree to construct the radiative transfer cells. We construct RT cells that contain a maximum of $N_{\text{max}} = 12$ SPH particles, and we use an additional 2-dimensional grid around the central star. In Figs. 6.9-6.10, we present the results of the radiative transfer simulation. We plot the disk density and temperature on the $x - y$ plane (Figs. 6.9a,b), on the $x - z$ plane (Figs. 6.9c,d), and the SED of the system at different viewing angles (Fig. 6.10).

We notice by comparing Figs. 6.7 and 6.9 that the radiative transfer cells do not seem to capture the smallest density variations, indicating that smaller cells are needed. However, even with this resolution, we can see (Fig. 6.9b,d) that the disk is not heated axisymmetrically. In Fig. 6.9b the upper left part of the disk is hotter than the lower right part of the disk, because of the existence of a density minimum towards the upper left direction. As in the case of the axisymmetric disk, the disk mid-plane is colder than the disk surface, but the heating now is not axisymmetric (see Fig. 6.9d).

In Figs. 6.10 and 6.11 we present the spectral energy distribution of the the star/disk system at different polar and azimuthal viewing angles. We calculate the SED for polar angles $\theta_{\text{obs}} = 0^\circ$, 

...
Figure 6.9 Radiative transfer simulations of a perturbed disk model representing GM Aurigae. (a) Disk density profile on the $x - y$ plane (disk mid-plane). (b) Disk temperature profile on the $x - y$ plane. (c) Disk density profile on the $x - z$ plane. (d) Disk temperature profile on the $x - z$ plane.
**Figure 6.10** SEDs of a perturbed disk model for GM Aurigae at different polar and azimuthal viewing angles. The SEDs fall into five groups. Each group corresponds to the same polar angle $\theta_{\text{obs}}$ for 4 different azimuthal angles $\phi_{\text{obs}}$, with $\phi_{\text{obs}} = 0^\circ, 90^\circ, 270^\circ$ and $180^\circ$ (from top to bottom in the same group) (there is a total of 4 curves per group but they are hard to distinguish). The highest group corresponds to $\theta_{\text{obs}} = 0^\circ$ and $\theta_{\text{obs}} = 20^\circ$ (there are 8 indistinguishable curves), the second highest to $\theta_{\text{obs}} = 50^\circ$, the third highest to $\theta_{\text{obs}} = 70^\circ$, and the lowest group to $\theta_{\text{obs}} = 90^\circ$. The dotted line corresponds to the intrinsic SED of the central star. The green squares correspond to the observational data. The red line corresponds to the best fit curves ($\theta_{\text{obs}} = 50^\circ$ and $\phi_{\text{obs}} = 180^\circ, 270^\circ$).

**Figure 6.11** The IR region of the SED (same as in Fig. 6.11). The azimuthal density perturbation results in a small $\phi$ dependence for the SED.
20°, 50°, 70° and 90°, and for 4 different azimuthal angles $\phi_{\text{obs}} = 0°, 90°, 180°$ and $270°$. The SED is similar to that of the axisymmetric system, apart from a small excess at wavelengths 10-200 $\mu$m. There is a small $\phi$-dependence that is more prominent at polar angles $60° - 80°$ (see Fig. 6.11). The best fit to the GM Aurigae SED is obtained for $\theta_{\text{obs}} = 50°$ and $\phi_{\text{obs}} = 180° - 270°$ (red line in Fig. 6.11).

6.4 Discussion

In this chapter we apply our Monte Carlo radiative transfer method to SPH snapshots. We construct flared protostellar disks using density and temperature profiles chosen from complementary theoretical and observational arguments. We study the specific case of GM Aurigae, a typical T Tauri star with a circumstellar disk. We examine an axisymmetric disk and a perturbed, non-axisymmetric disk, which both have a central gap near the star. For the axisymmetric disk, we find that the disk mid-plane is colder than the disk surface, as previous studies have indicated (e.g. Chiang & Goldreich 1997). The SED of GM Aurigae is consistent with an observing angle $\theta_{\text{obs}} = 50°$ (see Rice et al. 2003). For the perturbed disk, we find that the SED of the system is similar to the previous case, but shows a small dependence on the azimuthal angle $\phi$. The SED of GM Aurigae is consistent with an observing polar angle $\theta_{\text{obs}} = 50°$ and azimuthal angle $\phi_{\text{obs}} = 180° - 270°$.

