Seeing Through The Dark
Probing Structure and Processes Across Galactic Scales Using Monte Carlo Radiative Transfer

by

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Submitted for the degree of Doctor of Philosophy in Astrophysics

15/7/2013
Declaration

I, John Morrison MacLachlan, hereby certify that this thesis, which is approximately 33,000 words in length, has been written by me, that it is the record of work carried out by me and that it has not been submitted in any previous application for a higher degree.

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For my parents.
Ah, but a man’s reach should exceed his grasp,
Or what’s a heaven for?
from Andrea del Sarto by Robert Browning.
Abstract

Radiative transfer methods provide a path to uncover the intrinsic properties of astronomical objects from observations. The determination of the shape, size and brightness of many objects is complicated by the interaction of photons with the material in the intervening medium.

In this thesis I have explored the use of 3D Monte Carlo radiative transfer codes to investigate a variety of astronomical objects. A model has been created to calculate the transfer function for a simple model of the X-ray irradiated accretion disk around a massive black hole. I have reconciled the observationally derived accretion disk transfer function with a simple geometric model for the structure of the accretion disk in the active galactic nuclei Zw229-15. The results suggest that a change in the amount of flaring in the disk at \( \approx 600 \text{AU} \), possibly due to the emergence of a disk wind, can explain the observations.

By coupling a Monte Carlo photoionization code to a series of static snapshots of a numerical simulation of a star forming cloud I have been able to estimate the impact of photoionizing feedback on the stellar masses. It is estimated that the stellar mass formed over the course of the simulation is reduced by up to 38% by the action of photoionization feedback. I also illustrate the possible problems associated with stochastic sampling of the stellar initial mass function in clusters, on the number of ionizing photons produced.

I have utilized multi-wavelength data for three low surface brightness disk galaxies to show that their dusty interstellar medium has a scale height equal to that of the stellar disk. This is in contrast to the structure seen in higher mass disk galaxies and may play a role in their low star formation rates.

Collaborations

Chapter 3 of this thesis is based on work done in collaboration with I. A. Bonnell, K. Wood and J. E. Dale and submitted for publication to Astronomy and Astrophysics. The majority of the work was performed by the author. The co-author contributions to the work were as follows. I. A. Bonnell performed the original smoothed particle hydrodynamics simulations and provided the outputs for further investigation. K. Wood wrote the Monte Carlo photoionization code that was modified and applied to the data. J. E. Dale provided a set of simulations which were used to test the procedure implemented here. All co-authors provided comments on a draft of
Chapter 4 is based on work published in MacLachlan, Matthews, Wood and Gallagher, ApJ, 741:6, 2011. The majority of the work was performed by the author. The co-author contributions were as follows. L. D. Matthews provided observational data in the optical and advice on the reduction of far-infrared data. K. Wood wrote the Monte Carlo Radiation transfer code which was modified and used to model the data. J. S. Gallagher, L. D. Matthews and K. Wood provided comments and suggestions on a draft of the published work.
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I would never have made it to this point without the friendship of a great many people at the University of St Andrews. So thanks to Christine Liebig, Paul Browne and Peter Dodds for sharing an office with me at various points. Grant Miller, Joe Llama, Jack O’Malley James, David Brown, William Lucas, Pauline Lang, Craig Stark, Neil Parley and Carsten Weidner along with everyone else in the astronomy department for making this whole thing possible. Everyone at the Aberdour shinty club, especially Lisa, Katy, Ross, Doug and Fred for keeping me sane and reminding me there’s a world outside St Andrews. Thanks to Ian Taylor for his work to keep the computers running.

Finally I would like to thank my family for supporting me though the whole journey. Without my parents and my sister Katy I would not have been able to reach this point.
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At its heart astronomy is the study of light. From early naked eye observations of the stars and planets to modern observatories scanning the skies with large telescopes, light serves as the messenger which brings us information about the cosmos. The vast distances between the stars and galaxies means that the journey is often long with even the light from the nearest stars taking years to reach us. Light from the Andromeda galaxy ($\text{M31}$), nearby in cosmological terms, takes around 2.5 million years to reach us. The propagation of photons through space is not always straightforward, however. Material between a light source and an observer can scatter and absorb photons complicating the interpretation of the observations made by astronomers.

We experience these effects in everyday life as well. On a sunny day we can see the sun in the sky directly as a bright source of light. On an overcast day it can be almost impossible to locate the sun in the sky but sunlight still illuminates both the sky and the ground around us. In this case sunlight incident on the atmosphere has been scattered and absorbed by molecules and dust until it reaches the surface as an almost uniform illumination. Even the colours we see are caused by the interaction of photons with different material. Plants appear green
Chapter 1. Introduction

Figure 1.1: A sunset as viewed on Earth (left) and Mars (right). The martian image was taken by the Spirit rover (Credit: Mars Exploration Rover Mission, Texas A&M, Cornell, JPL, NASA). Due to the different composition of the atmosphere on Mars the sky appears red and becomes bluer closer to the sun in the sky. This is the opposite to what we view on Earth.

because their surfaces absorb red and blue light but efficiently reflect green light. In figure 1.1 sunsets on Earth and Mars are shown. Due to the different atmospheric compositions affecting the sunlight differently the colours seen in the sky are reversed.

From an astronomical perspective in order to be able to study the intrinsic properties of stars, planets and galaxies the radiation transfer effects due to the medium between the observer and the source must be understood. We must also strive to understand the impact of photons on the medium. Photons carry energy and so provide a mechanism to heat and cool gas and dust in space where conduction and convection can be extremely inefficient. High energy photons can ionize gas species by removing electrons while lower energy photons can excite electrons into different energy levels. Complicating matters is the fact that the interaction of photons with the medium is able to alter the way the medium interacts with the photons themselves leading to a very complex problem to solve.

1.1 The Radiative Transfer Equation

The formal equation of radiative transfer for a beam of light traversing a medium can be written as:

\[
\frac{dI_v}{d\tau_v} = -I_v + S_v
\]

(1.1)
where \( I_\nu \) is the intensity, \( S_\nu = \frac{j_\nu}{\kappa_\nu} \) is the source function and \( \tau_\nu \) the optical depth. Here \( j_\nu \) is the emissivity (erg s\(^{-1}\)g\(^{-1}\)). The optical depth along a path from 0 to some point \( x \) is given by

\[
\tau_\nu = \int_0^x \kappa_\nu \, ds
\]

with \( \kappa_\nu \) the total mass extinction coefficient (cm\(^2\)g\(^{-1}\)). In the case where \( S_\nu(\tau_\nu) = \text{constant} \) then the solution of the radiative transfer equation can be written as

\[
I_\nu = I_\nu(0) \exp(-\tau_\nu) + S_\nu(1 - \exp(-\tau_\nu)).
\]

It can be understood as the initial intensity \((I_\nu(0))\) being gradually replaced by the intensity within the medium \((I_\nu = S_\nu)\) as the optical depth increases. In the limit of \( \tau_\nu \gg 1 \) the observed intensity of the beam will just be the source function and \( I_\nu = S_\nu \).

Finding the solutions of the radiative transfer equation in astronomical objects can often be very complex. The source function is often not known in advance and can be a function of the radiation field itself and includes scattering terms. The density distributions involved in astronomical objects can be very complex and calculating the optical depth in the radiation transfer equation is often complex and time consuming. Coupled to the problems of solving equation [1.1] for a single beam of photons is the fact that objects are often composed of emitting material spread out in space. The line of sight variations between observer and source means that in essence the radiative transfer equation must be solved along many lines of sight and the results combined before comparisons to observations can be made.

**1.2 The Impact of Radiation**

As well as providing a probe of the conditions within astronomical objects radiation can play an important part in shaping their structure and evolution. Photons carry momentum and in some circumstances they are able to dynamically affect the medium they traverse. In the idealised scenario of a constant density, spherically symmetric, fully ionized accretion flow onto an isotropic point source of radiation the equation of radiation pressure can be solved to give the luminosity required for radiation to overcome gravity and halt accretion. This is known as the Eddington luminosity and is given by

\[
L_E = \frac{4\pi GMm_p c}{\sigma_T}
\]
where $G$ is the gravitational constant, $M$ is the central mass, $m_p$ the proton mass, $c$ the speed of light and $\sigma_T$ the Thompson scattering cross section for the electron. If the luminosity of the central object exceeds this value then radiation pressure will be sufficient to halt the inflow of material. This is of particular interest in the inner regions around massive black holes (see chapter 5). Although this is an idealised situation it provides an order of magnitude estimate of the maximum accretion rates in such objects.

Photoionization by high energy photons can also provide a mechanism for the radiation sources to impact their surroundings. Where the photon energy is sufficient to remove bound electrons from the atom, the gas will become ionized. The electrons which are liberated will carry away an energy that is the difference between the incident photon energy and the ionization potential (for hydrogen $h\nu - 13.6\text{eV}$) and the ionized gas will have kinetic temperatures of $8 - 10 \times 10^3\text{K}$ in most cases. This hot gas can have a significant impact on the surrounding medium. These effects are most often seen in the H II regions in sites of massive star formation and can play a role in regulating star formation in these regions.

1.3 The Monte Carlo Method

Originally conceived to solve problems in neutron scattering during the early development of thermo-nuclear weapons by utilising the speed of early computers, the Monte Carlo method has also been adapted to the task of radiation transfer. By probabilistically sampling the paths of many photons, using random numbers, the solution to the radiative transfer equation can be achieved implicitly. A full description can be found in chapter 2. The first simulations of Monte Carlo radiative transfer (MCRT) in astronomy were carried out in an effort to understand the effects of multiple scattering on observations of nebulae within the Milky Way (e.g. Mattila 1970; Witt 1977) and the method has grown in importance as the power of computers has made many more problems tractable.

Due to its flexibility and simplicity as well as astronomy, other fields have adopted MCRT to understand radiative transfer problems such as those found in atmospheric modelling (Deutschmann et al., 2011) and medical physics (Valentine et al., 2011).

1.3.1 Ray tracing

Another method widely used to calculated the transfer of radiation in astronomical environments is the ray tracing method (Kylafis & Bahcall 1987; Steinacker et al. 2013; Popescu 2013).
1.4. Concluding Remarks

et al., 2000; Xilouris et al., 1998; Misriotis et al., 2001b). It involves solving the radiative transfer equation (1.1) along a line of sight between a source and a particular position in space, in order to estimate the properties of the radiation field at that position. It can be used with analytic or spatially gridded density distributions and has proved to be flexible and efficient. As with MCRT its use has become more widespread with the advent of more powerful computers.

Ray tracing can have distinct advantages over MCRT in some circumstances. By directly calculating the radiation field for a given set of positions ray tracing can avoid some of the problems of low signal to noise which can cause large uncertainties in MCRT solutions in regions of low radiation field strength. It is also often faster to obtain a solution using a the RT method rather than the slightly more time consuming MCRT. The advantages of MCRT include the ability to treat complex geometries more easily, as often ray tracing relies on symmetry in the density profile that is not always realistic and the fact that images are produced as a by product of the simulation while in ray tracing they are not.

1.4 Concluding Remarks

In this thesis I will explore the application of 3D MCRT codes to further the understanding of processes occurring at a variety of scales. Chapter 3 focuses on the impact of photoionizing radiation from young, massive stars and its ability to reduce the stellar masses in young clusters. The clues to the structure of the dusty, cold interstellar medium in low surface brightness galaxies that can be found in far-infrared observations coupled to MCRT models are discussed in chapter 4. In chapter 5 I will examine the time resolved signature of reprocessed X-ray emission in the accretion disks around supermassive black holes to help uncover the structure of the inner disk.
Monte Carlo Radiative Transfer

In some situations it is possible to calculate the transfer of radiation through a medium analytically, although this often requires assumptions of symmetry and extent to allow the calculations of density/optical depth required. Monte Carlo Radiative Transfer (MCRT) recreates the transfer of radiation by simulating a large number of individual photons or energy packets. The path followed by each photon is determined by sampling from probability distribution functions (PDFs) which represent the physical processes at work. By utilizing a large number of photons, MCRT allows a robust picture to be built up of the emergent properties of the radiation. Unlike analytic methods complex geometries are able to be treated as well as simple ones with little increase in computational time. The accuracy of the MCRT solution will be determined by the number of photons which have been followed and consequently how well sampled the PDFs have been.

\[\text{A Monte Carlo energy packet actually represents a large number of real photons but in this thesis I will refer to energy packets as photons.}\]
Figure 2.1: An illustration of the possible paths of Monte Carlo photons emitted from a star surrounded by scattering material (grey). Some photons are able to escape the region directly while others have interacted several times before escaping.
2.1 Monte Carlo Sampling

2.1.1 Basic principles

The PDF of a variable \( x \) can be sampled using a random number between 0 and 1 (\( \xi \)) and knowledge of the cumulative distribution function. The PDF is a measure of the probability that a parameter will take on a particular value. If \( P(x) \) is the value of the PDF for variable \( x \) then the cumulative distribution function is the integral of \( P(x) \) between the lower limit and \( x \):

\[
C(x) = \int_a^x P(x) \, dx. \tag{2.1}
\]

The cumulative distribution function gives the probability that the value \( x \) will be found between \( a \) (the lower limit) and \( X \). Values can be sampled from a given PDF in the following way:

\[
\xi = \frac{\int_a^X P(x) \, dx}{\int_a^b P(x) \, dx} \tag{2.2}
\]

(with \( a \) and \( b \) the lower and upper limits of \( x \)) and the equation must be solved for the value of \( X \).

An example is the determination of \( \tau \) the optical depth that a photon should travel before interaction. The change in intensity along a beam of length \( dx \) is

\[
dI = -I\kappa \rho \, dx \tag{2.3}
\]

which has the solution

\[
I = I_0 \exp(-\kappa \rho x) \tag{2.4}
\]

for an initial intensity \( I_0 \) after traveling a distance \( x \) through a medium of constant density \( \rho \) and opacity \( \kappa \). \( \kappa \) gives the total interaction cross section (absorption and scattering) per unit mass and has units of cm\(^2\)g\(^{-1}\). The probability of a photon interacting with material between \( x \) and \( x + dx \) can be written as

\[
P(x) = (\exp(-\kappa \rho x))\kappa \rho \, dx \tag{2.5}
\]
and the cumulative probability

\[
C(x) = \int_0^x \exp(-\kappa \rho x) \kappa \rho \, dx = 1 - \exp(-\kappa \rho x) = 1 - \exp(-\tau)
\]  

(2.6)

where \(\tau = \kappa \rho x\). A random number can then be sampled and set equal to the cumulative distribution function

\[
C(x) = 1 - \exp^{-\tau} = \xi
\]

(2.7)

which can then be mapped to a value of the optical depth by inverting the equation giving

\[
\tau = -\log(1 - \xi).
\]

(2.8)

This can then be used within the MCRT code to determine a physical distance that the photon will travel by integrating through a given density distribution. In a similar way it is possible to sample the outcome of any physical process for which there is an understanding of the underlying physics, by constructing the PDF.

Often it is not possible to easily invert the PDF and in this case rejection sampling can be used to sample the PDF. Rejection sampling involves selecting pairs of values, one in the range \(x = [a, b]\) and the other in the range \(y = [0, P_{\text{max}}]\) where \(P_{\text{max}}\) is the maximum of the PDF. If \(y < P(x)\) then the value \(x\) is kept else it is rejected and a new pair of \(x\) and \(y\) values chosen. By accepting only values that fall below \(P(x)\) the PDF is built up as more values are sampled. The efficiency of rejection sampling is determined by the relative areas above and below \(P(x)\) and in some cases it may be highly inefficient, requiring a large number of samples to be drawn before one is accepted.

### 2.1.2 Random numbers

One of the features of Monte Carlo methods is the need to sample a large number of values of \(\xi\) in the range \([0:1]\). Computers are unable to produce truly random sequences of numbers and instead create pseudo random sequences based on a seed value. The sequence of “random” numbers is entirely determined by the choice of algorithm and initial seed. The random number generators \(\text{ran2}\) and \(\text{ran4}\) from Press et al. (1992) are used throughout this work.

In the case of code which has been parallelized, using the openMP\(^2\) extensions to fortran, the random number generator must be modified slightly. As the pseudo random sequence

\[^2\text{www.openmp.org}\]
2.2. Monte Carlo Radiation Transfer

MCRT is based on the concept of a Monte Carlo photon which contains a certain energy and depending on frequency, may represent a large number of real photons. Packets are tracked as they are emitted from a source and propagate through a medium. They are generally tracked until they exit the region of interest or meet another termination criteria. It is also possible to use the MCRT routines to evaluate the properties of the medium through which the photons are traveling. In the case of a dusty galactic ISM this may be the dust temperatures or the ionization structure of the gas exposed to ionizing photons. The steps involved in the journey of an individual photon are:

- The emission from a source.

- Propagation through a medium including: scattering, absorption and possible reemission.

- Binning of properties upon exiting the region of interest and evaluation of properties of the medium.

2.2.1 Emission

2.2.1.1 Location

The initial location of the photon will be dependent on the type of source involved. If the source is a well resolved star in a proto-planetary disk, then a location on the surface of the star will be selected as the point of emission. If instead the source is unresolved, say stars in the stellar disk of a galaxy, then the emission can be approximated as a large number of point sources located at a random positions within the disk. As with almost all aspects of MCRT it is possible to accommodate complex emission sources.
Chapter 2. Monte Carlo Radiative Transfer

2.2.1.2 Initial Direction

The initial direction of the photon is another source dependent quantity. The well resolved star in the previous example will have its photons emitted in an outward direction from the stellar surface at the point of emission. Unresolved point sources within a galactic disk would be simulated by emitting the photons isotropically in all directions. In general any desired initial emission distribution can be used appropriate for the situation. Cashwell & Everett (1959) provide methods to sample directions for isotropic emission and emission from a spherical surface which can be easily integrated into existing codes.

2.2.1.3 Wavelength

The starting photon wavelength (or frequency) will be sampled from a PDF appropriate for the source of interest. In astrophysical problems this will often be the spectral energy distribution (SED) of a star or stellar population. In general any arbitrary source spectrum can be easily included within the procedure. It is simply a case of acquiring the appropriate emission template in a form that can be interpreted by the MCRT codes. For some scattered light codes only a single wavelength is considered in each run to increase speed.