The simulations in this chapter show that the method we have developed for performing radiative transfer simulations on SPH snapshots using PHAETHON, works reasonably well. However, there are still some areas that need further study and development:

- Regions close to stars. Such regions are characterised by high temperature gradients, and hence small RT cells are needed to record these gradients. The required linear size of the RT cells is on the order of the star radius. This size is much smaller than the SPH resolution, defined by the smoothing length $h$ in the neighbourhood of the star. We treat this problem by using an additional 2-dimensional grid around the star. In this way we achieve a better resolution for the RT simulation in the region very close to the star. However, the SPH simulation does not give any information about the density distribution at such small scales and the choice of the density distribution close to the star is rather ad hoc. A more satisfactory (but more computationally expensive) way to treat the problem would be to increase the SPH resolution by using a larger number of SPH particles.
• RT resolution vs SPH resolution. This is similar to the problem discussed in the preceding paragraph but it is more general. In many cases the SPH resolution is not adequate for the RT simulation (e.g. in regions with high temperature gradients). There are two ways to increase the resolution of the RT simulation. The first way is to further subdivide the RT cells that were constructed using the SPH tree. The second way is to increase the number of SPH particles used in the simulation, so that the RT cells constructed using the SPH tree are smaller. The second way is the more appropriate, especially when we are interested in the effects of radiation transfer on the disk evolution (e.g. in a future SPH-RT scheme).

• Code efficiency. The running time of the code is critical for the method. In many cases, for example in regions with large temperature gradients, very small RT cells are needed. Thus, a large number of $L$-packets must be simulated in order to have a large number of absorption events per RT cell and a low statistical noise when calculating the temperature of each cell. Most of the computational time is used to propagate $L$-packets in the computational domain, and thus a robust algorithm is needed for this purpose. In the case that RT cells constructed using the SPH tree are further subdivided into smaller cells, the propagation of the photons should be done using the larger RT cells that were constructed using the SPH tree. That is because there are no density variations at smaller scales. Thus, in effect there would be two sets of cells: (i) the “density cells” used to propagate photons (i.e. the RT cells constructed using the SPH tree), and (ii) the “temperature cells” (i.e. the smaller RT cells constructed by subdividing the density cells) that interact with the $L$-packets.
Chapter 7

Discussion & Future Prospects

In this thesis we implement a Monte Carlo radiative transfer code with frequency distribution adjustment and use it to study systems related to the initial stages of star formation. We examine spherical and non-spherical prestellar cores that are illuminated by an external radiation field. We study both non-embedded cores and cores embedded inside molecular clouds. We extend the radiative transfer method to treat systems with arbitrary geometries resulting from SPH simulations. We test our code thoroughly and use it to study perturbed protostellar disks in SPH simulations. In this chapter, we summarise the main results and the future prospects of this work.

7.1 Monte Carlo radiative transfer with frequency distribution adjustment

We implement a Monte Carlo radiative transfer code (PHAETHON) which uses a large number of monochromatic luminosity packets to represent the radiation transported through a medium. The $L$-packets are injected into the medium and interact stochastically with it. The medium itself is divided into a number of cells, each with given mass and uniform temperature. The $L$-packets propagate into the medium and when they reach an interaction point they either get scattered or absorbed, depending on the albedo of the dust at the frequency of the $L$-packet. If the $L$-packet is scattered from a cell, then a new direction is chosen using the Henyey & Greenstein (1941) scattering phase function. If the $L$-packet is absorbed it raises the local temperature. The packet is directly reemitted, so as to conserve energy. The temperature of the cell is determined by
equating the absorbed luminosity
\[ \Gamma_i^\text{abs} = k_i \delta L, \]  
(7.1)
to the emitted luminosity
\[ \Gamma_i^\text{em} = 4\pi m_i \int_0^\infty \kappa_\nu B_\nu (T_i) \, d\nu, \]  
(7.2)
where the index \( i \) refers to the cell where the absorption takes place, \( k_i \) is the number of packets that have been absorbed by the cell, \( T_i \) the temperature of the cell, \( m_i \) the mass of the cell, and \( \delta L \) the luminosity of each packet.

The frequency of the reemitted \( L \)-packet is chosen using a probability distribution function so as to correct for the \( L \)-packets that were reemitted previously from the cell with an incorrect frequency distribution. The probability distribution function is constructed from the difference in the emissivity of the cell before and after the emission of the \( L \)-packet (Bjorkman & Wood 2001)
\[ p(\nu)d\nu = \frac{\kappa_\nu [B_\nu (T + \Delta T) - B_\nu (T)]d\nu}{\int_0^\infty \kappa_\nu [B_\nu (T + \Delta T) - B_\nu (T)]d\nu}, \]  
(7.3)
provided that the cell is in radiative equilibrium (Baes et al. 2003). Using this procedure the correct temperature distribution and spectrum of the system are obtained at the end of the simulation, when all the packets have been propagated through the medium and escaped, without iteration.