2.2.2 Propagation

The initial wavelength of the photon will often determine the properties of the medium through which it propagates. In the case of astrophysical dust both the opacity ($\kappa_\nu$) and albedo ($a_\nu$) of the dust are frequency dependent quantitates (the albedo in this case is simply the ratio of scattering to total opacity). $\kappa_\nu$ will be used to calculate the distance that a photon will travel through the medium before interaction. An optical depth, $\tau$, is sampled randomly (see section 2.1.1) and the physical distance the photon will travel ($L$) can then be calculated. In some circumstances, say a constant density medium, $L$ can be calculated immediately from $\tau$. However, in most environments $\rho(x,y,z)$ and the density must be numerically integrated along the photon’s direction of travel in order to find $L$. The codes used here utilize discretized density grids to aid in the calculations of $L$. The density distribution is tabulated at gridded values of $x$, $y$ and $z$ (or other appropriate co-ordinate system) and the density is assumed to be constant within each grid cell. The optical depth traversed by the photon can then be calculated by taking the sum $\kappa_\nu \sum \rho_i x_i = \tau$, where $\rho_i$ and $x_i$ are the density and distance travelled through cell $i$ respectively. The accuracy of the numerical integration is dependent on the size of the grid used. The size of the grid cells should be small enough to adequately...
2.2. Monte Carlo Radiation Transfer

resolve changes in the density, but not overly small. This is because the integration of optical
depths is generally the most time consuming process in the radiation transfer calculations.
Smaller grids slow this process as the integration takes place over a larger number of small
steps, each taking a certain amount of processor time. Advantages in this respect can often
be found by selecting the most appropriate coordinate system for the grid. Spherical and
cylindrical grids can take advantage of symmetries in the geometry to increase speed.

Once the photon has reached its interaction location it will either be scattered or absorbed.
This outcome is randomly sampled by selecting a random number ξ and if ξ > α, then the
interaction will be an absorption event, else the photon will be scattered.

In the case of scattering from astrophysical dust the photons direction (and polarization
if required) are changed by sampling from an appropriate phase function (see section
2.3.2). The methods of Chandrasekhar (1960) are used throughout this work to update the Stokes
vectors of the photon. A new interaction optical depth is sampled and the photon is tracked
as before to a new interaction point.

In absorption events the photon’s energy is absorbed by the medium. In most cases it is
required to be in radiative equilibrium and so we immediately re-emit the photon’s energy at a
new frequency, determined by the properties of the absorber. Based on the new frequency κν
and αν (and any other frequency dependent properties) are updated and the photon continues
its journey. The photons may be scattered or absorbed multiple times before they finally leave
the region of interest.

2.2.3 Exit

As the photons leave the grid they can be binned in direction and frequency to produce images
and spectra. Images can be produced by locating an image plane exterior (or interior) to the
simulation and projecting photons which leave the simulation in an appropriate direction into
the plane. In this way an image is built up photon by photon as the simulation runs. The S/N
of the results is dependent on the number of photons that have been used in the simulation.
A larger number of photons will better sample the PDFs involved and so reduce noise due
to under-sampling. The errors on binned properties in MCRT obey poisson statistics and so
the error on each bin $\sigma_i \propto 1/\sqrt{N_i}$, where $N_i$ is the number of photons in bin $i$. In order to
produce high quality images and spectra it will often be necessary to follow the propagation
of at least $10^6$ individual photons and in some cases many more.

Any properties of interest within the grid can also be calculated at this point. If the
temperature of the dust within the grid cells is to be calculated (see section 2.4) then it can be estimated at this point in the simulation. Some properties of the grid, such as the ionization fraction, can affect the properties of the medium that the photons encounter. In this case it is necessary to iterate the simulation to converge on the equilibrium solution.

2.2.4 Computational Tricks

2.2.4.1 Forced first scattering

The concept of forced first scattering (Cashwell & Everett, 1959; Witt, 1977) can be very useful in increasing the efficiency of calculations in regions of low optical depth. If $\tau_1$ is the total optical depth from a photon’s source location to the edge of the region of interest, then each photon is forced to interact at an optical depth $\tau < \tau_1$ by

$$\xi = \frac{\int_0^\tau e^{-\xi} d\xi}{\int_0^{\tau_1} e^{-\xi} d\xi} = \frac{1 - \exp(-\tau)}{1 - \exp(-\tau_1)}$$

(2.9)

$$\tau = \ln(1 - \xi[1 - \exp(-\tau_1)])$$

(2.10)

To correct the unphysical situation of every photon scattering at least once the weighting of the photon is changed from 1 to $W = 1 - \exp(\tau_1)$. In this way all photons contribute to the scattered light component, even in the case of low optical depth. The remaining weight, $W_0 = \exp(-\tau_1)$, can also be projected directly out of the system and into any images or spectral bins it intersects. To understand the motivation behind this method it is simply necessary to remember that each MCRT photon actually represents a large number of real photons and in reality a fraction $W_0$ of these would have escaped directly with the remainder indeed being scattered before escape.

2.2.4.2 “Peeling-off”

Yusef-Zadeh et al. (1984) introduced the concept of “peeling-off” where at each interaction location the probability of the photon being scattered toward the observer and the subsequent photon reaching the observed is calculated. A photon weighted by this probability is then projected into the observing plane. The original photons weight is reduced and it continues on its normal probabilistic path. This technique has the advantage that high S/N observations can be made at one particular observer location utilizing a smaller number of photons than standard methods would require. However, only one observer location can be used per run
2.3. Scattering

and so if multiple observations are required then the entire simulation must be re-run. Peeling-off is often combined with forced first scattering to quickly compute images in low optical depth simulations.

2.2.4.3 Calculating the mean intensity

Lucy (1999) introduced a method for speeding the computation of the mean intensity within a radiative transfer calculation. Here instead of a photon only contributing to the calculation of the mean intensity if it is absorbed in a cell the estimator

\[ J_i = \frac{\varepsilon}{4\pi \Delta t V_i} \sum I_i, \tag{2.11} \]

is used. Where \( \varepsilon \) is the energy of each photon, \( \Delta t \) is the time interval of the simulation, \( V_i \) the volume of cell \( i \) and the sum is over the path lengths of all photons that passed through cell \( i \) during the simulation. In this way all photons that pass through a cell contribute to the mean intensity and the computation is significantly speeded up.

2.3 Scattering

When a photon is scattered during an interaction then it is assumed that only its direction is changed and its wavelength remains constant. It is then necessary to calculate the new direction of travel for the photon based on the initial direction and the material which the photon encountered.

2.3.1 Isotropic scattering

Isotropic scattering refers to scattering in which the new direction of travel is selected uniformly from all directions. In choosing a new direction for the photon it is simply a matter of sampling a location on a unit radius sphere and the routines of Cashwell & Everett (1959) can be utilized to achieve this simply.

2.3.2 Dust Scattering

In the case of scattering from astrophysical dust the Henyey-Greenstein scattering phase function (Henyey & Greenstein, 1941) is used to calculate the scattering angle \( \theta \):

\[ p(\theta) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - 2g \cos(\theta))^{3/2}}. \tag{2.12} \]
Chapter 2. Monte Carlo Radiative Transfer

This function depends on the single parameter $g$ to determine its behavior. $g = 0$ represents isotropic scattering while $g = -1$ and 1 give backward and forward scattering respectively. The function can be expressed in terms of $\mu = \cos(\theta)$ and inverted to yield:

$$\mu = \frac{1}{2g} \left( 1 - g^2 - \left( \frac{1 - g^2}{1 + 2g\xi - g} \right) \right), \quad (2.13)$$

to allow sampling.

2.4 Dust Emission

2.4.1 Astrophysical Dust

Dust from an astrophysical perspective can be described as small (sub-micrometer) particles which are efficient at scattering and absorbing light. Dust can be found in almost all astronomical environments in which conditions allow its formation/survival, from around young stars to galaxies in the early universe (Rucinski [1985], Lapi et al. [2011], Dent et al. [2013]). Due to the ubiquitous nature of dust it is believed to be composed of condensations of the most abundant metals found in the ISM. Carbonaceous grains, such as graphite, as well as silicate grains and other refractory minerals have been proposed to explain the optical properties of dust (Mathis et al. [1977], Mezger et al. [1982], Weingartner & Draine [2001]). The rise in the extinction seen between the UV and near-IR suggests that the dust grains should have a wide range of sizes (Draine [2009]). Polycyclic aromatic hydrocarbons molecules (PAHs) have also been identified as an important constituent of interstellar dust and they contribute a number of emission features in the mid-infrared.

By adopting a composition, either a single substance or a mixture, a size distribution can be inferred by fitting the observed extinction properties of interstellar dust (see figure 2.2) simultaneously with the emission seen from galactic cirrus clouds. The average interstellar extinction curve is plotted in figure 2.2 using data from Whittet (1992). The properties of the curve can change when observations of different regions and along different sight lines are used with some features being absent in a given direction. A number of authors have proposed dust models based on different compositions and size distributions based on observations of the Milky Way and other nearby galaxies (e.g. Mathis et al. [1977], Weingartner & Draine [2001], Draine & Li [2007, 2001], Kim et al. [1994]). Unfortunately it has been found to be a degenerate problem with many different compositions and size distributions able to fit the observed extinction and emission properties (Zubko et al. [2004]).
2.4. Dust Emission

Figure 2.2: The average extinction curve for the Milky Way. Data from table 3.1 in Whittet (1992).

The interstellar dust is thought to be a combination of grains which formed in stellar processes and those which have formed directly in the ISM. Dust grains may form in the cool dense winds of low mass AGB stars (Ferrarotti & Gail 2001), be expelled during the formation of a planetary nebula (Stanghellini et al., 2007) or even during supernovae explosions (Sugerman, 2006; Ercolano et al., 2007). Given an appropriate seed particle dust grains may also grow within the dense regions of the ISM itself. In fact it is likely that a majority of the mass in dust grains was grown in the ISM rather than originating in stars (Draine, 2009). This is because grain destruction in the ISM by sputtering in supernovae shocks and other processes can destroy dust grains at a faster rate than it is believed that they are supplied by stellar processes. Hence, dust grain growth in the ISM is thought to provide a mechanism to maintain the observed dust masses and this has been supported by observational findings (Grootes et al., 2013; Dunne et al., 2011).
Chapter 2. Monte Carlo Radiative Transfer

2.4.2 Large Grains

When a photon packet is absorbed by a large dust grain in a simulation the absorption and re-emission are treated by assuming radiative equilibrium and that the grains are in local thermodynamic equilibrium (LTE). Absorption by VSG’s and PAH’s does not make these assumptions and the treatment in this case is discussed in 2.4.3. Radiative equilibrium describes the situation when all of the energy transport in the system is by radiation. In this case the total energy absorbed by a cell must also be emitted by the cell. The condition of radiative equilibrium in LTE is that (Mihalas, 1978):

\[
\int_0^\infty \kappa_\nu B_\nu(T) d\nu = \int_0^\infty \kappa_\nu J_\nu d\nu
\]  

(2.14)

where \(\kappa_\nu\) is the opacity, \(B_\nu(T)\) the Planck function for temperature \(T\) and \(J_\nu\) the mean intensity. The Planck function is

\[
B_\nu(T) = \frac{2h\nu^3}{c^3} \exp\left(\frac{h\nu}{k_B T}\right) - 1
\]  

(2.15)

Hence the local temperature in a cell is determined by the mean intensity of the radiation field within the cell.

Bjorkman & Wood (2001) introduced the frequency distribution adjustment (FDA) method for re-emitting photons from dust in radiative equilibrium. Traditional techniques require iteration to correctly calculate the temperature and emergent spectrum from a system. The method of FDA does away with the requirement to iterate to a solution and so is more time efficient than traditional methods. Baes et al. (2005) investigated the generality of FDA and found that it provided a robust estimate of the frequency distribution but noted that it would fail under certain circumstances, most notably in the treatment of small dust grains that are not in radiative equilibrium (see section 2.4.3).

When a photon packet is absorbed by dust within a cell the new temperature of the cell must be calculated. This is achieved for LTE dust grains by equating the absorbed and emitted energies resulting in the formula

\[
\sigma T^4 = \frac{N_i L}{4N_i \kappa_p(T)m_i}
\]  

(2.16)

where \(L\) is the total luminosity, \(N_i\) the total number of photon packets, \(N_i\) the number of photon packets absorbed by cell \(i\), \(\kappa_p(T)\) is the Planck mean opacity and \(m_i\) is the mass within
cell $i$. As the temperature of the cell has changed it means that all previous photons emitted from the cell have been emitted using the previous emissivity $j'_\nu = \kappa_\nu B_\nu(T - \Delta T)$ where $\Delta T$ is the change in temperature. In the FDA approach the energy will be emitted from a frequency distribution that corrects the previously emitted spectrum to the new cell temperature. To do this the emissivity should be:

$$\Delta j_\nu = j_\nu - j'_\nu = \kappa_\nu (B_\nu(T_i) - B_\nu(T_i - \Delta T)) \tag{2.17}$$

which can be seen as the shaded region in figure 2.3. Assuming $\Delta T$ is small then $\Delta j_\nu = \kappa_\nu \Delta T (dB_\nu/dT)$ and $\Delta j_\nu$ is always positive as $\Delta T > 0$ and $B_\nu(T)$ is a monotonically increasing function of $T$. We can then sample the new photon frequency $\nu$ from $\Delta j_\nu$ so that it corrects the previously emitted photons to the new cell temperature.

The result of this FDA approach to the radiative equilibrium grains is that the emergent spectrum at the end of the simulation is correct for the temperature distribution at the end of the simulation, without the need for iteration.

### 2.4.3 VSG’s and PAH’s

Very small grains (VSGs) and PAHs are an important source of emission in the mid-infrared ($5-40\mu m$) but their complex nature can cause problems when including their effects in MCRT codes. In contrast to the radiative equilibrium temperatures seen in the large dust grains small dust grains and PAH molecules do not reach equilibrium temperatures. The absorption of a single photon can cause spikes in the temperature of the grains as the photons carry an energy that is comparable to the energy content of the grain itself. As the timescale for small grain interaction with a photon is much longer than the cooling timescale for the grain it will tend to go through a series of temperature spikes rather than attaining an equilibrium. In general the observed spectra of small grains and PAH molecules in astrophysical environments is a complex combination of both continuum emission and spectral features produced as the grains/molecules radiatively de-excite.

To treat the effects of VSGs and PAHs within the MCRT code the opacity encountered by a photon is split into different parts. Upon reaching an absorption point the probability that the photon will interact with grain type $j$ is:

$$P_j = \frac{\rho_j \kappa_j}{\sum \rho_i \kappa_i}, \tag{2.18}$$
the emissivity at the old cell temperature (photon packet. The spectrum of the previously emitted packets is given by previous emissivity where energy so that the heating always balances the cooling.

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The total energy that should be radiated frequency distribution corresponding to the previous tem-

perature, The previous photons emitted from the cell have been emitted with the spectrum of the lower curve, which is now incorrect for the new cell temperature. In order to correct the previous spectrum to the new

procedure statistically reproduces for

distributed the reemitted packets. Normalizing this shape of This procedure statistically reproduces for

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the distribution of the reemitted packets. Normalizing this shape of The procedure statistically reproduces for

emitted spectrum, we immediately reemit the packet (to

Figure 2.3: The frequency distribution prior to and after the absorption of a photon. The emissivity \( J_\nu = \kappa_\nu B_\nu \) is shown before the absorption as the lower curve and after in the upper curve. The previous photons emitted from the cell have been emitted with the spectrum of the lower curve, which is now incorrect for the new cell temperature. In order to correct the previous spectrum to the new one we must emit a photon using the “difference spectrum” (shaded area). Figure from Bjorkman & Wood (2001).
where there are $i$ different grain species. We can then simply sample a random number to determine the species of grain that the photon has interacted with. In the case of large grains we proceed as described in \[2.4.2\]. If the photon has interacted with a small grain then we proceed somewhat differently. Using the method of Wood et al. (2008) the photon is re-emitted with a frequency sampled from a pre-computed emissivity table from the calculations of Draine & Li (2007). Draine & Li (2007) have computed the emissivity of a realistic VSG/PAH mixture under a range of values for the mean intensity and a template for the mean intensity appropriate for the cell under investigation is chosen and used to sample the new frequency. As we require the mean intensity for this calculation we have to iterate the calculation to converge the mean intensity. Initially during the first iteration all cells have a value for the mean intensity equal to the value found by Mathis et al. (1983), and in subsequent iterations the value previously calculated for the cell is used. The mean intensity in the simulation is found to converge quickly due to the low fraction of photons that are processed by the VSG/PAHs and requires at most three iterations (Wood et al., 2008). The code also makes use of the methods of Lucy (1999) to speed the computation of the mean intensities (see \[2.2.4.3\]).

Grains larger than 200Å are treated as being in thermal equilibrium while smaller grains are taken to be heated transiently and processed as above. The cutoff is motivated by the fact that most grains achieve radiative equilibrium temperatures above this size (Draine & Li, 2007). The emissivity of the VSG/PAHs is also taken to be a function of only the mean intensity of the illuminating radiation field and not its shape. All VSG/PAHs templates are illuminated by a spectrum appropriate for the local interstellar radiation field (\(\Sigma\)) but scaled to higher or lower intensities.

\[2.5\] Photoionization

In order to calculate the photoionization of gas exposed to a source of ionizing radiation during its evolution we use the photoionization methods described in Wood & Loeb (2000) and extended by Wood et al. (2010). The routines are based on the work of Wood & Reynolds (1999) which have been modified to take into account the effects of hydrogen-only photoionization.

The techniques employ a simplified description of the photoionization problem by breaking the radiative transfer problem down into a description involving only two wavelengths. Photons in the simulation can be one of two different types: direct or diffuse. Direct photons have been emitted directly from the ionizing source while diffuse photons represent the
diffuse radiation field produced by the absorption of a direct photon followed by subsequent reemission as an ionizing photon. All photons in the simulation encounter an average opacity as they propagate which is given by
\[ n_{H_0} \bar{\sigma} + n_H \sigma_{dust}, \]
where \( n_{H_0} \) is the number density of neutral hydrogen, \( \bar{\sigma} \) is the flux averaged cross section and \( \sigma_{dust} \) gives the dust cross section per hydrogen atom (i.e. \( \text{cm}^{-2}\text{H}^{-1} \)). \( \sigma_H \) is the total hydrogen density and we assume that the dust is still present even if the hydrogen has been ionized.

Two different flux averaged cross sections are considered depending on whether a photon is direct or diffuse. The cross section for direct photons is averaged over the flux
\[ \bar{\sigma} = \frac{\int \nu \sigma \, d\nu}{\int F \, d\nu}, \]
where \( F \) is the source ionizing spectrum, \( \nu_0 \) is the frequency of the Lyman edge and \( \sigma \) is the absorption cross-section for Hydrogen. In the case of the diffuse ionizing spectrum the photon energies are strongly peaked at just above 13.6eV and so we set the cross section for the diffuse photons to the hydrogen cross-section just above 13.6eV, \( \bar{\sigma} = 6.2 \times 10^{-18} \text{cm}^{-2}. \)

The dust opacity is taken to be \( 1.3 \times 10^{-22} \text{cm}^{-2}\text{H}^{-1} \) which is a reasonable value for silicate grains at the wavelengths considered (Mathis & Wood, 2005).

Once a direct photon has been emitted and allowed to propagate to its absorption location it will then be re-emitted as either a a diffuse ionizing photon with energy \( E > 13.6\text{eV} \) or a non-ionizing photon with \( E < 13.6\text{eV} \). To calculate the probability of the photon being re-emitted as a diffuse photon we calculate the ratio of the energy in the diffuse ionizing spectrum to the total energy. Here this is simplified for the case of hydrogen only gas to the ratio of the recombination coefficient to the ground state (the only route to re-emit an ionizing photon) to total recombination coefficient to all levels. So \( P = \alpha_1/\alpha_A = (1 - \alpha_B/\alpha_A) \), where \( \alpha_1 \) is the recombination coefficient to the ground state, \( \alpha_A \) is the recombination coefficient to the all states (CASE A) and \( \alpha_B \) is the recombination coefficient to the excited states (CASE B).

The values for the recombination coefficients are taken from Osterbrock & Ferland (2006) for gas at \( 10^4K \) \( (\alpha_A = 4.18 \times 10^{-13}\text{cm}^3\text{s}^{-1} \) and \( \alpha_B = 2.59 \times 10^{-13}\text{cm}^3\text{s}^{-1} \) resulting in a value of \( P = 0.38 \). Hence we can simply sample a random number and if \( \xi < P \) the photon will be reemitted as a diffuse ionizing photon else it will be reemitted as a non-ionizing photon. In the case of non-ionizing photon emission we simply terminate the photon at this point.

As the direct and diffuse ionizing photons are propagated in the simulation we require to calculate the mean intensity within each cell in order to later calculate the ionization fractions
throughout the simulation. We utilize the methods of Lucy (1999) as described in 2.2.4.3 to speed the calculation of the mean intensity. Once all photons have been run through the simulation we are in a position to compute the ionization fraction of each cell from the photoionization equation:

\[ n_{H_0} \int_{v_0}^\infty \frac{4\pi J_\nu}{h\nu} \sigma_\nu \, dv = \sigma_A n_e n_p, \tag{2.20} \]

where the integral over all frequencies is approximated in our description with only two frequencies as:

\[ \int_{v_0}^\infty \frac{4\pi J_\nu}{h\nu} \sigma_\nu \, dv = \frac{Q(H_0)}{N} \frac{\Sigma l}{V} \bar{\sigma}, \tag{2.21} \]

where \( Q(H_0) \) is the number of photons able to ionize hydrogen. If we define the neutral fraction \( f_n = \frac{n_{H_0}}{n_{tot}} \), then we can re-express equation 2.21 as a quadratic and solve for the neutral fraction within each cell. This is done for a sufficient number of iterations to converge the ionization fractions within the cells. Initially all cells are taken to be fully ionized and photons see little opacity and so are able to freely travel though the simulation. The neutral fractions are then able to relax “up” to their equilibrium state. This is preferable to assuming that the simulation is completely neutral and provides much quicker convergence of the neutral fractions.

The output of the code is an estimate of the neutral fraction for every grid cell in the original input density distribution. This can then be used to compute the distribution of ionized gas within the simulation.

### 2.6 Time Resolved Response

The time resolved response in a MCRT simulation can be estimated by calculating the travel time for each photon and introducing an additional time dimension to the observed properties. The travel time for each photon can be calculated by maintaining a running total of the distance traversed by the photon as it propagates through the medium. This is easily achieved as a by-product of the optical depth integrations carried out during the simulations. For the purposes of this work it is assumed that any interactions, be they scatterings or absorptions and reemissions, are instantaneous and the distance travelled uniquely determines the travel time. In addition to the distance travelled through the grid we also include the distance from the photons final position to the image plane. In this way the travel times calculated will be those measured by a distant observer.

Calculating the travel time from the distance can be achieved simply by \( t = \frac{d}{c} \) where
Chapter 2. Monte Carlo Radiative Transfer

$t$ is the time, $d$ the distance and $c$ the speed of light. Images are then binned in the time dimension as well as space, producing a time series of images.
3.1 Introduction

Star formation is one of the most fundamental processes in the universe. It is responsible for transforming the primordial gas of the early universe into the wide and diverse range of stars that are seen in the present day universe and enriching the gas with the elements necessary for the formation of planets and life. It is a process that has been ongoing for a large fraction of the history of the universe, from the early stars which helped to re-ionize the universe after the cosmic “dark ages” (Ciardi & Ferrara, 2005) to current star formation that is observed in the local galactic neighborhood, such as in the Orion star formation region (Bally et al., 1998). Despite this the exact nature of the star formation process has remained somewhat unclear.

The main sites of star formation are the molecular clouds found primarily associated with the spiral arms in our own galaxy and also observed in many external galaxies. These clouds are massive ($M = 10^4 - 10^6 M_{\odot}$) and are formed primarily of cold $H_2$ gas which is rich in
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molecular chemistry. As well as widely ranging in size from a few to a few tens of parsecs, molecular clouds are observed to be highly structured on many scales with dense clumps of high density. Molecular clouds are normally cold (10 – 20K) and composed of dense (>\(10^2\)cm\(^{-3}\)) gas. Due to the lack of accessible H\(_2\) emission, molecular gas is generally traced using rotational transitions of CO which can be excited at the low temperatures found in the dense clouds.

It is in the highly structured, very dense cores of molecular clouds that star formation occurs. Here local densities can reach \(10^4 – 10^6\)cm\(^{-3}\) but normally only within a few percent of the clouds total volume ([Kato et al., 1999].

Studies of young stellar objects and young clusters associated with molecular clouds have revealed that the star formation efficiency is only a few percent ([Myers, P. C. et al., 1986] and this is a pivotal result as most of the material within molecular clouds appears to be not forming stars, rather than the other way around.

The process by which individual stars form in the dense cores is thought to proceed via gravitational collapse, opposed by thermal pressure, magnetic effects and turbulent motions. The cloud mass associated with the margin of stability can be crudely estimated applying the virial theorem to a constant density spherical cloud. This mass is usually referred to as the Jeans mass \((M_j)\) and is given by:

\[
M_j = \left(\frac{5kT}{G\mu m_H}\right)^{3/2} \left(\frac{3}{4\pi\rho}\right)^{1/2},
\]

where \(\mu\) is the mean molecular weight, \(m_H\) the mass of hydrogen, \(k\) the Boltzmann constant and \(T\) the temperature. For typical values of the density and temperature of molecular clouds \((n = 100\text{cm}^{-3}, T = 20\text{K})\) the thermal Jeans mass is \(M_j \approx 160M_\odot\) which is much less than the mass of a typical cloud. Hence a simple argument reaches the conclusion that giant molecular clouds (GMCs) should be globally unstable to collapse and form stars on a timescale comparable to the free fall time (\(\sim 3.4 \times 10^6\) yrs for typical GMC densities). If all GMCs in the galaxy were forming stars on this timescale then the star formation rate (SFR) of the galaxy would be \(\approx 250M_\odot\text{yr}^{-1}\) ([Bodenheimer 2011] which is a factor \(\sim 100\) larger than the observed rate ([Smith et al., 1978]; [Robitaille & Whitney, 2010]). There must therefore be additional support opposing gravitational collapse as well as thermal pressure as assumed in a basic analysis.

Magnetic fields provide one such possibility. The magnetic field in a molecular cloud can
3.1. Introduction

Figure 3.1: CO maps of several spiral galaxies showing molecular gas tracing the large-scale spiral structure. It is the dense molecular gas which is associated with ongoing star formation. Credit: Peter Teuben, CARMA.
be estimated by observing the Zeeman splitting of molecular absorption lines (such as the OH ground state transition at 1665.4MHz) and it has been found that most molecular clouds possess magnetic fields which place them very close to or in excess of the critical value to be supported against collapse \cite{Crutcher99,Sarma13,Bourke01} in clouds from $\sim 0.02 - 3$pc. So magnetic fields provide a mechanism for slowing the star formation but not preventing the collapse entirely.

Highly supersonic turbulent motions are also likely important to the star formation process. Observations of the molecular line widths in clouds often show molecular velocities of a few $\text{km s}^{-1}$. The thermal sound speed for the clouds at temperatures of $\sim 20\text{K}$ is only $c_s = \left( \frac{\gamma kT}{m_H} \right)^{1/2} \approx 0.3\text{km s}^{-1}$ and so the turbulent motions are supersonic. Turbulence can be described as highly chaotic and stochastic variations in the velocity field within a molecular cloud. It is believed that energy is fed into the system on the largest scales and then “cascades” down to the smaller scales. The large turbulent velocities will prevent the collapse of the gas except in dense, localized, regions where the density is sufficiently increased for a period of time. This picture leads to a view where star formation is an inefficient process, only occurring when a shock can increase the density and it will be controlled by the properties of the underlying velocity field.

Because the turbulent motions within the molecular cloud will dissipate over time some driving mechanism is required \cite{MacLow98}. Mechanisms such as magnetic driving \cite{Sellwood99}, supernova \cite{Hill12}, stellar winds \cite{MacLow04}, expanding HII regions \cite{Matzner02} and gravitational instabilities \cite{Wada02} have all been suggested. However, it is also possible that no driving is necessary. If molecular clouds are transient, short lived, objects which are globally unbound then no driving mechanism may be required. An initial input of turbulent velocity, or energy, may be enough to sustain the turbulent velocities for the relatively short lifetimes of molecular clouds. Simulations have suggested that molecular clouds may be formed out of the shocked gas flows of lower density clouds within the potential of spiral arms \cite{Bonnell06}. If the molecular clouds survive for only a short time before dispersing then the turbulent velocities can be caused by the initial formation of the cloud in the shock.

A protostar can form in the central dense region of the core, possibly surrounded by an accretion disk. As a molecular cloud normally contains many dense cores, each of which can also fragment into additional sub cores, young stars and protostars are normally found within
clusters rather than in isolation. Lada & Lada (2003) estimate that 70% of stars are formed in cluster environments and this fraction may be higher for high mass stars. Clusters are important for studies of stellar evolution as the population can generally be assumed coeval with all stars being of the same age.

Observationally the sites of star formation are often difficult to observe as they can be highly obscured. The dense gas and associated interstellar dust enshroud the sites of star formation and high attenuation makes visual observations of the inner regions of the cloud very challenging. Observers must then look to the longer infrared, sub-mm and radio wavelengths which can penetrate the obscuring dust to probe the very heart of the star formation process (Wood & Churchwell, 1989; Dunham et al., 2006; Rivera-Ingraham et al., 2013).

Although the star formation process is ubiquitous it is nevertheless a slow process by human standards taking of order $\sim 10^5$ yrs to progress. Little evolution can be observed...
Chapter 3. Photoionizing Feedback in Molecular Clouds

within individual objects over the course of decades and so analytical and numeric models of star formation must be utilized to fully understand its intricacies. Early works provided insights into the important physical processes occurring and their timescales. The advent of computers allowed the numerical models to provide additional insights. They allow us to encode our understanding of the physical processes occurring within star formation (SF) regions and follow the evolution of the gas as it evolves under their influence (Larson 1969; Boss & Bodenheimer 1979; Bate et al., 2003; Bonnell et al., 2011; Vazquez Semadeni et al., 2007).

The formation of massive stars in GMCs is likely to often have a profound impact on the structure and future evolution of the cloud. Feedback from young, massive stars can have a significant impact on their surroundings, from tens of AU to several kpc (Hollenbach et al., 2000; Whitworth, 1979; Franco et al., 1994; Tenorio-Tagle, 1979) and is often invoked to regulate SFRs (Ostriker et al., 2010; McKee, 1989). The emission of high frequency photoionizing (PI) photons from young, massive stars into the surrounding neutral gas may have a significant impact on the future evolution of both the gas and stars. On small scales the action of PI photons from the central star is a principal mechanism for the dispersal of circumstellar disks around massive stars (Hollenbach et al., 2000; Bally et al., 1998). In dense cluster environments the photo-evaporation by an external source can cause the destruction of circumstellar disks, even around low mass stars, if the cluster is large enough to host an O or B star.

The action of nearby massive stars may be sufficient to disrupt the star formation process within the molecular cloud by effectively removing the reservoir of available gas and starving future star formation. It is thought that a large fraction of stars form in clusters embedded within molecular clouds rather than in isolation (Lada et al., 1991; Lada & Lada, 2003) and so the action of massive stars can strongly impact the growth and evolution of other cluster members. In the case where ionized gas becomes unbound and is effectively able to be removed from the cluster (e.g. a blister HII region) then it can lead to the complete disruption of the stellar cluster (Hills, 1980; Baumgardt & Kroupa, 2007; Goodwin & Bastian, 2006).

In addition to limiting the ability of stars to accrete neutral gas the influence of ionized gas is also likely to promote the formation of new stars. This may be due to the “collect and collapse” mechanism in which neutral gas is swept up by the advancing ionization front and forms unstable clumps which undergo collapse and form stars (Whitworth et al., 1994).
3.1. Introduction

Figure 3.3: Schematic of the collect and collapse model of triggered star formation. As an ionization front sweeps up gas some regions can become gravitationally unstable and themselves collapse to form stars. Credit: Deharveng & Zavagno

[Elmegreen & Lada, 1977; Dale et al., 2007a]. Alternatively additional star formation may be caused by the radiatively driven implosion of pre-existing stable gas clumps which exist in the structure of the undisturbed molecular cloud (Kessel-Deynet & Burkert, 2003; Bisbas et al., 2011).

It has been shown by previous authors (Dale et al., 2005; Krumholz et al., 2005; Dale & Bonnell, 2011) that the underlying structure of the neutral gas in which an ionizing source is embedded will have a strong influence on the propagation of ionizing photons. If the source is accreting down high density accretion flows then these will strongly inhibit the flow of PI photons in certain directions and effectively shield portions of the surrounding medium from the direct effects of the source. The ionizing photons will more easily escape into the low density cavities of the surrounding gas and the accretion flows can remain mostly neutral.

In order to model the evolution of a molecular cloud the methods of smoothed particle hydrodynamics (SPH) provide a powerful tool. The large density contrasts involved in the gas dynamics can be easily handled due to the Lagrangian nature of SPH codes but traditional methods for evaluating the transfer of radiation in such environments are best suited to Eulerian schemes, where the density can be more simply integrated along directions of photon travel. Several authors have implemented radiation transfer methods in SPH simulations to
Chapter 3. Photoionizing Feedback in Molecular Clouds
treat PI radiation (e.g. [Dale et al., 2005, 2007b; Gritschneder et al., 2009; Kessel-Deynet & Burkert, 2000]). While methods exist to implement radiation transfer in SPH codes many simulations still neglect such effects for the sake of computational speed and complexity.

MCRT methods have been used to calculate the ionized gas fraction at discrete times throughout the SPH simulation and apply corrections to the accreted gas masses. The advantage of this method is that there is no additional computational overhead during the SPH simulation as all photoionization calculations are performed once the simulation is completed. In this way the reduction in star formation rates and efficiencies caused directly by PI feedback can be characterized.

The aim of this work is to provide an estimate of the first order effects of feedback from PI radiation on the star formation efficiency in a large star forming complex in the spiral arm of a disk galaxy.

3.2 SPH Simulations

The starting point for the investigation are the SPH simulations carried out by Bonnell et al. (2013). These were designed to track the small scale star formation process as well as the large scale evolution of the interstellar medium on galactic scales. Three simulations were carried out: the first a large scale simulation of an annulus within a galactic disk, the second a higher resolution re-simulation of a dense cloud which formed in the previous simulation, and the last a high resolution self-gravitating simulation to follow the star formation process. The properties of the three simulations can be found in table 3.1.

The galactic scale simulation was carried out with a mass of $\sim 10^9 M_\odot$ of gas located within an annulus between 5 and 10 pc within a galactic disk. The gas was evolved for 370 Myrs under the influence of a four arm spiral potential (Dobbs et al., 2006). Initially the gas was given a uniform temperature of $10^4$ K and then it was allowed to cool following the treatment of thermal physics described in Bonnell et al. (2013) which produced a complex, multiphase, interstellar medium. Dense clouds were formed as warm gas flowed through spiral shocks much as GMCs are thought to form within our own galaxy.

A single dense cloud formed during this process was then selected by eye for a higher resolution re-simulation (the Cloud simulation). The particles contained in the cloud were traced back through $\approx 1/4$ of a galactic orbit and then each was split into 256 lower mass particles, in order to simulate the formation of the original cloud with greater resolution. The rest of the global annulus simulation was not included in the re-simulation and its effects were
accounted for with appropriate boundary conditions (see Bonnell et al., 2013). This Cloud simulation was then evolved for 54Myrs as the gas flowed through the shock and reproduced the initial cloud in higher resolution.

The high resolution cloud was then re-simulated with the inclusion of self-gravity (Gravity simulation). Within the Gravity simulation the star formation process is tracked using sink particles (Bate et al., 1995). In this case when a region of gas becomes self gravitating the mass and momentum of the particles is collected into a sink particle which interacts gravitationally with the rest of the simulation. It may accrete additional mass during the remainder of the simulation. The sink particles are a way of tracking star formation without the difficulties involved in treating the very high densities found during the collapse phase and possible resolution issues. This allows the fragmentation and collapse of the gas to be tracked as it forms stellar clusters. Due to the mass resolution of the Gravity simulation the sinks that form are too massive to be considered individual stars but are instead better described as stellar clusters. The lowest mass clusters that form are $\approx 11\, M_\odot$ in mass, limited by the mass resolution and the details of the formation of the sink particles (Bonnell et al., 2013). A graphical representation of the three simulations and how they relate to one another can be found in figure 3.4.

The Gravity re-simulation is approximately 250pc in size and contains $\approx 1.7 \times 10^6 M_\odot$ of gas. During the time evolution of the Gravity simulation the properties of each SPH particle (position, velocity etc.) were printed out to file at several times. It is on these outputs the analysis regarding the effects of photoionization on the star formation process is based.