We test this method using the Ivezić et al. (1997) benchmark calculations, the Bjorkman & Wood (2001) calculations, and also using the thermodynamic equilibrium test, in which the system is illuminated by an isotropic blackbody radiation field. All tests indicate that the code is very accurate.

The Monte Carlo radiative transfer method with frequency distribution adjustment accounts for both absorption and scattering, it is robust, it is very accurate, it can be parallelised easily and it can treat systems with arbitrary geometries. However, a large number of \( L \)-packets must be simulated in order to minimise the statistical noise in the results.

### 7.2 Radiative transfer in spherical prestellar cores

We use PHAETHON to study prestellar cores, which are condensations in molecular clouds. These systems have no internal source of radiation. We represent prestellar cores by Bonnor-Ebert spheres, i.e. isothermal spheres in which the gravity is balanced by the thermal pressure of
the sphere. We first assume that the cores are directly exposed to the interstellar radiation field (non-embedded cores) as estimated by Black (1994). Our code predicts that the temperature inside these cores drops from \( \sim 17 \) K at the edge, down to \( \sim 7 \) K at the centre, depending on the total optical depth. Our results are similar to those of previous studies (Evans et al. 2001, Zucconi et al. 2001). We also calculate intensity profiles of prestellar cores at different wavelengths. The core is seen in absorption at MIR wavelengths (e.g. \( 90 \mu m \)). Observations at submm and mm wavelengths (e.g. \( 850 \mu m \)) map mainly the column density through the core and the intensity at these wavelengths drops from the centre to the edge of the core. At wavelengths near the peak of the core emission (150-250 \( \mu m \)) the intensity increases slightly towards the edge of the core due to the temperature increase near the edge.

We also explore models of spherical cores that are embedded in molecular clouds. The radiation field incident on embedded cores is different from the radiation incident on non-embedded cores. The ambient molecular cloud absorbs the UV, optical and NIR part of the radiation and re-emits it in the FIR and submm region (Mathis et al. 1983). We study cores with different density profiles embedded in molecular clouds with various optical extinctions and we calculate temperature profiles, SEDs and intensity profiles. Our study indicates that the temperature gradients in embedded cores are less steep than those in non-embedded cores. Deeply embedded cores (ambient cloud with visual extinction larger than 15-25) are almost isothermal at around 7-8 K. The temperature inside cores surrounded by an ambient cloud of even moderate thickness (\( A_V \sim 5 \)) is less than 12 K, which is lower than previous studies have assumed. Thus, previous mass calculations of embedded cores (for example in the \( \rho \) Ophiuchi protocluster), based on mm continuum observations, may underestimate core masses by up to a factor of 2.

We also calculate intensity profiles of embedded cores at different wavelengths. At 90 microns the core is seen in absorption against the background. The intensity decreases slightly towards the centre of the core, and therefore very sensitive (say \( \sim 1 - 3 \) MJy sr\(^{-1} \)) observations are needed to detect cores in absorption at 90 \( \mu m \). At wavelengths near the peak of the core emission (150-250 \( \mu m \)) the intensity increases by a small amount (\( \sim 5 - 20 \) MJy sr\(^{-1} \) above the background) towards the edge of the core. The higher the increase in the intensity near the core boundary, the less embedded is the core. Thus, very sensitive observations of embedded prestellar cores at 170-200 \( \mu m \), might allow us to determine the extinction of the cloud surrounding the core. Finally, at submillimetre and millimetre wavelengths (400-1300 \( \mu m \)) the intensity drops towards the edge of the core considerably. The core can be observed at 400-500 \( \mu m \), where the contrast
with the background is quite large (~ 50 – 150 MJy sr\(^{-1}\)). At wavelengths longer than ~ 600 \(\mu\)m the background radiation becomes important and the core emission is not much larger than the background emission (~ 20-50 MJy sr\(^{-1}\) larger). However, most of the background radiation is the CMB and can easily be subtracted. The upcoming \textit{Herschel} mission (ESA, launch date 2007) will, in principle, be able to detect these features and test our models.

## 7.3 Models of non-spherical prestellar cores

We extend our work on prestellar cores by studying non-spherical cores. We examine flattened cores (disk-like asymmetry) that are either directly exposed to the interstellar radiation field or embedded inside ambient molecular clouds, and also cores with a “south-pole asymmetry”, i.e. where the “south” part of the core is denser than the “north” part. These models may represent more realistic density distributions than the commonly used spherically symmetric Bonnor-Ebert model. We calculate core temperature profiles, SEDs at different viewing angles, and isophotal maps at different viewing angles and different wavelengths.

Our radiative transfer simulations using \textsc{phaethon} demonstrate the features that even mild deviations from spherical symmetry can produce on the isophotal maps of such cores, and emphasise the importance of mapping at wavelengths near the peak of the SED. We find that SEDs of flattened cores (equatorial-to-polar optical depth ratio \(e = 1.5\) and 2.5) are essentially independent of the viewing angle. However, isophotal maps depend strongly on the viewing angle. When the core is viewed edge-on it appears elongated on 850 \(\mu\)m maps, which effectively trace column-density. At wavelengths near the peak of the core emission (e.g. 200 \(\mu\)m), isophotal maps are strongly affected by the temperature of the core and they are not solely column density tracers. There are interesting features on these maps, which depend on the observer’s viewing angle, and the detailed density and temperature structure of the core. Hence, they contain complementary information to the 850 \(\mu\)m maps. South-pole asymmetric models (south-to-north pole optical depth ratio \(e = 1.5\) and 2.5) yield similar results. The predicted characteristic features are on scales 1/5 to 1/3 of the overall core size, and high resolution observations are needed to observe them. They are also weaker when the core is embedded inside a molecular ambient cloud. \textit{Herschel} will in principle provide the resolution at 170-250 \(\mu\)m that is required to detect such features.
7.4 Monte Carlo radiative transfer and SPH

We extend PHAETHON to treat radiative transfer in systems with arbitrary geometries resulting from SPH simulations. SPH is a Lagrangian method that uses a large number of particles to represent a fluid. Particles interact with each other via gravity, pressure and viscous forces. The physical properties of the fluid are calculated as weighted local averages. SPH uses a tree structure to calculate gravity forces. The SPH tree is a hierarchical division of the computational domain into cells and subcells, until each cell contains just one particle or no particles at all. This hierarchical structure is used to speed up the computation of the gravitational forces between particles. To calculate the gravitational force on a given particle \( i \), particles which are close to \( i \) contribute individually to this force but particles that are far away contribute collectively.

We use the SPH tree to construct radiative transfer cells, i.e. cells that interact with the radiation. The SPH cells, from the root cell to lower level cells, serve as potential radiative transfer cells. If the number of particles belonging in a given SPH cell is smaller than a maximum value, \( N_{\text{max}} \), then this SPH cell is also a radiative transfer cell. \( N_{\text{max}} \) is chosen to be \( \sim 70 - 100 \) particles, i.e. a bit larger than the mean number of SPH neighbours. This procedure naturally creates cells with linear size on the order of \( 4h \) (where \( h \) is the local SPH smoothing length). Thus, the resolution provided by the radiative transfer cells is about the same as the SPH resolution.

We test our method against the thermodynamic equilibrium test. A uniform density sphere is represented by a large number of SPH particles, and it is illuminated by an isotropic blackbody radiation field. The temperature calculated from the simulation is accurate, i.e. the same as the temperature of the illuminating field. There are some deviations near the edge of the sphere, due to the presence of irregular cells, i.e. cells with only a small part within the actual sphere. These cells are a side effect of representing a sphere by an ensemble of cubic cells.

We also test the method using the Ivezić et al. (1997) tests, where a star is surrounded by a spherical envelope. The temperature is not calculated correctly close to the star because the RT cells are not small enough to capture the large temperature gradient in this region. To solve this problem, we propose the construction of a spherical grid around the star (the star grid), comprising concentric cells with width on the order of the dust destruction radius. With the addition of the star grid the code reproduces the results of Ivezić et al. (1997).

The method developed for performing continuum radiative transfer simulations on SPH snapshots is useful for comparing the results of hydrodynamic simulations directly with observations.
7.5 Radiative transfer in protostellar disks

We apply the extended version of PHAETHON to study the radiative transfer in axisymmetric and perturbed disks in SPH simulations. Our goal is to test the adaptability of the code in treating systems with arbitrary geometries in SPH simulations.

We construct realistic models of protostellar disks, using information from theoretical models and observations. To test our radiative transfer method, we model GM Aurigae, a T Tauri star with a circumstellar disk. Initially, we construct an axisymmetric disk model with a surface density profile that falls off as $R^{-1}$ along the disk mid-plane. The disk thickness is calculated by balancing the vertical component of the gravitational forces of the star and the underlying disk, against the disk thermal pressure gradient. The disk produced in this way is flared and the degree of flaring depends on the disk mass; more massive disks are less flared than less massive disks.

We examine an axisymmetric disk, and a perturbed disk with an $m = 1$, $A = 0.5$ azimuthal density perturbation. The axisymmetric disk is heated axisymmetrically and the disk mid-plane is colder than the disk surface. On the other hand, the perturbed disk is heated asymmetrically due to the existing density perturbations. The resulting SED in both cases depends strongly on the polar viewing angle. For the perturbed disk there is also a weak dependence on the azimuthal viewing angle, when the disk is viewed at polar angles $\gtrsim 40^\circ$. The best fit of the SED of GM Aurigae is obtained for an observing polar angle $\theta_{\text{obs}} = 50^\circ$ and azimuthal angle $\phi_{\text{obs}} = 180^\circ - 270^\circ$.