During the formation and evolution of the SPH sink particles a 100% efficiency for star formation is assumed, so that all gas that is accreted onto sinks is completely converted into stars. Star formation efficiencies are unlikely to be this high and evidence suggests that they are in the region 25 – 50% (Olmi & Testi, 2002) which would lead to the star formation rates being upper limits by a factor 2 – 4.

From the work of Bonnell et al. (2013) with the original, non-ionizing simulations, it is found that the global star formation rate surface densities can be explained by the heating of gas within a spiral shock coupled to the cooling rates in the interstellar gas.

### 3.3 Monte Carlo Photoionization Code

The Monte Carlo photoionization (MCPI) code described in Chapter 2 is used here to investigate the effects of ionizing feedback within the SPH simulations. The code has been modified...
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3.3. Monte Carlo Photoionization Code

Figure 3.4: An illustration of the initial SPH simulations. The global disk simulation (left) represents an annulus of material within a galactic disk. The formation of a dense cloud within the global simulation is then re-simulated in higher resolution in the Cloud simulation (centre). Finally in the Gravity (right) simulation self-gravity is introduced and the star formation progresses.
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to accept the input from the individual SPH density dumps.

3.4 Ionizing Photon numbers

In the Gravity simulation the mass resolution means that sink particles do not represent individual stars but instead small stellar clusters even at the least massive size. This complicates the estimation of the PI feedback as an estimate of the number of ionizing photons produced by the stellar cluster is required and this can be a highly uncertain value.

The number of ionizing photons, able to ionize hydrogen, produced by a stellar cluster per second is referred to as the $Q_H$ value. The locations of the sink particles are taken as the cluster locations and the $Q_H$ values estimated from the cluster mass. Only sinks which exceed 600$M_\odot$ are allowed to become sources of ionizing photons. This is a somewhat arbitrary limit but it is likely that less massive clusters will not host a massive O or B star and these are the major source of ionizing photons in young clusters. The mean intensities and neutral fractions within the grid of the MCPI codes must be converged within each run. The greater the number of sources and the larger the spread in $Q_H$ the more iterations and MC photon packets that must be used to achieve convergence. Truncating the ionizing sources at 600$M_\odot$ helps significantly reduce the computational requirements of the MC simulations. High mass clusters are expected to have the greatest impact on their surroundings but the possible impact of low mass clusters cannot be ruled out here.

3.4.1 Dale method

Dale & Bonnell (2011) introduced a simple method to estimate the $Q_H$ value for sinks by calculating the total mass in stars with masses $M > 30M_\odot$ and dividing this mass by $30M_\odot$. This gives an approximate measure of the number of $30M_\odot$ stars, $N_{30}$. The number of massive stars is calculated by integrating the Salpeter (Salpeter, 1955) initial mass function (IMF) between the limits $0.1 – 100M_\odot$ and with a power law slope of $-2.35$. The total mass in stars $M > 30M_\odot = M_{30}$ is then equal to

\[
M_{30} = N_0 \int_{30}^{100} M^{-1.35} dM \quad (3.2)
\]

where $N_0$ is a normalization which depends on the total cluster mass by $N_0 = M_{tot}/5.826$. This mass can then be divided by 30 to get the approximate value of $N_{30}$. $Q_H$ is estimated from the O-star data of Conti et al. (2008) (Table 3.1) and Diaz-Miller et al. (1998) (Table 1). From
this a $Q_{H}^{30}$ of $2.78 \times 10^{48}\text{s}^{-1}$ is estimated. Although this method is crude it is expected to give a reasonable approximation to $Q_{H}(M)$ and will allow the comparison with earlier work. Any parameterization of the cluster ionizing flux will be uncertain due to the poor sampling of the high mass end of the IMF in all but the most massive clusters. Due to the form of the Salpeter IMF and its lack of turnover at low masses the estimates for the mass in stars $> 30M_{\odot}$ will be slight over-estimates of the true value, but the effect will be small compared to the other approximations employed to estimate the ionizing flux for each cluster, such as the assumed 100% star formation efficiency which likely overestimates the total stellar mass by a factor $2-4$.

### 3.4.2 The Number of Ionizing Photons Produced in a Stellar Cluster: the $Q_{H} - M_{\text{cluster}}$ relation

In this section an attempt is made to quantify a more robust $Q_{H} - M_{\text{cluster}}$ relation and illustrate some of the difficulties in its calculation. The number of ionizing photons produced in a stellar cluster is a quantity that is dependent on a number of factors: the mass of the cluster, the assumed IMF, the upper and lower mass limits of the IMF and the stellar atmosphere models used to name a few. Stochastic sampling effects can also come into play quite strongly (Villaverde et al., 2010b,a; Cervino et al., 2003).

For an individual cluster stochastic effects are likely to be very important unless the cluster is sufficiently massive to well sample the IMF at all masses. For instance a cluster of $50M_{\odot}$ may be composed entirely of low mass stars, $M \leq 5M_{\odot}$, which produce negligible numbers of ionizing photons. Alternatively it may contain one massive star of say, $40M_{\odot}$, which is capable of producing a large number of ionizing photons. In real terms this means that the value of $Q_{H}$ for the cluster may vary from $1.2 \times 10^{42} - 1 \times 10^{49}\text{s}^{-1}$, a range of almost seven orders of magnitude for a single cluster. Of course this is an extreme example but it illustrates the problems faced when randomly sampling from an IMF.

In Figure 3.5 the difference in sampling the IMF for a 100 and $1 \times 10^{5}M_{\odot}$ stellar cluster is shown. The less massive cluster contains mainly low mass stars and the IMF above $\sim 5M_{\odot}$ is not sampled at all. The $1 \times 10^{5}M_{\odot}$ cluster is well sampled at all masses up to the upper limit, $M_{\text{upper}}$. Figure 3.6 shows another pair of randomly sampled clusters but in this case the low mass cluster contains a single massive star ($> 50M_{\odot}$) and the low mass end of the IMF is less well sampled. There is little difference in the high mass cluster and, as before, it is well sampled at all masses. This small change in the sampling would create a very large difference.
Figure 3.5: An example of two clusters randomly sampled from a Kroupa (Kroupa, 2001) IMF. The lower mass cluster (black) contains $100M_\odot$, with a cluster of $1 \times 10^5 M_\odot$ shown in red. The low mass cluster contains no massive stars while the high mass cluster is populated at almost all stellar masses.
Figure 3.6: Clusters of the same mass as figure 3.5 but for a different random sampling of the IMF.
Figure 3.7: The analytic relation between $Q_H$ and stellar mass from Schaerer (2002) (dashed line) along with the observational data from Diaz-Miller et al. (1998) and Conti et al. (2008).

In order to evaluate the effects of this stochastic sampling on the number of ionizing photons produced by a stellar cluster the mass of a star must be translated into an output of ionizing photons. To achieve this the relation between stellar mass and ionizing photon output from Schaerer (2002) is used. The author provides an analytic fit to the $Q_H(M)$ relation in terms of a polynomial:

$$\log_{10}(Q_H) = 27.89 + 27.75x - 11.87x^2 + 1.73x^3,$$  \hspace{1cm} (3.3)

where $x = \log_{10}(M/M_\odot)$. This relation was calculated for solar metallicity stars between $7-120M_\odot$ and is shown in Figure 3.7 plotted along with observational data for massive stars.

With this relation it is possible to estimate the total number of ionizing photons produced by a cluster. By simply assigning a value of $Q_H$ for each star in the cluster and summing these to get the total $Q_H$ value. In this calculation an assumption that no ionizing photons emerge from stars with a mass $< 7M_\odot$ is made. This is a reasonable assumption as the major source of ionizing photons are high mass young stars and the number of ionizing photons produced falls very steeply with decreasing stellar mass (see Figure 3.7). In order to evaluate the effects
3.4. Ionizing Photon numbers

Figure 3.8: The range of $Q_H$ values produced as a function of total cluster mass. The color of the cell indicates the number of clusters that fall in the cell with white meaning no clusters were produced with the combination of properties. It can be seen that the relation starts out with a wide spread at each cluster mass but the relation becomes much tighter at high masses due to more complete sampling of the IMF. The black dashed line shows the median value.

of stochastic sampling of the IMF a series of randomly sampled clusters at a range of total cluster masses was produced and the spread of the $Q_H$ values obtained were noted. Clusters were produced between 10 and $1 \times 10^4 M_\odot$, with 1000 individual clusters produced at each cluster mass. The IMF was a two part Kroupa IMF (Kroupa, 2001) between $0.1 - 150 M_\odot$.

It can be seen that at each cluster mass a large range of $Q_H$ values is possible. The spread is caused by the large effect of massive stars on the total $Q_H$ for a cluster, as one massive star can produce a large fraction of the total number of ionizing photons (this is especially true for low mass stellar clusters). Then small changes in the stellar population will cause large changes in the $Q_H$ values. The theoretical lower limit in this prescription is $Q_H = 0$ for all masses, as it is entirely possible (although improbable in most cases) to produce a randomly sampled cluster of any mass that contains no stars with $M > 7 M_\odot$. Even high mass clusters which are likely to be the most well sampled show a significant range in the number of ionizing photons they produce due to stochastic effects.

Randomly sampling the IMF for a given cluster mass can be somewhat complex. As stellar
masses are being sampled a running total of the stellar cluster mass is kept. If this falls in the range $98 - 102\%$ of the required value then the sampling is stopped and the stellar masses accepted. If the cluster mass exceeds the target mass then sampling is stopped and the entire cluster repopulated. This is the “hard” sampling of Parker & Goodwin (2007). A consequence of this method is that the number of high mass stars is slightly underestimated as if a high mass star is chosen when the cumulative cluster mass is near the target value, it will cause the cluster to be repopulated.

In this work there is no upper mass limit on the most massive star which may form in a given cluster. It has been proposed that as well as an absolute upper mass limit of around $150 M_\odot$, low mass clusters may have a limited ability to form massive stars (Larson, 1982; Weidner & Kroupa, 2013; Weidner et al., 2010). In this scenario the most massive star which can be formed in a cluster may be constrained by the total cluster mass, to a value $M_{\text{max}} < 150 M_\odot$. No constraint is included here and the most massive star in a cluster is constrained only by the upper mass limit $M < 150 M_\odot$ and the total cluster mass.

The black dashed line in figure 3.8 is the result of a polynomial fit to the median cluster $Q_H$ as a function of mass. This provides a reasonable value that can be used to estimate the most likely $Q_H$ for a stellar cluster of a given mass. The relation is:

$$\log_{10}(Q_H) = 5.0754 + 42.0340x - 15.0797x^2 + 2.4439x^3 - 0.1474x^4,$$

for $x = \log_{10}(M_{\text{cluster}}/M_\odot)$. This will be referred to as the clusterQ relation from here on. In comparison, the values of Dale et al. (2012b) fall below the $Q_H$ values computed here at all masses and likely represent a lower limit on the true $Q_H$.

### 3.5 Coupling the MCPI to SPH data

The SPH data that are being investigated are static as the dynamical evolution of the system has already been computed. As the original simulations did not include the possible effects of ionizing feedback, it is necessary to approximate the feedback effects as best as possible. By linking the MCPI codes to the individual time dumps of the SPH code it is possible to investigate the effects that photoionization by young stars can have on the mass accretion rates during the course of the simulation.

At each time dump from the Gravity simulation the density is discretised onto a cartesian grid and an independent MCPI run is performed, using the stellar cluster masses to calculate
the positions and $Q_H$ values for each individual cluster. The regions of gas within the Gravity simulation likely to be ionized at the time in question can then be identified.

The fundamental thinking behind this approach is that gas which is ionized in HII regions is dynamically hot, with temperatures in the region $8 - 10 \times 10^3\text{K}$ (Rodríguez & García-Rojas, 2010). This hot gas is unlikely to be accreted onto stellar sinks as its kinetic energy is much increased, leading to a reduction in the mass accreted over the course of the simulation compared to the original simulation which did not account for this possibility. This leads to an overall reduction in the stellar masses of the sinks when PI feedback is included.

Each SPH Gravity simulation dump is discretised into a $200^3$ grid of cells. The grid is centered on the centre of mass of the system at each time step and the grid extends to $\pm 0.1\text{kpc}$ in all three axes, to fully encompass the central region of the cloud with sufficient resolution. Increasing the resolution of the MCPI simulations was found to have little impact on the results obtained but significantly increased the computational time requirements.

The investigation is begun at the point in the simulation where at least one stellar sink has a mass $\geq 600 \text{M}_\odot$, as this will provide the first source of ionizing photons as described in section 3.4. The output of the MCPI code is a grid containing the ionization fraction throughout the Gravity simulation at the time step of interest. Importantly, each time step is treated independently by the MCPI code and the ionization state of the gas is purely determined by the distribution of gas and ionizing sources at an individual time step with no memory of the previous ionization state.

Once the MCPI code has calculated the ionization fraction, the SPH particles that are located within highly ionized cells are identified. If a gas phase SPH particle is located in a cell with a neutral fraction, $f_n < 0.5$ then it is classified as an ionized particle. It has been found that in general the results obtained are relatively insensitive to the exact value of $f_n$ at which particles are classed as ionized, as the mass of ionized particles is dominated by grid cells that are almost fully ionized ($f_n < 0.1$).

The accretion rates are adjusted by removing any mass accreted that originates in an “ionized” SPH particle, as such gas is unlikely to be gravitationally bound to the accreting sink. The stellar cluster masses are recalculated by removing an amount of mass from the sink equal to the mass of the ionized particle multiplied by $(1 - f_n)$. In this way if an accreted ionized particle was found in a cell with $f_n = 0.4$ then 60% of its mass would be prevented from accreting onto the stellar sink.
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<table>
<thead>
<tr>
<th>Run</th>
<th>Mass ($M_\odot$)</th>
<th>Radius (pc)</th>
<th>$v_{RMS}$ (km s$^{-1}$)</th>
<th>$t_{ff}$ (Myr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$10^6$</td>
<td>180</td>
<td>5.0</td>
<td>19.6</td>
</tr>
<tr>
<td>I</td>
<td>$10^4$</td>
<td>10</td>
<td>2.1</td>
<td>2.56</td>
</tr>
</tbody>
</table>

Table 3.2: The initial properties of the test cases from [Dale et al. (2012b)](#) (full details can be found within).

Tests are also carried out to check for the ionization of the SPH particles that are used to initially form stellar sinks. If, when a sink particle is formed, more than 50% of the gas particles that took part in its formation were classified as ionized, then the sink will be removed from further calculations and assumed not to form.

This method allows the investigation of the effects of ionization feedback on the accretion onto stellar clusters as the simulation progresses and comparison with the results with the initial distributions, that do not include any effects of photoionization by massive stars.

### 3.6 Tests

In order to validate the assumption that the methods will provide a reasonable approximation to the effects of PI feedback on the stellar masses a comparison to the work of [Dale et al. (2012b)](#) (hereafter referred to as D12) has been performed. D12 implement a Strömgren volume technique to calculate the ionization structure directly within the SPH simulations. This is outlined in detail in [Dale et al. (2007b)](#) and [Dale & Bonnell (2011)](#) and includes additions to account for multiple ionizing sources. The Strömgren volume technique involves estimating for each SPH gas particle whether or not it would be contained in the Strömgren sphere (a theoretical, spherically symmetric ionization region) of an ionizing source. The calculation involves using the line of sight density profile only to estimate the ionization state of a particle, without considering any other radiative transfer effects. Particles which are ionized during the course of the simulation are immediately heated to $10^4$K and the dynamical effects followed using standard SPH techniques. Ions also have the possibility to recombine with an electron and return to being neutral if shielded from the ionizing sources. This method has been tested against a MCRT code and is found to be in good agreement [Dale et al. (2007b)](#).

The D12 method of including PI feedback has the advantage of explicitly including the dynamical effects of the hot gas on the SFR. However, it means that the SPH simulation can take up to 50% longer to run than when no ionization effects are included. The MCPI method of including PI feedback has no overheads on the SPH simulations as all calculations are performed after the SPH simulation is completed. Also, with MCPI, different methods of calculating the $Q_H$ values can be investigated for their effects without running the entire SPH
3.6. Tests

Figure 3.9: Run A (left) and run I (right) at the point of formation of the first ionizing source in each case.

The methods outlined here have been applied to runs A and I from D12 (data kindly provided by Jim Dale). The simulations were performed in the absence of ionization effects (Control runs) and including ionization (Dale runs). The initial properties of the two clouds can be seen in table 3.2.

Run A has the largest radius of the simulations of D12 to form any stars and shows diffuse structure. It contains a few tens of clusters, with a number that are massive enough to become sources of ionizing photons. Run I is physically much smaller and more compact than run A and possesses the lowest escape velocity of any of the simulations investigated. In run I the mass resolution is sufficient to consider the sinks that form as individual stars and so the number of ionizing photons can be directly calculated. The method of D12 is followed in this case and $Q_H$ values are assigned to all sinks of mass greater than $20M_\odot$ according to the relation

$$\log(Q_H) = 48.1 + 0.02(M_* - 20M_\odot),$$

which is a fit to the $Q_H$ values of solar mass stars as found in Diaz-Miller et al. (1998). These two clouds represent two extremes in the sample of D12 and so provide a good way to test the effectiveness of the treatment. Figures 3.9 and 3.10 illustrate the gas distribution in the control runs of D12 at the point when the first ionizing source forms and at the end of the simulation.
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3.6.1 Total Stellar Mass

In the case of the diffuse Run A (figure 3.11) it can be seen that there is a good agreement between the method used here and the full implementation of PI feedback, in terms of the total stellar mass formed as a function of time. The relative difference is less than 10% at almost all times in the simulation. The relative difference increases rapidly near the end point of the simulation due to what appears to be triggered star formation in the D12 run which cannot be accounted for by the MCPI routines.

Run I shows a larger discrepancy between the D12 and MCPI routines in terms of the total stellar sink mass, as seen in figure 3.12. The difference initially grows quickly between the two methods up to around 5.4Myrs then stabilizes at approximately 10% for a short time before growing to reach a maximum level of $\approx 20\%$ by the end of the simulation. The difference in this case appears to be caused by the greater dynamical impact of the ionized gas causing some triggered star formation, similar to the case for Run A.