The results indicate that PHAETHON works reasonably well in treating arbitrary SPH systems. However, regions with large temperature gradients introduce difficulties into the radiative transfer calculations, and further study is required in this direction.

7.6 Future prospects

Radiative transfer is important for the study of all astrophysical systems. Monte Carlo radiative transfer with frequency distribution adjustment is an efficient and accurate method that can be used to treat a variety of systems with arbitrary geometries. The method solves for the dust temperature and calculates SEDs at different viewing angles, and intensity maps at different viewing angles and wavelengths. Thus, the method produces results that, after being convolved with the telescope’s observing beam, can be directly compared with observations.
7.6. FUTURE PROSPECTS

PHAETHON, our implementation of Monte Carlo radiative transfer, works reasonably well in treating a variety of systems. The code could be further optimised, so as to

- Improve the treatment of low-density regions. These regions absorb a small number of photons and thus the statistical noise in calculating the temperature is large. One way to solve this problem is to construct larger cells in regions of low density. However, this deteriorates the spatial resolution of the RT simulation. Another way is to use the mean intensity of the local radiation field to determine the energy absorbed in each cell (Lucy 1999).

- Produce isophotal maps when there is a strong luminosity source in the computational domain. Consider for example a star surrounded by a spherical envelope. Most of the radiation escaping from the system comes from the region close to the star. Thus, the isophotal maps of the spherical envelope are very noisy, even though the temperature is computed reasonably well in the envelope. To solve this problem a post-radiative transfer analysis could be done to directly calculate the intensity reaching the observer from each cell. Another option is to calculate the probability a reemitted/scattered photon has of reaching the observer, at each absorption/scattering event. Then, we could weight the luminosity of the packet by this probability and assume that the weighted luminosity reaches the observer (peeling-off technique).

- Propagate \(L\)-packets and determine the RT cell of each \(L\)-packet more efficiently within SPH. The RT cells are cubic cells constructed using the SPH tree. During the building of the tree we can record information about the neighbours of each cell. Thus, as a packet propagates through the medium in small steps, the search for its new cell could be confined to the neighbours of the cell that the packet is currently in. The code could also easily be parallelised. In the Monte Carlo radiative transfer method each \(L\)-packet is treated independently. Thus, each processor of a parallel computer can be used to treat a single \(L\)-packet. We expect that the code running time should decrease almost linearly with the number of processors used.

We plan to apply PHAETHON to the study of other asymmetric systems, like circumbinary disks, protostellar jets, and turbulent clouds. We also intend to treat the effects of radiation transport on the evolution of such systems by integrating Monte Carlo radiative transfer with an energy equation, within Smoothed Particle Hydrodynamics.
Appendix A

$L$-packet Scattering Angle

Assume that before a scattering event the unit vector of an $L$-packet (i.e. the direction in which it propagates) in the fundamental reference frame $(x, y, z)$ is

$$\hat{k} = \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}.$$  \hfill (A.1)

In the photon’s idiosystem $(x'', y'', z'')$ this unit vector is

$$\hat{k}'' = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$  \hfill (A.2)

The above relation defines the $L$-packet’s idiosystem as the system in which the unit vector of the packet is along the $z''$-axis. The other two axes are on a plane perpendicular to the $z''$-axis but they are not uniquely defined. We can therefore define them arbitrarily (i) by rotating the fundamental reference frame $(x, y, z)$ through an angle $\phi$ about $z$ to produce an intermediate frame $(x', y', z')$, and then (ii) by rotating this frame through an angle $\theta$ about $y'$ to produce the photon’s idiosystem $(x'', y'', z'')$. Any vector in the photon’s idiosystem can then be transformed back to the fundamental reference frame by first rotating about $y''$ through an angle $-\theta$, which
requires the transformation

\[ T_1 = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}, \]  

(A.3)

and then rotating about \( z' \) through an angle \(-\phi\), which requires the transformation

\[ T_2 = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \]  

(A.4)

Assume that after scattering the \( L \)-packet’s unit vector in the \( L \)-packet’s pre-scattering idiosystem is

\[ \hat{e}'' = \begin{pmatrix} e''_x \\ e''_y \\ e''_z \end{pmatrix}, \]  

(A.5)

whereas in the fundamental reference frame it is

\[ \hat{e} = \begin{pmatrix} e_x \\ e_y \\ e_z \end{pmatrix}. \]  

(A.6)

The scattering of the \( L \)-packet happens at a random azimuthal angle \( \phi_{\text{scat}} = 2\pi R_\phi \) and at a polar angle \( \theta_{\text{scat}} \) calculated using the Henyey & Greenstein (1941) phase function as described in Section 2.10. We note that both of them are given in the \( L \)-packet’s idiosystem. Thus, the unit vector of the \( L \)-packet’s post-scattering direction (in the \( L \)-packet’s pre-scattering idiosystem) is

\[ e''_x = \cos(\phi_{\text{scat}}) \sin(\theta_{\text{scat}}) \]
\[ e''_y = \sin(\phi_{\text{scat}}) \sin(\theta_{\text{scat}}) \]  

(A.7)
\[ e''_z = \cos(\theta_{\text{scat}}). \]
We calculate this vector in the fundamental reference frame, using the transformations $T_1$ and $T_2$. After the first rotation we obtain

\[
e'_x = \cos(\theta)e''_x + \sin(\theta)e''_z
\]
\[
e'_y = e''_y
\]
\[
e' = -\sin(\theta)e''_x + \cos(\theta)e''_z .
\]

After the second rotation we obtain the direction of the $L$-packet in the fundamental reference frame

\[
e_x = \cos(\phi)e'_x - \sin(\phi)e'_y
\]
\[
e_y = \sin(\phi)e'_x + \cos(\phi)e'_y
\]
\[
e_z = e'_z .
\]
Appendix B

Isophotal Maps

B.1 General case

Let us assume that the direction to the observer is

\[ \hat{\mathbf{r}}_O = \begin{pmatrix} \cos \phi \sin \theta \\ \sin \phi \sin \theta \\ \cos \theta \end{pmatrix}. \]  \hspace{1cm} (B.1)

Also assume that the direction of the L-packet escaping from the system is

\[ \hat{\mathbf{k}}_p = \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}, \]  \hspace{1cm} (B.2)

and the last interaction point of the L-packet before escaping from the system is

\[ \mathbf{r}_p = \begin{pmatrix} x_p \\ y_p \\ z_p \end{pmatrix}. \]  \hspace{1cm} (B.3)

The escaping L-packet will be observed if its direction is the same as the direction of the observer. In practice, in order to improve statistics we count L-packets that escape within a tolerance angle.
Figure B.1 Observer’s view of the system.

\[ \Delta \theta \text{ of observer's direction. Thus, the condition for an } L\text{-packet to be observed is} \]

\[ \vec{k}_p \cdot \vec{r}_O = \cos(\vec{k}_p, \vec{r}_O) \geq \cos(\Delta \theta) \quad (B.4) \]

To construct an isophotal map we need to know where each \( L \)-packet that reaches the observer comes from. To do this we construct a new coordinate system \((x'', y'', z'')\), in which the observer lies along the \( z'' \)-axis of the new system and the other two axes are perpendicular to \( z'' \)-axis and to each other. This means that the observer’s direction vector in the new system is

\[ \vec{r}_O'' = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (B.5) \]

We can construct such a system by rotating the fundamental reference frame \((x, y, z)\) through and angle \( \phi \) about \( z \) to produce an intermediate frame \((x', y', z')\), and then rotating this frame through an angle \( \theta \) about \( y' \) to produce the observer’s system \((x'', y'', z'')\). The transformation is the inverse of that presented in Appendix A. It is easy to check that \( T_2^{-1}T_1^{-1} \) transforms \( \vec{r}_O \) to
\( \mathbf{r}_0'' \). Then the position of the last interaction, in the observer’s coordinate system, is given by the same transformation:

\[
\mathbf{r}_p'' = \begin{pmatrix}
\cos \phi \cos \theta x_p + \sin \phi y_p - \cos \phi \sin \theta z_p \\
-\sin \phi \cos \theta x_p + \cos \phi y_p + \sin \phi \sin \theta z_p \\
\sin \theta x_p + \cos \theta z_p
\end{pmatrix}
\]  \hspace{1cm} (B.6)

Now, the only thing we have to do is construct a grid on the \( x''y'' \)-plane of the observer’s system and place the escaping \( L \)-packets in the cells of this grid. If \( N_{ij} \) is the number of \( L \)-packets coming from the \((i, j)\) cell and \( \Delta x^{ij}, \Delta y^{ij} \) are the dimensions of the cell, then the intensity coming from this cell is

\[
I_\lambda = \frac{N_{ij} \delta L}{\Delta x^{ij} \Delta y^{ij} \delta \lambda \Delta \Omega},
\]  \hspace{1cm} (B.7)

where \( \delta \lambda \) is the width of the wavelength bin, \( \Delta \Omega = \pi \Delta \theta^2 \) the solid angle of the \( L \)-packets contributing to the observer’s direction, and \( \delta L \) the luminosity of each \( L \)-packet.