3.6.2 Star Formation Rates

In figures 3.13 and 3.14 the comparison of the derived SFRs in the control runs to the ionization simulation of D12 and these calculations using MCPI is shown. For run A there is a good agreement between these calculations and D12 over most of the time covered by the simulation. Both methods show a reduction in the SFR to around 40% of the value in the control run shortly after the formation of the first ionizing source and then a mostly flat SFR there after,
Figure 3.11: The total stellar mass formed in Run A in the Control (black), Dale (green) and the MCPI runs described here.
Figure 3.12: Same as figure 3.11 but for the Run I simulation.
Figure 3.13: The instantaneous SFR for the Run A simulation. The Control is shown in black with the Dale run in green and the MCPI in blue.
Figure 3.14: The instantaneous SFR for the Run I simulation. The Control is shown in black with the Dale run in green and the MCPI in blue.
permeated by sharp spikes in the SFR caused by the formation of individual sink particles. These spikes are a numerical effect caused by the prescription used to form sink particles and the mass resolution of run A. Some of the SFR events can be seen in all three simulations while some are prevented by PI feedback entirely or have their magnitude reduced. Some triggered star formation can be seen in the D12 simulation as spikes which do not appear in the control.

The integrated SFR, calculated from the total stellar mass formed during the simulation, is

\[ SFR_{\text{control}} = 3.6 \times 10^{-3} \, M_\odot \, \text{yr}^{-1} \]

in the control and drops to

\[ SFR_{\text{Dale}} = 2.8 \times 10^{-3} \, M_\odot \, \text{yr}^{-1} \]

and

\[ SFR_{\text{MCPI}} = 2.5 \times 10^{-3} \, M_\odot \, \text{yr}^{-1} \]

in the D12 and MCPI simulations respectively.

The comparison between the MCPI and D12 SFRs for run I are presented in figure 3.14. The agreement is generally good until about 6.5Myrs after which there are significant differences. Both the MCPI and D12 SFRs follow a similar course until around 6.5Myrs where they begin to diverge. The MCPI shows a significant drop in SFR while the D12 value continues to grow and in fact reaches a value that is almost equal to the control run at this point. Both then show a slight drop in SFR just before the end of the simulation. The difficulties of the MCPI method in accurately treating run I are unsurprising as this is the simulation which is dynamically most affected by ionizing feedback. The integrated SFR for the control is

\[ SFR_{\text{control}} = 1.1 \times 10^{-4} \, M_\odot \, \text{yr}^{-1} \]

and drops to

\[ SFR_{\text{Dale}} = 7.1 \times 10^{-5} \, M_\odot \, \text{yr}^{-1} \]

for the D12 simulation and

\[ SFR_{\text{MCPI}} = 5.7 \times 10^{-5} \, M_\odot \, \text{yr}^{-1} \]

in the MCPI run.

3.6.3 Sink Mass Distributions

It is now possible to look at the sink masses produced in both simulations. As can be seen in figure 3.15 for run A the agreement is good, although the low number of sinks formed means that the distribution is noisy. But, overall, there appears to be a good agreement between the two methods across all masses. Run I shows a more marked difference, especially for lower mass sinks. The MCPI method seems to prevent the growth of lower mass sinks more effectively than is seen in the Dale run. It is not immediately obvious why this should be the case, as the sinks in question are mostly not massive enough to become ionizing sources. This means that the more massive sources are having a more wide-spread impact in the MCPI runs. This is likely due to the dynamical impact of the ionized gas which is neglected in the MCPI method. The ionizing photon escape fraction reported by D12 for run I is 0.90, meaning that the majority of ionizing photons are escaping the region. The high escape fraction can be attributed to the dynamical effects of the ionized gas creating large cavities in the neutral material, which allow the escape of ionizing photons through these low density paths. The
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Figure 3.15: The stellar (sink) mass function for runs A (left) and I (right).

MCPI methodology is unable to create these channels for the escape of ionizing photons and as a result the majority of the photons (~99%) are locally absorbed in the cloud. This increases the impact of the PI by allowing a larger number of gas phase particle to become ionized before they can be accreted by sinks.

The fact that the MCPI results are in reasonable agreement with the more sophisticated D12 treatment gives us encouragement that this method is able to treat the ionization feedback on stellar growth in a satisfactory way. It should also be noted that mostly the MCPI method predicts a SFR that is equal to or lower than D12. The MCPI treatment can then be interpreted as providing an upper limit to the effects of ionizing feedback by only allowing it to reduce the SFRs and not accounting for the possible triggering of star formation.

3.7 Results

The methods outlined above have been applied to a series of static snapshots of the SPH simulations of Bonnell et al. (2013) to investigate the effects on the stellar mass formed. Three different simulations with different average gas surface densities have been investigated. The results from the low ($\Sigma_{gas} = 0.4M_{\odot}pc^{-2}$), standard ($\Sigma_{gas} = 4M_{\odot}pc^{-2}$) and high ($\Sigma_{gas} = 40M_{\odot}pc^{-2}$) surface density simulations will now be discussed.
3.7. Results

3.7.1 Standard Surface Density

Here results are presented for the standard surface density SPH simulation with a value of $\Sigma_{gas} = 4M_\odot pc^{-2}$. In figure 3.16 the time evolution of the ionized gas mass and number of ionizing photons emitted per second ($Q_H$) is plotted for both methods of calculating the number of ionizing photons. $Q_H$ values calculated using the more robust clusterQ relation, which takes account of stochastic sampling effects, are significantly higher than those calculated using the D12 relation (see section 3.4.1). The $Q_H$ values grow steadily throughout the simulation reaching $6.6 \times 10^{49}s^{-1}$ for the D12 relation and $2.6 \times 10^{50}s^{-1}$ for the clusterQ case. Each step in the ionizing luminosity represents a new sink particle (or particles) exceeding the minimum mass required to become an ionizing source. The decrease in ionizing luminosity at $\sim 354.3$Myrs is due to an ionizing source exiting the region of interest. In the simulations the ionized gas mass is representative of the total number of SPH particles which have been ionized and therefore excluded from the star formation process. The ionized gas mass shows an initial fast growth as the first ionizing sources appear, followed by a modest growth as the simulation progresses. A similar trend is seen for both methods of estimating the number of ionizing photons. As each MCPI simulation is independent, the ionized gas mass can decrease in time due to the exact distribution of sources and neutral gas in each case.

Figure 3.17 shows the locations of the sink particles at the end of the simulation. Many of the sinks are clustered in the central regions of the cloud in a large star forming complex which also contains many ionizing sources. However, ionizing sources can also be found in the outer regions of the cloud.

3.7.1.1 Morphology of the gas

Figures 3.18 and 3.20 show the distribution of the neutral and ionized gas for the clusterQ relation. Even just after the first ionization source forms ionized gas fills a large region of the cloud. However, the ionized particles tend to be in low density diffuse regions which are not actively star forming. It can be seen from the lower left panel in figure 3.20 that the ionizing source is located above the galactic plane and PI photons are only able to penetrate into the heart of the cloud down a few low density channels. By the end of the run ionized gas is found throughout the cloud. The densest regions of ionized gas are located close to the major sites of star formation in the centre of the cloud but lower density ionized gas can be found throughout the cloud. Several regions are visible, however, which appear to be relatively free of ionized gas. These are often shielded from the effects of the ionizing sources by dense gas in
Figure 3.16: The time evolution of the ionized gas mass and total number of ionizing photons with time. The solid lines show the results when the D12 $Q_H$ relation is used and the dashed lines show the clusterQ relation results.
Figure 3.17: Positions of the stellar sink particles (black circles) and the ionizing sources at the end of the Gravity simulation (356,04 Myrs) with $\Sigma_{\text{gas}} = 4 M_\odot \text{pc}^{-2}$. Particles massive enough to be sources of ionizing photons are marked with red crosses.
Figure 3.18: The distribution of neutral gas at the point the first source of ionizing photons forms (above left) and at the end of the simulation (above right) as viewed from above the galactic plane and as viewed from within the plane initially (below left) and at the end (below right). Results of using the clusterQ relation.

The overall morphology seen in the simulations using the D12 \( Q_H \) relation is similar to that produced by the clusterQ method, but as the clusterQ method produces higher values of \( Q_H \) the ionized gas is slightly more widespread in that run and the PI photons are able to ionize some of the gas that remains unaffected using the D12 \( Q_H \) values.

3.7.1.2 Cumulative stellar mass

Figure 3.22 shows the cumulative mass which has been accreted by the stellar sink particles from the point at which the first ionizing source forms, until the end of the simulation. It can be seen that there is a steady divergence of the control and photoionized cases due to the ionization of gas particles, which are then prevented from accreting onto stellar sinks.
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Figure 3.19: The same as figure 3.18 but for the D12 relation.
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Figure 3.20: The distribution of ionized gas at the point the first source of ionizing photons forms (above left) and at the end of the simulation (above right) as viewed from above the galactic plane and as viewed from within the plane initially (below left) and at the end (below right). Results of using the clusterQ relation for values of $Q_H$. 
Figure 3.21: The same as figure 3.20 but for the $Q_{ij}$ values calculated using the D12 relation.
Figure 3.22: Cumulative stellar mass as a function of time for the control (red) and the MCPI runs using the D12 \( Q_H \) relation (blue) and clusterQ relation (black).
3.7. Results

In total after the inclusion of photoionization effects the final mass accreted by all sinks falls from $M_{\text{Control}} = 2.20 \times 10^{5} M_{\odot}$ to $M_{D12} = 1.68 \times 10^{5} M_{\odot}$ using the D12 $Q_{H}$ relation which is a reduction in the stellar mass of $\approx 24\%$ (shown by the blue line in figure 3.22). The clusterQ relation is able to reduce the total stellar mass to $M_{\text{clusterQ}} = 1.36 \times 10^{5} M_{\odot}$ a slightly larger reduction of 38\% (the black line in figure 3.22). This larger reduction is due to the larger $Q_{H}$ values estimated using the clusterQ relation allowing a larger amount of the neutral gas to be ionized.

3.7.1.3 Star formation rates

The SFRs over the course of the simulation can also be estimated by taking the total stellar mass in the region of interest at the end of the simulation and dividing by the total length of time the simulation has been allowed to form stars. The Control run has a mean SFR of $SFR_{\text{Control}} = 4.2 \times 10^{-2} M_{\odot} \text{yr}^{-1}$ while the MCPI run using the D12 relation reduces this to $SFR_{D12} = 3.2 \times 10^{-2} M_{\odot} \text{yr}^{-1}$. Again the larger $Q_{H}$ values in the clusterQ run allow more gas to be ionized and the SFR falls to a value of $SFR_{\text{clusterQ}} = 2.6 \times 10^{-2} M_{\odot} \text{yr}^{-1}$. The changes are due to feedback from ionizing sources which have previously formed ionizing gas before it can be accreted onto stellar sinks or from new sinks. In the case of the clusterQ run the integrated SFR is reduced to 62\% of its value in the control run which is a significant reduction.

The time evolution of the global instantaneous SFR is shown in figure 3.23. Instantaneous SFRs between each SPH dump have been calculated by dividing the total mass increase in the stellar sinks divided by the time period between the dumps. The time starts just before the first sink becomes an ionizing source, before this point the SFR is identical in all simulations. In the top panel of figure 3.23 the red line shows the control run, the blue line the D12 $Q_{H}$ run and the black line the clusterQ run. Both the MCPI runs show a SFR which is initially around 5\% lower than the control until $\approx 353.5\text{Myrs}$ when a steady divergence of the SFRs begins due to the formation of ionizing sources. The divergence continues for the duration of the simulation and has reduced the MCPI SFRs to around 62\% of the control run for the D12 $Q_{H}$ relation and 47\% for the clusterQ relation.

3.7.1.4 Stellar Cluster Masses

Figure 3.24 shows a cumulative histogram of the final stellar sink masses for both the control and MCPI simulations. It shows the total number of sinks formed by the end of each simulation as a function of their mass. It can be seen that fewer sinks have formed in the MCPI runs compared to the control but all follow a similar distribution. There are a larger number of
Figure 3.23: The instantaneous SFR of the simulation in the control and MCPI runs. The red line shows the control run, the blue line the SFR derived from the D12 \(Q_H\) relation and the clusterQ relation is shown in black.
3.7. Results

Stellar Sink Mass ($M_{\odot}$)

<table>
<thead>
<tr>
<th>Number</th>
<th>Control</th>
<th>MCPI D12</th>
<th>MCPI ClusterQ</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1000</td>
<td>10</td>
<td>100</td>
</tr>
<tr>
<td>10</td>
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</tr>
<tr>
<td>1</td>
<td>10</td>
<td>100</td>
<td>1000</td>
</tr>
</tbody>
</table>

Figure 3.24: The cumulative mass distribution at the end of the simulation. The red line shows the control simulation and the blue line the distribution in the MCPI simulation using the D12 $Q_{ij}$ relation. The black line illustrates the results using the clusterQ relation.
Figure 3.25: The final sink mass distribution for the three runs. It shows number of sinks present in a given mass bin at the end of the simulation.

Sinks formed in the control run at nearly all masses, the exception being at the very low mass end where there are a higher number of low mass sinks in the MCPI runs due to the action of PI feedback. The most obvious change in the sink mass distribution is at the high mass end where the action of PI feedback is able to reduce the numbers of high mass sinks. As has been seen before the increased number of ionizing photons in the clusterQ run leads to a stronger impact on the stellar sink masses.

Figure 3.25 contains the mass distribution for the final stellar sinks masses. It can be clearly seen that the MCPI simulations form fewer sinks at all masses, except at the low mass end where they form an excess compared to the control run. The D12-$Q_H$ run forms a slightly greater number of stellar sinks at all masses than the clusterQ run which is consistent with the lower overall stellar mass formed. There does not seem to be any specific mass range that is more affected by the increased $Q_H$. The maximum mass attained by a stellar sink falls from $1968\,M_\odot$ in the control to $1154\,M_\odot$ in the D12-$Q_H$ run and $1050\,M_\odot$ in the clusterQ run.
3.7. Results

Figure 3.26: Accretion histories for the sinks with final masses $M \geq 600M_\odot$ in the Control run, after the inclusion of ionization in the MCPI clusterQ run. The dashed black line marks a mass of $600M_\odot$ which all sinks plotted exceed in the control run.

3.7.1.5 Accretion History

To better understand the impact of PI feedback on individual sinks the accretion histories of the individual sinks as they form and grow with time can be plotted. Figure 3.26 shows the growth of all sinks which achieved a mass $M \geq 600M_\odot$ by the end of the control run, during the MCPI simulation. It can be seen that many of the sinks now fail to grow to the point they will be considered as ionizing sources (as shown by the black dashed line) and in fact there are only 19 ionizing sources by the end of the MCPI run compared to 36 in the control. There appear to be two different behaviors within the accretion histories with one set of sinks continuing to grow throughout the time the simulation runs (even in some cases after the sink has become an ionizing source) while others have their growth truncated. The truncation can be seen as the flattening of the lines at a constant value of sink mass. For
some sinks this happens at a small mass and one sink reaches a mass of only 280$M_\odot$, less than half its value in the control run. Other sinks appear to have accretion shut off as they become ionizing sources and this can be seen in the large number of sinks with final masses of just over 600$M_\odot$. This is most likely caused by the ionizing output of the sinks ionizing the material surrounding it and effectively starving the sink of material to accrete.

### 3.7.1.6 Distance from the nearest ionizing source

The data in figure 3.27 show the fractional mass lost by sinks against the distance of the sink from the nearest source of ionizing photons in the MCPI clusterQ run. Ionizing sources are included in the plot and in this case the distance to the nearest ionizing source is 0pc. Sinks which are prevented from forming and would show a fractional mass change of 1.0 are not included, however. While most of the sinks which have been prevented from accreting a large fraction of their mass are located close to an ionizing source it should be noted that a number of sinks that have had their final masses reduced by a large fraction are located a significant distance from an ionizing source. This is illustrative of the ability of ionizing photons to travel large distances within the cloud.

The sinks that were prevented from forming (aborted sinks) are plotted in figure 3.28 showing the distribution of distances to the nearest ionizing source. As would be expected sinks that were aborted are more concentrated at small distances and show less of a tail at large distance than the overall sink population. However, there are a couple of examples of sinks which have been prevented from forming at a distance of $\approx 90$pc from the nearest ionizing source.

### 3.7.2 High Surface Density

In addition to the case outlined above the effects of PI feedback on the SPH simulation when the mean surface density is ten times higher ($40M_\odot$pc$^{-2}$) than the standard case have also been investigated. The clusterQ relation was used to calculate the number of ionizing photons in the high surface density run.

In the case of the high surface density run the SPH simulation ran for a shortened period of time due to the high densities producing prohibitively short time-steps within the SPH code. However, a large number of sink particles were able to form and grow in mass until they became sources of PI photons. A total stellar mass of $2.54 \times 10^6M_\odot$ formed in the region of interest within the $\approx 1.3$Myrs which the simulation was evolved for. Even in this short timescale the PI photons are able to strongly affect the star formation in the region. Figure
3.7. Results

Figure 3.27: The above plot shows the fractional change in the stellar sink masses against the distance to the nearest source of ionizing photons.
Figure 3.28: A plot of the distribution of distances to the nearest ionizing source for the sinks which were prevented from forming as well as for the rest of the sinks.
3.7. Results

Figure 3.29: Cumulative stellar mass formed as a function of time in the high surface density run for the control (red) and MCPI (black) simulations. The mean SFR over the simulation falls from $SFR_{\text{Control}} = 1.94M_\odot\text{yr}^{-1}$ in the control run to $SFR_{\text{MCPI}} = 1.01M_\odot\text{yr}^{-1}$ for the MCPI run. In figure 3.30 the instantaneous SFR during the high surface density run is plotted as a function of time. The sharp decrease in the star formation rate at a time of $\approx 351.6$Myrs appears to be caused by the coalescence of the ionized regions around several sources within the centre of the cloud to form one large ionized complex. This effectively ionizes the majority of the gas near the sinks and removes the reservoir of neutral star forming gas. At some points of the simulation a decrease in the SFR of over 60% can be seen.
Figure 3.30: The SFR as a function of time in the case of the high surface density ($40\,M_\odot pc^{-2}$) simulation. The black line shows the control run and the red line the MCRT run.
3.7.3 Low Surface Density

In the case of the simulation with mean surface density ten times less than the standard (0.4$M_\odot$pc$^{-2}$) the situation is more complicated. The low surface density causes the simulation to suffer from a lack of star formation due to a more limited reservoir of gas available for accretion and a lack of dense clumps where the gas can cool effectively \cite{Bonnell2013}. The result is a much reduced SFR and a lack of high mass sinks within the simulation. No sink is able to grow beyond 75$M_\odot$ in mass and so there are no sources of PI photons as described in section 3.4.

However, to gauge the possible effects of PI feedback a MCPI simulation was performed as follows. When the most massive sink in the simulation grows to a mass of > 40$M_\odot$ it is assumed that a 30$M_\odot$ star is formed in the cluster. The star is assigned an $Q_H$ of $2.78 \times 10^{48}$s$^{-1}$ as previously used in section 3.4. While this is a somewhat arbitrary setup it should at least allow an assessment of the possible impact of the formation of a high mass star in such an environment.

The effect of the PI feedback can be seen in figure 3.31. There is a small reduction in the stellar masses at late times but for most of the simulation there is little change. Partly this is due to the fact that the sink containing the massive star does not form until 354.8Myrs so there is no ionizing source until this point in time. The PI feedback then causes a small steady divergence from the control run. The integrated SFR drops from $SFR_{control} = 1.55 \times 10^{-4}M_\odot$yr$^{-1}$ to $SFR_{MCPI} = 1.53 \times 10^{-4}M_\odot$yr$^{-1}$ over the course of the simulation. This is a modest reduction and in fact most of the stellar mass which is lost is removed from the sink which is the source of PI photons with virtually no reduction in the mass of any other sinks.

3.7.4 SFRs vs Surface Density

In trying to understand the effects of PI feedback on the accretion processes it is useful to compare the results with the observed properties of star forming regions. It has been shown that there is a strong observed link between star formation and the local cold gas density \cite{Schmidt1963, Kennicutt1998b, Kennicutt2012, Bigiel2010} at galactic scales. In the case of disk averaged properties of local galaxies this can be fitted by a power-law relation of the form

$$\Sigma_{SFR} = A\Sigma_g^N,$$  \hspace{1cm} (3.6)
**Figure 3.31:** The cumulative stellar mass formed in the low surface density simulation after the introduction of a single high mass star.
Figure 3.32: The gas surface density versus star formation rate surface density of the MCPI simulation as viewed along the three axes of the cartesian grid. The SFRs have been calculated as the instantaneous rates at the end of the simulation. Colored points (see key in top left) show the effects of increasing the cell size up to the size of the entire region (200pc). The numbers associated with the red contours indicate the fraction of the points that lie within the contour. The dashed black line shows the extra-galactic relation, the black crosses the observational data of Heiderman et al. (2010) and the blue line is the best fit power law found by Bonnell et al. (2013) when fitting the entire Gravity dataset.

where $\Sigma_{SFR}$ is the star formation surface density, $\Sigma_g$ the total cold gas mass surface density and the power-law slope $N$ has a value of $\approx 1.4$ (Kennicutt, 1998b) and the constant $A \approx 2.5 \times 10^{-4}$. Observations of molecular clouds within the local environment in the Milky Way have suggested that the star formation surface density is a factor 10 – 20 higher than that predicted by the extragalactic relation (Evans et al., 2009; Heiderman et al., 2010) but this is possibly partially due to the methods used to observationally determine the values.

In figure 3.32 the final instantaneous SFR and neutral gas mass surface density in the photoionization simulation as viewed along the three axes of the simulation grid are shown. The instantaneous SFRs have been calculated from the final $\approx 0.05\text{Myrs}$ time step in the SPH simulation. This does not give a true reflection of the instantaneous SFR but it is the shortest
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Figure 3.33: The gas surface density versus star formation rate surface density of the MCPI simulation as viewed along the three axes of the cartesian grid. Here the SFRs have been calculated as the integrated rates for the duration of the simulation. Colored points (see key in top left) show the effects of increasing the cell size up to the size of the entire region (200pc). The numbers associated with the red contours indicate the fraction of the points that line within the contour. The dashed black line shows the extra-galactic relation, the black crosses the observational data of Heiderman et al. (2010) and the blue line is the best fit power law found by Bonnell et al. (2013) when fitting the entire Gravity dataset.
timescale over which the SFR can be estimated here. The colored diamonds represent the results obtained by viewing the simulation on progressively larger scales. Orange diamonds show values viewed in “pixels” with a linear size of 25pc, green are 50pc, blue 100pc and the single purple diamond represents the entire simulated region. The values were calculated using grids of neutral gas density and SFR. Each grid was a $200^3$ cube of cells which was re-gridded to the required cell size before calculating the observed surface densities, as viewed along the three axes of the grid. In this way the entire cloud is covered at each resolution. Cells with no star formation activity have been omitted from the plot. Also shown are the observations of [Heiderman et al. (2010)] of local molecular clouds and YSO derived star formation rates (black crosses), as well as the extra-galactic relation of [Kennicutt (1998b)] (black dashed line) and the fit from [Bonnell et al. (2013)] (blue line) to the entire Gravity simulation. The fit from Bonnell et al. (2013) was made to the non-ionized SPH simulations and combines the high ($40\, M_\odot\, pc^{-2}$), normal ($4\, M_\odot\, pc^{-2}$) and low ($0.4\, M_\odot\, pc^{-2}$) surface density data. Firstly it can be seen by comparing the three panels that the orientation of the cloud can have an effect on its observed properties. All three panels show a similar distribution at the scales investigated, although they show significant differences at smaller scales due to projection effects. There is a significant scatter in the data points in all orientations, which is more apparent when small scale observations are made. As the cell size over which the properties are averaged is increased in general all three figures move into better agreement. Many regions in the cloud can be seen which overlap with the observed data of Heiderman et al. (2010) as well as many which seem to lie at lower gas surface densities.

Figure 3.33 is identical to figure 3.32 except that the SFRs have been calculated as integrated rates over the history of the simulation. This increases the derived SFR for most sinks and so offsets the results to higher SFR surface densities. It is also possible to observe sinks at low gas surface densities that have relatively high integrated SFRs. This can partly be explained by sinks forming and accreting early in the simulation and then migrating to regions of low gas density, or regions of highly ionized gas.

### 3.7.5 Hα derived SFRs

Observationally Hα emission is often used to estimates the SFR. The emission originates in the ionized gas near massive stars and based on the observed Hα luminosity it is possible to calculated the number of massive stars and hence the SFR. The PI simulations have as one of their outputs a grid of ionized gas density throughout the region. Using the relation of [Aller](#)
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(1984) (eq. 16):

\[ E(\text{H}\beta) = 1.387 \times 10^{-25} N_{H} N_{e} t^{-0.983} 10^{-0.0434} \tau \]  

(3.7)

where \( N_{H} \) and \( N_{e} \) are the number density of ions and electrons respectively and \( t \) is the temperature in units of \( 10^4 \)K, the H\( \beta \) emissivity (\( \text{erg s}^{-1} \text{cm}^{-3} \)) is calculated. The H\( \alpha \) emissivity can then be calculated from the ratio of emissivities as estimated for a case B nebula at \( 10^4 \)K by Osterbrock & Ferland (2006) as \( \frac{E(\text{H}\alpha)}{E(\text{H}\beta)} = 2.87 \).

A scattered light Monte Carlo code was then used to produce images of the region in H\( \alpha \) light and the results can be seen in figure 3.34. The morphology is very similar to that seen in the ionized gas (see figure 3.20) with the emission centered on the massive stars. Large regions of low density ionized gas also fill the outer regions of the cloud.

The SFR has also been estimated from the H\( \alpha \) images, using the relations of Kennicutt (1998b):

\[ \text{SFR} \left[ \frac{\text{M}_\odot}{\text{yr}^{-1}} \right] = 7.9 \times 10^{-42} L(\text{H}\alpha) \left[ \text{erg s}^{-1} \right] \]  

(3.8)

to convert the observed fluxes to SFRs in a similar way to real observations. Figure 3.35 shows a comparison of the SPH and H\( \alpha \) derived SFRs when viewed along the three axes of the simulation and at different spatial scales. It can be seen that the SFR derived from H\( \alpha \) is lower in almost all cases. The primary reason for this is that it is only the massive sinks which are able to influence the ionized gas and so positional information on the low mass sink star formation is lost. The derived H\( \alpha \) SFR surface densities agree well with the SPH SFR surface densities if only sinks with \( M > 600 \text{M}_\odot \) are considered, but fall below the total SPH SFR surface densities. As can be seen from figure 3.36 the massive sinks only contribute a fraction of \( \approx 8\% \) of the total star formation over the course of the simulation.

The SFR-H\( \alpha \) relation of Pflamm-Altenburg et al. (2007) has also been used to calculate the SFRs from the H\( \alpha \) images. Pflamm-Altenburg et al. (2007) attempt to account for the under sampling of the high mass end of the IMF and provide a non-linear relation between H\( \alpha \) luminosity and SFR where

\[ \log(\text{SFR} \left[ \frac{\text{M}_\odot}{\text{yr}^{-1}} \right]) = a_{0} + a_{1} x + a_{2} x^{2} + a_{3} x^{3} + a_{4} x^{4} + a_{5} x^{5} \]  

(3.9)

with \( x = \log(L_{\text{H}\alpha} \left[ 10^{41}\text{erg s}^{-1} \right]) \) and the coefficients taking their values from table 3.3.

The results are shown in figure 3.37 and there is a good agreement at the largest cell size (blue and purple points). The agreement is not as good at small sizes and this is most
3.7. Results

Figure 3.34: Images of the PI simulation when viewed in the H\(_\alpha\) emission line along the three principle axes of the cartesian grid. Fluxes have been calculated for an observer distance of 1 kpc.
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**Figure 3.35:** The integrated SFR surface densities calculated directly from the SPH simulation (x-axis) and derived from the Hα images (y-axis). Hα SFRs have been calculated using the relation of Kennicutt (1998b). Colored points show the effects of calculating the SFRs within pixels of different spatial sizes (see the key in the top left corner). Pixels which encompass no star formation have been assigned a value of $10^{-6}$. In almost all cases the Hα derived SFR is lower than the actual SFR.

**Figure 3.36:** The cumulative SFR as a function of the sink mass.
Table 3.3: Coefficients of the Hα-SFR relation of Pflamm-Altenburg et al. (2007).

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$</td>
<td>0.438</td>
</tr>
<tr>
<td>$a_1$</td>
<td>0.964</td>
</tr>
<tr>
<td>$a_2$</td>
<td>$3.21 \times 10^{-2}$</td>
</tr>
<tr>
<td>$a_3$</td>
<td>$-8.47 \times 10^{-3}$</td>
</tr>
<tr>
<td>$a_4$</td>
<td>$-9.30 \times 10^{-4}$</td>
</tr>
<tr>
<td>$a_5$</td>
<td>$-2.67 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

likely because the low mass sinks do not influence the distribution of Hα emission so while they are accounted for in the total SFR, their spatial distribution is not. There are also slight differences in the way the IMF is sampled to obtain $Q_H$ values which may also contribute to the scatter.

Any star formation that occurs in low mass sinks, that do not host a massive star, will be missed by Hα SFRs derived using relations that do not account for stochastic sampling of the IMF. This effect has been exaggerated here by the sharp cut-off in PI sources at lower masses but may still be an issue in observations especially when SFRs are low. The possibility that several close, low mass sink particles which may in reality be better described as a single more massive cluster has also been neglected here.

3.8 Discussion

From the results shown in Figure 3.22 it is clear that the total mass accreted onto sinks throughout the simulation is overestimated by standard SPH methods when PI feedback is ignored. The final total stellar sink mass in the simulations including photoionization is reduced by $24 - 38\%$ depending on the prescription used to calculate the $Q_H$ value for each cluster. This is a significant change and suggests that it is likely very important to include photoionization effects to accurately model the SFRs and efficiency within SPH simulations.

3.8.1 Limitations

It has been suggested that the feedback from massive stars may act to trigger additional star formation under certain conditions. The expansion of the ionized HII region into surrounding neutral gas can sweep up a dense shell of material which can become self-gravitating (Whitworth et al., 1994; Elmegreen & Lada, 1977; Dale et al., 2007a). Observationally it has proved difficult to definitively find evidence for triggered star formation surrounding massive stars but several authors have presented compelling arguments based on multi-wavelength datasets (Deharveng et al., 2005; Dirienzo et al., 2012). The extent to which these triggered star formation processes may counteract the reduction in star formation caused by the heating and ionization of neutral gas is also unclear but simulations suggest they are likely second order effects (Dale et al., 2012b, 2013). It is also important to note that some triggered star formation events would occur even in the absence of PI feedback, but this is a small fraction.
There are also additional mechanisms in which the dynamical effects of ionized gas can allow the PI feedback to have a greater effect than estimated here. The penetration of the ionizing photons into dense regions of gas can be increased due to the streaming of hot ionized gas out of the cloud. Whitworth (1979) explored this scenario and found that the removal of ionized gas allows the ionization front to penetrate deeper into dense gas and may increase the effects of ionizing photons beyond those discussed here.

In addition to assuming a 100% efficient star formation process the SPH simulation studied here also neglects several physical processes which are likely to affect the overall star formation process. There is no treatment of magnetic fields which may cause a reduction in the star formation rate (Price & Bate 2008, Arthur et al. 2011, McKee 1999) by providing an additional support mechanism to overcome self-gravity and prevent the collapse of less massive clouds to form stars. Self gravity is also not included in the initial disk simulation from which the dense star forming region originates. This will lead to a reduced kinetic energy which, again, will enhance star formation rates. The reduction in the star formation rates caused by the inclusion of such effects may provide a mechanism to move the simulated values into better agreement with observed relations.

There is no inclusion of a source of ionizing photons outwith the bounds of the star forming cloud. In reality there will be a non zero background of ionizing flux produced by previous bouts of star formation in the galactic disk. The effects of background FUV heating are included in the SPH code (Vazquez Semadeni et al. 2006) but without account for the ionization of the gas Reynolds (1990) found that the diffuse ionized gas (DIG) in the local environment requires a diffuse ionizing flux of \( \approx 4 \times 10^{-5} \text{ergs s}^{-1}\text{cm}^{-2} \) to maintain it. This additional source of PI photons may be able to affect the outer regions of the cloud, but is
unlikely to penetrate into the dense cloud centre. While this is unlikely to affect the star formation in the cloud interior it may impact the initial stages of cloud formation during compression within the spiral shock.

3.8.2 Localization of stellar signatures

The clumpy gas distribution produced by the SPH calculation has been found to produce a highly structured complex of HII regions which, due to low density paths, provides an illustration of a possible source of ionizing photons required to maintain the DIG seen in the Milky Way and external galaxies. At the final time-step of the simulation the photoionization code suggests that $\approx 15\%$ of ionizing photons escape into the ISM from this star forming complex. This escape fraction may also be important for observations of H$\alpha$ as a localized star formation indicator. If a significant fraction of the ionizing photons are able to escape the star forming cloud then it also suggests there would be a corresponding drop in the H$\alpha$ luminosity. This effect will lead to H$\alpha$ emission that is non-coincident with the star formation. In turn this may cause deviations from the observed power law relation between star formation and gas surface densities at small scales (Relaño et al., 2012). Indeed Schruba et al., (2010) and Onodera et al., (2010) have found observational evidence of such deviations in high spatial resolution studies of the star formation in the nearby spiral galaxy M33. Based on analysis of CO emission maps and H$\alpha$ imaging Schruba et al., (2010) estimate that the star formation law observed at large scales breaks down at scales below $\sim 300$pc. It is not possible to verify this effect here due to the size of the region studied.

3.9 Future

In this work a simple hydrogen only MCPI code has been utilized but the method proposed can easily be extended to use radiation transfer codes which provide a more realistic treatment of the photoionization physics (Ercolano et al., 2008; Wood et al., 2004). The simplified treatment likely only provides a first order correction as it focuses on the ionization of hydrogen and the impact of Lyman continuum photons only, neglecting the effects of Helium as a source of opacity. There is, however, no reason that more complex radiation transfer codes which include these effects could not be added to provide more accurate gas physics at the cost of computation time. The possibility to also self-consistently include calculations of star formation indicators, such as H$\alpha$ and 24$\mu$m dust emission would allow the direct comparison with observational data.
The Stability of Low Surface Brightness Disks
Based on Multi-Wavelength Modeling


4.1 Introduction

Low surface brightness (LSB) disk galaxies, whose central, face-on surface brightnesses fall below \( \mu_{B,0} \gtrsim 23.0 \) mag arcsec\(^{-2} \) in the B band, account for an important fraction of the luminosity and galactic mass densities of the local universe (Driver, 1999; Minchin et al., 2004; O’Neil & Bothun, 2000). LSB disk galaxies show a range of masses and morphologies (e.g., Sprayberry et al., 1997; Auld et al., 2006), but the most common are bulgeless, late-type LSB disks with Hubble types Sd-Sdm. These galaxies frequently show signs of being dark matter dominated at nearly all radii (e.g., de Blok & McGaugh, 1997; de Blok & Bosma, 2002; Banerjee et al., 2010). This is in contrast to many disk galaxies where the luminous matter can dominate the dynamics of the inner disk regions (Persic et al., 1996).

LSB galaxies have been extensively studied in the H\(_I\) 21-cm line. Often their total H\(_I\) masses are comparable to or larger than their high surface brightness (HSB) counterparts,
while their H I surface densities are lower by a factor of $\sim 2$ [van der Hulst et al., 1993]. In fact, LSB galaxies are usually found to have most of their H I disk at surface densities below the Kennicutt [1989] critical values for the formation of massive stars [van der Hulst et al., 1993]. This fact may lead to a lower than expected star formation efficiency causing LSB galaxies to evolve more slowly than HSB galaxies. A lack of high mass stars will slow metal production and indeed McGaugh [1994] find LSB galaxies have metal abundances of $\sim 1/3$ solar. H II regions are observed in LSB galaxy disks as traced by H$\alpha$ emission [Rand, 1996; McGaugh et al., 1995; Matthews et al., 1999] and blue disk colours indicating young stars are present [McGaugh et al., 1995; Matthews et al., 1999; Matthews & Uson, 2008] suggesting LSB galaxies do have ongoing star formation. However, the conditions and structure of the interstellar medium (ISM) in LSB disk galaxies are still uncertain.

While observations of H$\alpha$ and H I have revealed information on the ionized and atomic gas, little is known about the dust and molecular hydrogen in the ISM. Based on observations of $^{12}$CO(1-0) emission in several LSB disk galaxies [Matthews et al., 2005] find that the CO emission, and hence the molecular hydrogen content, depends strongly on the rotational velocity. It appears that the rotational velocity, as well as the surface density, play an important role in shaping the structure and content of the ISM. This is also suggested by the work of Dalcanton et al. [2004] who find that the gas and dust disk of a galaxy is more stable to the effects of radial instabilities at lower rotational velocity. This limits the ability of perturbations to cause the collapse of the ISM into a thinner layer and may inhibit global star formation by
preventing the formation of large numbers of giant molecular clouds.