If the system has some kind of symmetry we should exploit that symmetry to improve \( L \)-packet statistics.
B.2 Spherical case

A spherical symmetric system (Fig. B.2) appears the same independent of the viewing angle and, thus, the only thing we need to know is the impact parameter $b$ of the escaping $L$-packets,

$$b = \left[ |\mathbf{r}_p|^2 - (\mathbf{r}_p \cdot \hat{k}_p) \right]^{1/2} \tag{B.8}$$

If $N_b$ is the number of $L$-packets with impact parameter between $b$ and $b + \delta b$ then the intensity coming from an annulus of radius $b$ and width $\delta b$ is

$$I_\lambda = \frac{N_b \delta L}{2\pi b \delta b \, 4\pi \delta \lambda}, \tag{B.9}$$

where $\delta L$ is the luminosity of each $L$-packet, $\delta \lambda$ is the width of the wavelength bin and the factor $4\pi$ accounts for considering $L$-packets that escape in any direction.

![Diagram](image)

**Figure B.2** Observer's view of a spherical system.
Appendix C

Photon Injection Angle

We assume a spherical system embedded in an isotropic radiation field. We inject all photons from the point \((0,0,R)\) \((R \text{ is the radius of the sphere})\). If \(N_b\) is the number of photons injected having impact parameter between \(b, \ b + db\) \((\text{or}, \text{equivalently, between angles } \omega, \ \omega + d\omega)\) \((\text{Fig. 3.3, } \omega = \pi - \theta)\) that correspond to the above impact parameters, then the intensity of radiation coming from impact parameter \(b\) is

\[
I(b) = \frac{N_b \delta L}{2\pi b \ db \ 4\pi} .
\]  

(C.1)

Setting

\[
b = R \sin(\omega) , \ db = R \cos(\omega) \ d\omega .
\]  

(C.2)

and using Eq. (3.17) we get

\[
I(\omega) = \frac{N_\omega}{N} \frac{I_0}{2\sin(\omega) \cos(\omega) \ d\omega} ,
\]  

(C.3)

where \(N_\omega = N_b\). The probability that a photon is injected at an angle between \(\omega\) and \(\omega + d\omega\), is

\[
p_\omega d\omega = N_\omega/N
\]  

(C.4)

The radiation field is isotropic, so at every angle

\[
I(\omega) = I_0
\]  

(C.5)
Thus, from Eqs. (C.3)-(C.4), we have

\[ p_\omega d\omega = 2 \sin(\omega) \cos(\omega) d\omega . \]  \hfill (C.6)

Considering that \( \theta = \pi - \omega \), thus \( d\omega = -d\theta \), \( \sin(\theta) = \sin(\omega) \), \( \cos(\theta) = -\cos(\omega) \), we get for the injection angle probability:

\[ p_\theta d\theta = 2 \cos(\theta) \sin(\theta) d\theta , \quad \frac{\pi}{2} \leq \theta \leq \pi \]  \hfill (C.7)

We can sample the distribution of injection angle \( \theta \) using random numbers. If we apply the general Monte Carlo formula (Eq. 2.1) for \( p_\theta \), we get

\[ \int_{\pi/2}^{\theta} p_\theta d\theta = \mathcal{R}_\theta \Rightarrow \theta = \cos^{-1}\left[-\mathcal{R}_\theta^{1/2}\right], \]  \hfill (C.8)

where \( \mathcal{R}_\theta \) is a random number between 0 and 1.
Appendix D

Distribution of SPH Particles in a Disk

To calculate the distance $R$ of the particle on the disk mid-plane we assume

$$\frac{M(R)}{M_{\text{disk}}} = R_1.$$  \hspace{1cm} (D.1)

We set $\omega = R^2/R_0^2$, $\omega_0 = R_{\text{disk}}^2/R_0^2$, and then substituting in Eq. (D.1), using Eq. (6.3) and Eq. (6.4), we obtain

$$
\left[(1 + \omega)^{1-(\nu/2)} - 1\right] = \left[(1 + \omega_0)^{1-(\nu/2)} - 1\right] R_1.
$$

Solving for $\omega$, we get

$$\omega = \left\{1 + R_1 \left[(1 + \omega_0)^{1-(\nu/2)} - 1\right]\right\}^{2/(2-\nu)} - 1.$$  \hspace{1cm} (D.2)

Substituting for $\omega_0$ we find

$$\omega = \left(1 + R_1 \frac{M_{\text{disk}}}{\pi R_0^2 \Sigma_0}\right)^{2/(2-\nu)} - 1.$$  \hspace{1cm} (D.3)