Due to the difficulties of directly detecting molecular gas in low-mass LSB spirals (cf. Matthews & Gao [2001]; Matthews et al. [2005]; Das et al., 2006), an alternative method to investigate the composition and structure of their molecular ISM is to observe far-infrared (FIR) emission produced by dust. The dust and gas are expected to be well mixed and so the highest dust densities should trace the high density, cool phases of the ISM. In order to interpret the distribution of FIR emission a radiation transfer model is required to produce synthetic images and spectral energy distributions based on galactic stellar and dust distributions.

4.1.1 Dust in galaxies

The role of dust in galaxies is a critical factor to understand and correctly interpret observations in terms of underlying physical properties. Dust will attenuate the stellar output by varying amounts at different wavelengths, with results affected by the distribution of the stars and dust as well as the properties of the dust grains themselves. The emission of thermal photons by the cool dust grains gives information about the distribution of the dense phases of the ISM, often associated with star formation, and the long wavelengths of the emission mean that, for the most part, the photons are free to escape the galaxy without scattering or absorption by the galactic material. The emission from cool dust also provides important information about the diffuse ISM. Far infra-red and sub-mm wavelengths are readily absorbed by the water in the earth’s atmosphere (except in a few windows) so space based observatories play a key role in observing the dust emission.

In the simplest case the dust provides a continuum opacity source that can absorb and scatter UV/optical photons. This effect can be observed clearly in the dark patches that are visible in the band of our own Milky Way on a dark night. Even along what appear to be empty sight lines interstellar dust is reddening and attenuating the light received from stars. In the presence of dust the sizes and shapes of galaxies derived from observations will differ from their intrinsic values. Measured scale lengths of galactic disks will be larger than the intrinsic values, the central surface brightness will be fainter (Möllenhoff et al., 2006; Gadotti et al., 2010; Pastrav et al., 2013) and it becomes necessary to correct our observed properties in order to gain understanding of the true intrinsic structure of galaxies.

Estimating the dust content of disk galaxies observationally has proved to be a difficult problem. Optical surveys of local galaxies showed that the surface brightness vs. inclination relation was flat suggesting that galactic disks should be regarded as optically thick at these
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Figure 4.2: The observed spectral energy distribution in the absence of dust (blue) and after inclusion of dust effects. Energy that is absorbed at UV/optical wavelengths re-emerges in the FIR and sub-mm. Figure from [Conroy (2013)] wavelengths ([Valentijn, 1990]). These early results however were plagued by sample biases which hid the true nature of the relation. More recently large optical surveys with a greater completeness have allowed the empirical estimation of the opacity of disk galaxies in the local universe ([Driver et al., 2007]). The results of [Driver et al. (2007)] suggest that the mean face-on, B-band optical depth of spiral disks is $\tau_B = 3.8 \pm 0.7$ meaning that spiral disks are optically thick. Other observational efforts used the serendipitous alignment of overlapping galaxy pairs to probe the dust content of the foreground galaxy directly ([White & Keel, 1992; White et al., 2000; Keel & White, 2001]). Estimates have also been made using the number counts of distant background galaxies through the galactic disk ([Holwerda et al., 2013]) to estimate the opacity of nearby galactic disks, where high resolution data are available.

A full treatment of the radiation transfer problem can provide a wide range of model predictions to compare to observations as well as giving insight to the physical processes at work. Modeling efforts have often focussed on fitting the optical and near-infrared (NIR) extinction of nearby HSB galaxies ([Kylafis & Bahcall, 1987; Xilouris et al., 1997, 1998, 1999; Bianchi et al., 2000; Bianchi, 2007]) and treating the dust absorption and reemission processes to model the full UV/optical to sub-mm spectral energy distribution (SED) ([Popescu et al., 2000; Misiriotis et al., 2001a; Bianchi, 2008; Baes et al., 2010; Popescu et al., 2011]).

When modeling the optical appearance of a disk galaxy an edge-on orientation is advantageous. This viewing geometry allows both the vertical and radial ISM structure to be constrained simultaneously and small scale features of the galaxy are smoothed out due to overlapping sight lines. The effects of dust become more apparent and dark dust lanes can
often be seen obscuring stellar emission where the central regions of the galactic disk have become optically thick. This makes the quantification of dust masses and distributions much more straightforward than the more degenerate case of a less inclined disk that is optically thin across most of its area.

In this Chapter the effects of dust, ISM geometry and mass on the UV/optical - FIR SEDs of edge-on LSB galaxies will be further constrained using Monte Carlo radiation transfer techniques. In section 4.2 the sample of galaxies to which the analysis is applied will be introduced followed by a description of the the data available at various wavelengths in section 4.3. Section 4.4 includes a description of the model used in the analysis. The results for the sample of galaxies can be found in section 4.5 and a discussion of the key results is presented in section 4.6.

4.2 Galaxy Sample

Three LSB galaxies have been selected that have been observed at a wide range of wavelengths to allow the best determination of the shape of the SED. The galaxies are nearby (≤10 Mpc) and are well-resolved in optical imaging. The selected galaxies span a range of central face-on surface brightness (μ_B,0 = 22.6 - 23.6 mag arcsec^{-2}) as well as rotational velocity (V_{rot} = 88 - 105 km s^{-1}). Face-on surface brightnesses in this case have been estimated based on inclination-surface brightness relations derived for normal galaxies. The three galaxies have similar total H I masses but observations indicate that their molecular hydrogen content decreases with decreasing rotational velocity (V_{rot}) (Matthews et al., 2005), suggesting that the ISM conditions may be different across the sample. Table 4.1 contains the properties of the galaxies as gathered from the literature. High resolution optical imaging of the three galaxies can be seen in Figure 4.3.

4.2.1 UGC 7321

UGC 7321 is one of the best studied edge-on LSB galaxies. It shows a very thin disk (a/b ~ 10.3\textsuperscript{1}) with signs of clumping of the stellar and dust distributions in the inner galaxy (Matthews & Wood, 2001) and a more uniform structure in the outer disk. The disk shows strong (B − R) color gradients in both horizontal and vertical directions that cannot be explained by the effects of dust (Matthews & Wood, 2001) and appear to be due to stellar population or metallicity gradients within the disk itself. Hα imaging shows ionized gas is present in a very thin

\textsuperscript{1}a/b is the disk axial ratio measured at the 25.0 mag arcsec^{-1} R-band isophote
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layer that has very little structure and shows no signs of large scale star forming regions (Matthews et al., 1999). The estimated stellar mass is $3 \times 10^8 M_\odot$ (O’Brien et al., 2010) and its distance is 10 Mpc (Matthews, 2000). The H I gas content of UGC 7321 has a greater radial extent than the optical disk of the galaxy (Uson & Matthews, 2003) and shows indications that the H I disk is also vertically extended (Matthews & Wood, 2003). Observations of the CO(1-0) line emission by Matthews & Gao (2001) confirm the presence of molecular gas in UGC 7321 and this measurement leads to a molecular hydrogen mass of $M_{H_2} \sim 3.2 \times 10^7 M_\odot$ assuming a Galactic CO-H$_2$ conversion factor $X = 3.0 \times 10^{-20} \text{cm}^{-2} \left( \text{K km s}^{-1} \right)^{-1}$ (Young & Scoville, 1991). The X-factor converts a measured velocity integrated CO line intensity to a column density of H$_2$ gas. It is necessary to use CO as a tracer of H$_2$ in cool, dense clouds as molecular hydrogen lacks low excitation emission lines.

4.2.2 IC 2233

IC 2233 is another example of a thin, bulge-less galaxy viewed close to edge on. It shows no signs of a dust lane in the central regions of its disk with only a few dark clouds visible. Rand (1996) detected Hα emission associated with H II regions across the disk of IC 2233, including a large complex in the outer region of the galaxy, indicating that there is ongoing star formation. In contrast to UGC 7321 the H II regions in IC 2233 are often located out of the mid-plane at up to $\sim 0.5 Z_s$ in the outer parts of the galaxy (Matthews & Uson, 2008). Observations by Matthews & Uson (2008) find that H I in IC 2233 is extended vertically and horizontally beyond the optical disk, with evidence for flaring in the outer gas disk. Attempts by Matthews et al. (2005) to detect CO emission from IC 2233 were unsuccessful leading to a 3-$\sigma$ upper limit on the mass of molecular hydrogen of $1.4 \times 10^6 M_\odot$. The distance to the galaxy is estimated to be 10 Mpc (Matthews & Uson, 2008).

4.2.3 NGC 4244

NGC 4244 is the closest galaxy in the sample lying at an estimated distance of only $\sim 4.4 \text{Mpc}$ (Seth et al., 2005a). It has a stellar mass estimated at $6 \times 10^9 M_\odot$ (Strickland et al., 2004). NGC 4244 shows many dark clouds in optical imaging of its central regions. Despite this, based on NIR photometry (Kodaira & Yamashita, 1996) conclude that the disk of NGC 4244 suffers from little internal extinction (although the NIR is less affected by dust extinction). Continuum subtracted Hα imaging obtained by Hoopes et al. (1999) shows H II regions extending up to $\sim 990 \text{pc}$ from the disk mid plane. The two largest H II regions are found in the outer galactic

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2This value has been re-scaled to the distance adopted in this paper (4.4 Mpc)
4.3 Data

Figure 4.3: High resolution imaging of the inner regions (approximately $\sim 3.4 \times 1.5\text{kpc}$) of the three galaxies studied. WFPC2 $F702W$ and $F814W$ composite image of UGC 7321 (top). ACS WFC $F606W$ filter images of IC 2233 (middle) and NGC 4244 (bottom). The white bar in the top right corner of each image has a length of 500pc, assuming the distances in Table 4.1. UGC 7321 and NGC 4244 show the presence of dark clouds in their nuclear regions that are seen in lower numbers in IC 2233.

disk. The work of Olling (1996) investigating the H$_1$ distribution in NGC 4244 shows that the gas distribution appears to be slightly extended radially compared to the stellar disk. Both Matthews & Gao (2001) and Sage (1993) report the detection of CO emission from NGC 4244 and the estimated H$_2$ mass is $1.4 \times 10^7M_\odot$.

4.3 Data

All three galaxies have been observed in the optical by the Sloan Digital Sky Survey (SDSS) in $u, g, r, i$ and $z$ bands and the data are available under data release seven (Abazajian et al., 2009). The images were downloaded from the SDSS archive and fluxes in each band were extracted using GAIA’s aperture photometry tool. It was necessary to reanalyze the SDSS images to extract reliable photometry as each galaxy appeared to have been split into multiple components during the SDSS photometric reduction, which can be a common feature of automated reduction in large surveys when dealing with large galaxies.

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3http://www.SDSS.org/dr7/
This work has also made use of $B$ band imaging of UGC 7321 and IC 2233 obtained at the 3.5m WIYN telescope at Kitt Peak, AZ. These observations are described in Matthews et al. (1999) (UGC 7321) and Matthews & Uson (2008) (IC2233). The images have been flux calibrated and are of a higher resolution than the SDSS imaging available. In the case of NGC 4244 no high resolution data is available and so the SDSS $r$ band imaging will be used for the optical comparisons.

High resolution Hubble Space Telescope (HST) imaging is also available for the three galaxies. NGC 4244 and IC 2233 have previously been observed using the Wide Field Channel (WFC) of the Advanced Camera for Surveys (ACS) with the $F606W$ filter (Seth et al., 2005b). These data were accessed from the Multi mission Archive at STScI (MAST). Imaging of UGC 7321 is available from the Wide Field Planetary Camera 2 (WFPC2) and a composite $F702W$ and $F814W$ image previously presented in Matthews & Wood (2001) is used. HST images of the inner regions of each galaxy can be seen in Figure 4.3.

The MIR and FIR observations of the three galaxies were obtained with the Spitzer Space Telescope’s IRAC and MIPS imagers. Data were obtained for this project under Spitzer PID 20432 (PI: L. Matthews) along with observations taken from PIDs 3 (PI: G. Fazio) and 40204 (PI: R. Kennicutt). These data have recently been used as part of the Spitzer Local Volume Legacy (LVL) survey Dale et al. (2009). This provides imaging and photometry for a large sample of galaxies within ~11Mpc. Data are available for all four IRAC bands (3.6, 4.5, 5.8 and 8.0$\mu$m) as well as three MIPS bands (24, 70 and 160$\mu$m) with photometry provided for each band after foreground stars and background galaxies have been removed and aperture corrections applied.

Photometry is also available based on near-infrared (NIR) 2MASS$^5$ imaging using apertures matched to those used in the extraction of the IRAC and MIPS fluxes. Spitzer LVL survey imaging can be accessed via an online archive$^6$ and NIR, IRAC and MIPS fluxes are available in Table 2 of Dale et al. (2009).

Lee et al. (2011) provide a catalogue of matched far and near-UV observations for galaxies contained in the Spitzer LVL survey that have been observed with GALEX. The GALEX bands are centered at 1528Å (far-UV) and 2271Å (near-UV) (Morrissey et al., 2005) and fluxes have been extracted using the apertures obtained from the FIR Spitzer data for consistency. The UV

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4http://archive.stsci.edu/index.html
5http://www.ipac.caltech.edu/2mass/
6http://irsa.ipac.caltech.edu/data/Spitzer/LVL/
data provide a constraint on the emission from the young stellar population which, due to the higher opacity at UV wavelengths, will play an important role in heating the diffuse dust.

4.4 Radiative Transfer Model

In order to produce synthetic images and SEDs for comparison to the data a Monte Carlo radiation transfer modeling scheme has been adopted.

4.4.1 Emissivity and Dust Distributions

The model allows energy packets emitted within a smooth stellar emissivity distribution to be tracked as they propagate through a dusty medium. For both the emissivity and dust a smooth “double exponential” distribution is adopted:

\[
\rho(\sigma, z) \propto \exp(-|z|/Z) \exp(-\sigma/R),
\]

where \(\rho(\sigma, z)\) is the density at a point in the galaxy specified by \(\sigma\), the cylindrical radius, and \(|z|\) the height above or below the galactic plane. This analytic distribution has been shown to provide a good description of the observed brightness profiles of edge-on galaxies even in the presence of spiral arms (Misiriotis et al., 2000; Jurić et al., 2008). The scale lengths \(R\) and \(Z\) can be independently varied for both components as necessary. The stellar emissivity and dust density are discretised across a three dimensional spherical grid of cells to allow the Monte Carlo radiation transfer routines to be used. To reduce the number of free parameters in the model no attempt has been made to take account of clumpy substructure within either the emissivity or dust distributions, which may be important in reproducing the optical properties of galactic disks (Matthews & Wood, 2001; Bianchi et al., 2000; Pierini et al., 2004; Schechtman-Rook et al., 2012). This also allows the use of a lower resolution grid of cells, reducing the memory requirements of each radiation transfer simulation.

4.4.1.1 Emission Sources

To begin the radiative transfer process it is necessary to sample an initial wavelength of emission for each photon packet. Wavelengths are chosen to reproduce the intrinsic unattenuated stellar SEDs produced by the population of stars present in each galaxy. For this purpose a set of synthetic stellar SEDs was constructed using the GALEV\(^7\) codes (Kotulla et al., 2009). These are shown in Figure 4.4. The GALEV routines allow the user to provide input parameters describing the conditions under which to construct the models, allowing a wide variety

\(^7\)http://www.galev.org/
<table>
<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>B-band Luminosity</th>
<th>Distance (kpc)</th>
<th>Vrot (km/s)</th>
<th>µB, i</th>
<th>MH1</th>
<th>MH2</th>
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<td>95</td>
<td>4.4</td>
<td>3.6</td>
<td>SD</td>
</tr>
<tr>
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<td>88</td>
<td>10</td>
<td>8</td>
<td>SD</td>
</tr>
<tr>
<td>IC 7324</td>
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<td>1.1</td>
<td>105</td>
<td>1.1</td>
<td>105</td>
<td>SD</td>
</tr>
</tbody>
</table>

Table 4.1: Galaxy Properties
Table 4.2: The intrinsic stellar template model parameters. Columns are: (1) galaxy name (2) Fraction of remaining gas converted to stars during burst (3) Age of the galaxy at the time of the star formation burst (4) Age of the galaxy adopted to fit the broadband fluxes (5) SFR at adopted age.

<table>
<thead>
<tr>
<th>Name</th>
<th>Initial SFR $\left(\text{M}_\odot\text{yr}^{-1}\right)$</th>
<th>Burst Mass Fraction</th>
<th>Burst Time $\left(10^8\text{yr}\right)$</th>
<th>Age $\left(10^9\text{yr}\right)$</th>
<th>SFR $\left(\text{M}_\odot\text{yr}^{-1}\right)$</th>
</tr>
</thead>
<tbody>
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<td>0.1</td>
<td>7</td>
<td>8.6</td>
<td>0.02</td>
</tr>
<tr>
<td>IC 2233</td>
<td>0.005</td>
<td>0.1</td>
<td>8</td>
<td>9.1</td>
<td>0.04</td>
</tr>
<tr>
<td>NGC 4244</td>
<td>0.03</td>
<td>0.1</td>
<td>7.5</td>
<td>9.4</td>
<td>0.04</td>
</tr>
</tbody>
</table>

of galaxy types to be modeled. Each model used initially has a constant SFR for several Gyrs which is followed by an exponentially decreasing burst of star formation with an e-folding time of 1 Gyr. Table 4.2 lists the values used within the model for each galaxy. In all cases a Salpeter initial mass function with slope $\alpha = -2.35$ is used and the metallicity of the gas is allowed to change with time to remain chemically consistent. Also included are the effects of continuum and line emission from gas within the model SEDs as these may contaminate the broad band filters.

In searching for appropriate stellar populations to model the observed stellar SED it has been found that a wide range of ages can provide adequate fits. This has previously been noted by other authors (Zackrisson et al., 2005; Vorobyov et al., 2009) who have suggested that based on additional information, such as $H\alpha$ equivalent widths and oxygen abundance gradients, that old stellar populations are more probable in samples of blue LSB galaxies. The ages adopted here range from $8.6 - 9.4$ Gyrs which are in agreement with Jimenez et al. (1998) who suggest ages larger than 7 Gyrs for LSB galaxies. It should be noted, however, that the conclusions on the dust masses and distributions are most sensitive to the shape of the intrinsic stellar SED and will not be significantly altered by the exact age, metallicity or star formation history of the underlying stellar population which produces it.