Finally, $R$ is calculated from the equation

$$R = R_0 \omega^{1/2}.$$  \hspace{1cm} (D.5)
Then, we generate a second random number $R_2$ to calculate the azimuthal angle $\phi$:

$$\phi = 2\pi R_2.$$  \hfill (D.6)

Thus, the $x$ and $y$ coordinates of the SPH particle are

$$x = R \cos(\phi),$$  \hfill (D.7)

$$y = R \sin(\phi).$$  \hfill (D.8)

To calculate the vertical distance $z$ of the SPH particle from the disk mid-plane we assume

$$\frac{\Sigma(R, z)}{\Sigma(R, z_0)} = R_3,$$  \hfill (D.9)

where

$$\Sigma(R, z) = \int_{-z_0}^{z} \rho(R, z)dz$$  \hfill (D.10)

Substituting for $\rho(R, z)$ (Eq. 6.18), and solving the integral, we obtain

$$\Sigma(R, z) = \rho(R, 0)z_0 \frac{2}{\pi} \left[ \sin \left( \frac{\pi z}{2z_0} \right) \right].$$  \hfill (D.11)

$\Sigma(R, z_0)$ is calculated by setting $z = z_0$ in the previous equation:

$$\Sigma(R, z_0) = \rho(R, 0)z_0 \frac{4}{\pi}.$$  \hfill (D.12)

After substituting the two previous equations in Eq. (D.9), and solving for $z$, we obtain for the vertical distance of the particle:

$$z(R) = z_0(R) \frac{2}{\pi} \sin^{-1}(2R_3 - 1),$$  \hfill (D.13)

where $z_0(R)$ is calculated from Eq. (6.13).
Appendix E

Fourier Analysis of the Structure of a Disk

We decompose the structure of the disk into a sum of Fourier components following the procedure described in Sleath & Alexander (1996). Our goal is to compare the amplitudes of different modes, and discover the existence of modes that may be difficult to discern by eye, if their amplitude is much smaller than the amplitude of the dominant mode. We use as a basis a logarithmic spiral

\[ r = r_0 e^{-m \phi / \zeta}, \]  

(E.1)

where \( m \) is the mode of the perturbation (\( m = 1 \) corresponds to a single-armed spiral, \( m = 2 \) to a double-armed spiral), \( \phi \) is the azimuthal angle of the SPH particle and \( \zeta \) is a parameter that determines the pitch angle of the spiral. The pitch angle \( \beta \) is given by:

\[ \tan(\beta) = -m / \zeta, \]  

(E.2)

The Fourier transform can be written as:

\[ F(\zeta, m) = \int_{-\infty}^{\infty} \int_{-\pi}^{\pi} \sum_{j=1}^{N} \delta(u - u_j) \delta(\phi - \phi_j) e^{-i(\zeta u + m \phi)} du d\phi = \frac{1}{N} \sum_{j=1}^{N} e^{-i(\zeta u_j + m \phi_j)}, \]  

(E.3)

where \( u_j = \ln(R_j) \) and \( R_j = \sqrt{x_j^2 + y_j^2} \). We can then determine the relative strength of each mode by plotting \( F(\zeta, m) \) against \( \zeta \) (for \( m = 1, 2, 3, 4, \ldots \)).
Appendix F

Publications


Stamatellos, D. & Whitworth, A. P. 2003, IAU Symposium, 221


Bibliography


André, P. 1994, The Cold Universe, 179


Barnes, J. & Hut, P. 1986, Nature, 324, 446


Calvet, N., Hartmann, L., & Strom, S. E. 2000, Protostars and Planets IV, 377


Ebert, R. 1955, Zeitschrift Astrophysics, 37, 217


Hartmann, L. 1998, Accretion processes in star formation, Cambridge University Press


Inutsuka, S. 1994, Memorie della Societa Astronomica Italiana, 65, 1027


Jeans, J. 1902, Phil. Trans. R. Soc. 199A, 49


Königl, A. & Pudritz, R. E. 2000, Protostars and Planets IV, 759


Larson, R. B. 2003, ArXiv Astrophysics e-prints, 6595
Mathieu, R. D., Ghez, A. M., Jensen, E. L. N., & Simon, M. 2000, Protostars and Planets IV, 703
Mestel, L. 1965a, QJRAS, 6, 161
Mestel, L. 1965b, QJRAS, 6, 265
BIBLIOGRAPHY


Stahler, S. W., Palla, F., & Ho, P. T. P. 2000, Protostars and Planets IV, 327


Whitworth, A. & Boyd, D. 2003, IAU Symposium, 221

Williams, J. P., Blitz, L., & McKee, C. F. 2000, Protostars and Planets IV, 97