The SFRs for UGC 7321 and IC 2233 have previously been estimated based on the observed $H\alpha$ luminosity. SFRs of $\sim 0.02$ and $0.05 \text{M}_\odot\text{yr}^{-1}$ have been found for UGC 7321 (Matthews & Wood, 2003) and IC2233 (Matthews & Uson, 2008) respectively, which are in reasonable agreement with the values in Table 4.2. The SFR of NGC 4244 has been estimated based on the $H\alpha$ luminosity, $L_{H\alpha} = 10^{40}\text{erg s}^{-1}$ (Kennicutt et al., 2008), and the SFR - $H\alpha$ relation taken from Kennicutt (1998a). Together these yield a SFR $\sim 0.079 \pm 0.023 \text{M}_\odot\text{yr}^{-1}$ which is roughly consistent with the value adopted for the template stellar SED. The SFRs of the LSB galaxies studied here are significantly lower than estimates of the SFR for the Milky Way.

A single stellar SED is assumed for each galaxy modeled. No account of stellar gradients,
Figure 4.4: The intrinsic stellar emission templates used for our three galaxies. The fluxes have been scaled for comparison. The important property of each template is its shape, as this is used within our models to correctly sample the stellar emission. Each galaxy required a different intrinsic stellar template to match the observation in the UV, optical and NIR. The templates were produced using GALEV \cite{Kotulla2009} and model parameters can be found in Table 4.2.
4.4. Radiative Transfer Model

which may be important in LSB galaxies (Matthews & Wood, 2001) is made in order to reduce the complexity of the model. It is not believed that the stellar gradients will have a significant impact on the SED and derived dust disk properties.

Also included is a secondary emission component from obscured star formation regions that may be necessary to account for the total FIR emission. As such emission takes place from compact regions that are below the resolution of the spherical grid currently employed in the radiation transfer, a separate model has been created. The regions are approximated by a single central star surrounded by a shell of dust and gas. The shell has a $V$ band optical depth of $\tau_V \sim 88$ and extends from a distance $d = 10^{-4}$pc out to 2.3pc. The size of the shell was chosen to best reproduce the shape of the observed FIR emission of star forming regions observed by Chini et al. (1986). The shell is exposed to internal heating from a stellar source, with emissivity sampled from a model atmosphere of temperature $T = 36,000$K (Kurucz, 1993). The shell is also illuminated from the exterior by a radiation field approximating the mean intensity in the plane of the galaxy model. Due to the size of the clouds, however, the luminosity incident on the exterior is typically much smaller than the luminosity of the central source and hence diffuse illumination has little effect on the overall SED. The output SED can be seen in Figure 4.5 along with observed data points of 56 Galactic compact H II regions taken from Chini et al. (1986). A single SED is used to approximate all compact sources in the galaxy. The spatial distribution of compact sources is an exponential disk (Eq. 4.1) with $Z = 0.1$ kpc and $R = 1.8$ kpc in all models. This secondary emission component, from obscured star forming regions, has previously been found necessary to reproduce the FIR emission in HSB galaxies (Popescu et al., 2000; Misiriotis et al., 2001a; Popescu et al., 2011). Due to the high optical depth of the compact regions very few photons are able to escape from star forming regions into the diffuse ISM. This may lead to problems with reproducing the UV portion of the SED as in reality a fraction of the direct stellar photons would escape through the clumpy cloud structure (Indebetouw et al., 2006).

Other methods to account for such emission include utilizing sub grid resolution models for individual star forming regions (Jonsson et al., 2010) or the inclusion of adaptive grids to allow radiation transfer on the small size scales needed. Current adaptive grid models of an entire galaxy, however, lack the resolution to resolve individual star forming regions (Bianchi, 2008). The problem of resolution is one of the main issues with producing fully self-consistent radiative transfer models on galactic scales.
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Figure 4.5: The template for the emission from compact sources between 10 and 2000\(\mu m\). The solid line shows the model output SED as it varies with wavelength. The model comprises of a central star (\(T=36,000\)K) heating a constant density shell of gas and dust surrounding it. The shell extends from \(10^{-4} - 2.3\)pc and has a V band optical depth of \(\tau_v \sim 88\). The total luminosity included in each cloud model is \(2.5 \times 10^5 L_\odot\) and each has a dust mass of \(5 \times 10^4 M_\odot\). Data points represent the median observed properties of 56 compact H\(\text{II}\) regions found by [Chini et al. (1986)] at 12, 25, 60, 100 and 1300\(\mu m\). Error bars show the range of values observed at each wavelength.
4.4. Radiative Transfer Model

4.4.1.2 Dust Model

The radiative transfer of the stellar emission is treated with the methods described in chapter 2 in order to produce the full multi-wavelength SED. The composition and size distribution of the large grains is taken from the work of Kim et al. (1994) who used a mixture of silicate and graphite grains to fit the observed extinction in the Milky Way and the emission from PAH molecules and VSGs is calculated from precomputed emissivity files from Draine & Li (2007). This method was presented by Wood et al. (2008) to compute the SED of proto-planetary disks. This treatment of large dust grains, without the extensions added to treat transient heating of very small grains (VSG) and polycyclic aromatic hydrocarbon (PAH) molecules, has previously been used by Savoy et al. (2009) to investigate the dust content of early-type galaxies. One small caveat to this treatment is the fact that the Kim et al. (1994) dust models have been fitted to the observed properties of Milky Way dust without the inclusion of PAH/VSGs. This means that the PAH/VSGs are not included in the extinction component but are in the emission component. The ratio of absorption to scattering will therefore not be consistent between the two and this effect will be greatest in the UV where PAH/VSGs have the biggest impact.

As the ISM conditions of LSB galaxies are likely different from those found in the Milky Way, it is possible that the treatment of the PAH/VSG dust components may be inappropriate. It is known that the strength of the PAH emission relative to that from VSGs, estimated using the $f_{\nu}(8\mu m)/f_{\nu}(24\mu m)$ color, decreases with decreasing metallicity (Engelbracht et al., 2005; Madden et al., 2006). This is likely due to either the delayed formation of PAH molecules in low metallicity environments (Galliano et al., 2008) or destruction/processing caused by the harder radiation field (Gordon et al., 2008; Madden et al., 2006). It is therefore possible that the treatment, which assumes Milky Way abundances, may overestimate PAH emission relative to that of the VSGs. The fraction of the total dust mass contributed by PAH/VSGs is also fixed to a value inferred for the Milky Way (Draine & Li, 2007). This could affect the relative strength of the MIR and FIR emission. As mentioned before the PAH/VSGs are treated separately from the larger grains and this inconsistency may also contribute to the differences in the MIR colours. It is also possible for that changes in the in the SFR can impact the $f_{\nu}(8\mu m)/f_{\nu}(24\mu m)$ ratio (Bendo et al., 2008) and this effect is accounted for in this treatment of the dust emission.

To model the appearance and SED of each galaxy the following free parameters of the
model can be altered: stellar scale length, stellar scale height, dust scale length, dust scale height, stellar luminosity, total dust mass, inclination and the luminosity of the obscured star formation component.

The overall fitting process was done manually to find the set of parameters that could provide adequate fits to both the optical and the UV-FIR SED.

4.5 Results

Initial values for the fitting process were taken from sources in the literature. Matthews & Wood (2001) have previously investigated UGC 7321 using a three dimensional Monte Carlo scattered light code and their parameters for a smooth stellar and dust distribution were adopted as initial values in this case. Matthews & Uson (2008) and Fry et al. (1999) have previously estimated the scale lengths of IC2233 and NGC 4244 respectively, by fitting an exponential function to the observed surface brightness profiles. While the functions used take no account of the effects of dust on the galaxy profiles they should provide reasonable initial estimates for the stellar distributions assuming that dust effects are not severe. From the work of Xilouris et al. (1999) on high surface brightness, edge-on, galaxies the relation that the dust scale heights would be approximately half the stellar scale heights and the dust scale lengths around 1.4 times larger than the stellar values was initially adopted. We adopt a fixed stellar scale height for all wavelengths here when in reality the stellar scale height should be a function of wavelength, with younger stars having a smaller scale height than older ones. Ideally the scale height of the young stars that produce most of the UV emission would be equal to that of the disk of star forming regions as that is where they originate. Here we have opted to keep a fixed stellar scale height for simplicity and to reduce the number of free parameters.

One of the main difficulties in modeling the dust distributions of LSB galaxies is that their disks appear to be optically thin, even when viewed edge on. When modeling the appearance of HSB galaxies, the effects of the dust distribution can be quantified based on the presence of a dust lane along the galactic mid-plane. As none of the galaxy sample shows any sign of a dust lane the problem becomes more degenerate. Initially the dust mass was increased in the adopted geometry until the effects of the dust became obvious and the optical profiles of the model galaxy no longer matched the shape of the observed data. It was found that the dust mass required to reprocess the stellar light and reproduce the observed FIR emission could not be located in an average HSB type dust disk without revealing its presence by flattening

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4.5. Results

Figure 4.6: Observed (left) and synthetic (right) images of UGC 7321 at, from top to bottom: B band, 3.6\,\mu m, 8\,\mu m, 70\,\mu m and 160\,\mu m.

the optical profile in the central region of the galaxy. The inclination angle of the galaxies was initially set to 90 degrees and then altered to fit the optical profiles of each galaxy.

It has been discovered that the optical appearance and total FIR emission of the LSB galaxies can be reproduced by removing the constraint that the dust be more concentrated in the galactic mid plane than the stars. If the dust scale height is taken to be equal to the stellar scale height then it is also possible to fit the optical appearance of the galaxy adequately. In this case, however, a significantly larger dust mass can be accommodated within the dust disk without the appearance of a dust lane. In order to reproduce the observed FIR flux distribution it was also necessary to increase the dust scale length. When the dust is vertically extended into a disk with a larger scale height that is well mixed with the stellar population, the exact radial distribution of the dust becomes poorly constrained from optical data alone. The dust scale length was found to be between 1.8 – 2.6 times the stellar scale length for our LSB disk galaxies.

The best fit parameters for the models of each galaxy can be found in Table 4.3. $R_s$ and $R_d$ are the radial scale lengths of the stars and dust while $Z_s$ and $Z_d$ are the vertical scale heights. $L_s$ is the intrinsic bolometric luminosity of the stellar population. $M_d$ represents the total dust mass and $i$ the inclination angle. $L_{\text{cloud}}$ gives the luminosity emitted from the template of compact dust emission (see section 4.4.1.1). $\tau_{\text{face}}$ and $\tau_{\text{eq}}$ give the V band face-on and equatorial optical depths respectively.\(^8\)

Figures 4.6, 4.7 and 4.8 show a comparison of the B (or r), 3.6\,\mu m, 8\,\mu m, 70\,\mu m and 160\,\mu m data (left panel) and synthetic images (right panel). In general the B (or r) and 3.6\,\mu m model images match the large scale morphology of the data reasonably well. Differences are,\(^8\)

\[^{8}\] $\tau_{\text{face}}$ is the optical depth from the disk centre to the edge of the model grid perpendicular to the plane of the disk. $\tau_{\text{eq}}$ is measured from the disk center to the edge of the model grid parallel to the disk plane.
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Figure 4.7: Observed (left) and synthetic (right) images of IC 2233 at, from top to bottom: B band, 3.6\( \mu \)m, 8\( \mu \)m, 70\( \mu \)m and 160\( \mu \)m.

Figure 4.8: Observed (left) and synthetic (right) images of NGC 4244 at, from top to bottom: r band, 3.6\( \mu \)m band, 8\( \mu \)m, 70\( \mu \)m and 160\( \mu \)m.
4.5. Results

however, apparent in the longer wavelength emission at 8, 70 and 160\(\mu m\) that is dominated by emission from PAHs and dust grains. IC 2233 and NGC 4244 show significant structure in their 8 and 70\(\mu m\) images, suggesting that perhaps a more complex non-axisymmetric dust distribution is needed. In both galaxies several small point like sources in the outer disk are prominent sources at 70\(\mu m\). These are likely star forming regions as they appear brighter at shorter wavelengths and show associated emission in GALEX far-UV and H\(\alpha\) imaging. The 160\(\mu m\) emission from all three of the model galaxies shows a significant deviation from the data. The models predict a centrally concentrated 160\(\mu m\) image while the data suggest a more diffuse distribution. Figures 4.9, 4.10 and 4.11 show \(B\) (or \(r\)) band intensity profiles parallel to the minor and major axes of the galaxies at various points while figures 4.12, 4.13 and 4.14 show the output model SEDs for the three LSB galaxies.

Overall the models are able to reproduce the global properties of the data. The surface brightness slices parallel to the minor axis and along the major axis show a similarity to the data and deviations are likely caused by the comparison of smooth axisymmetric models to observations of a galaxy that shows a clear clumpy structure (see Figure 4.3). The main discrepancies found between the surface brightness of the model and data generally occur in the central regions of the galaxies. As can be seen in Figure 4.3 these are also the regions that show the greatest number of dark clouds and bright star clusters. Our smooth axisymmetric model is not able to reproduce such structures and so only a relatively poor fit can be achieved in the central regions.

The short dashed line in Figure 4.12 shows the result of fitting the optical imaging of UGC 7321 using the average HSB galaxy stellar-to-dust scaling relation of Xilouris et al. (1999). In order to produce the required 70\(\mu m\) emission a large luminosity is assigned to the obscured star formation template (see section 4.4.1.1). However, this scenario underestimates the 160\(\mu m\) emission by a factor \(\sim 2\).

In the SEDs the shorter wavelength data from the UV through to NIR originate in the underlying stellar populations and can be highly attenuated by the diffuse dust in the ISM. Most of the photons absorbed by the dust, in these models, originated as short wavelength UV emission. This can be seen in Figure 4.12 as the difference between the intrinsic stellar emission (long dashed line) and the observed emission (solid line) once the photons have propagated through the dusty ISM. The amount of absorption tends to decrease with increasing wavelength as the dust opacity decreases and the photons are able to travel through the
<table>
<thead>
<tr>
<th>Name</th>
<th>$R_s$</th>
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<th>$R_d$</th>
<th>$Z_d$</th>
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<td>33.5</td>
<td>2.38</td>
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Table 4.3: Fitted Galaxy Parameters
4.5. Results

Figure 4.9: The top two plots show UGC 7321 $B$ band surface brightness slices parallel to the minor axis at the galaxy centre (top), and 3 kpc radial distance along the major axis (middle). The lower panel shows the surface brightness variation along the major axis. All slices are average values taken across a $\sim 60$pc region. Solid lines show the predicted intensity based on our best fitting Monte Carlo radiation transfer models and crosses represent the data taken from the $B$ band image.
Figure 4.10: As in Fig. 4.9 but for IC 2233.
Figure 4.11: As in Fig. 4.9 but for NGC 4244 and utilizing SDSS $r$ band rather than $B$ band data.
Figure 4.12: The observed and modeled SED of UGC 7321. Square points indicate an observed flux from one of our data sources either GALEX, SDSS, 2MASS, SDSS, or Spitzer/IRAC/MIPS along with their associated errors. Error bars associated with SDSS imaging do not include the contribution of the sky subtraction or Spitzer/IRAC/MIPS along with their associated errors. Error bars associated with SDSS imaging do not include the contribution of the sky subtraction errors. The solid line shows the model overall SED as calculated from the best-fit to the WIYN B band image. Open circles show the predicted fluxes for Spitzer/IRAC/MIPS bands. The long dashed line indicates the input, unattenuated, stellar template plus compact dust emission template. The dotted line shows the input, unattenuated, stellar template plus compact dust emission template. The double line shows the best-fit model when an average stellar-dust distribution for HSB galaxies (Xilouris et al., 1999) is used in the optical imaging.
Figure 4.13: The above plot shows the model SED of IC 2233 (solid line) along with the available data (squares). Open circles indicate the predicted model fluxes for the filters used in the observations. The dashed line shows the intrinsic SED of the emissivity sources (both stellar and dust emission from unresolved sources).
Figure 4.14: Same as Figure 4.13 but for NGC 4244.
4.6. Discussion

ISM with a lower probability of interaction. The models can reproduce the observed optical and NIR fluxes well but show slight discrepancies in the FUV emission. The models are also unable to reproduce the $z$ band flux ($0.893\mu m$). It is believed this may be due to the lower S/N in the $z$ band combined with the intrinsic low surface brightness of the galaxies, leading to galaxy flux being lost during removal of the sky background.

The 5.8 and 8.0\mu m IRAC bands trace emission from PAH molecules while the MIPS 24\mu m emission is produced primarily by the VSGs in this case. Observationally it has been found that the 24\mu m emission is mostly produced by large grains heated near massive stars (Bendo et al., 2008) and the difference here is caused by the limitations of the resolution in the simulations. In all three cases the 8.0\mu m emission is over-predicted by our models. The 24\mu m flux is over-predicted by the model of UGC 7321, under-predicted for IC 2233. This behavior in the MIR is likely a result of our treatment of the PAH/VSG emission which is based on Milky Way abundances and illuminating radiation field shape (see 4.4.1.2). Both the relative abundances of PAH molecules and VSGs in LSBs and the shape of the ISRF in LSBs are likely different causing the discrepancies observed in the MIR.

The larger, cooler dust grains are responsible for the peak of the FIR emission bracketed by the MIPS observations at 70 and 160\mu m. In all three cases it has been possible to reproduce the FIR 70 and 160\mu m emission, within the quoted photometry errors, using these models.

4.6 Discussion

The model outputs suggest that it is possible to provide a good global fit to the optical appearance of LSB galaxies, while at the same time reproducing the observed FIR emission. At some locations, however, such as the central region of UGC 7321 (Figure 4.9, top) there is a clear discrepancy between the data and model. In most cases this is likely to occur due to structure in the galaxy that is not included in the models, such as star clusters, H\textsc{ii} regions, and optically thick dust clumps and other limitations of the simulations such as insufficient resolution.

4.6.1 Implications of the Models

In this analysis it has been found that in order to accommodate the mass of dust required to reprocess the FIR emission seen in this sample of three LSB galaxies it is necessary for the dust to be located in a diffuse disk with a scale height at least equal to that of the stellar population. This is in contrast to the dust distributions obtained by previous studies of HSB galaxies (see
Chapter 4. The Stability of Low Surface Brightness Disks Based on Multi-Wavelength Modeling

Section 4.5, which find the dust to be located in a diffuse disk with approximately half the scale height of the stellar disk. The main observational signature of the smaller vertical extent of the dust in HSB galaxies is the central dust lane observed when the inclination approaches edge-on. Dalcanton et al. (2004) have previously noted that in a sample of edge on galaxies that spans a range in $V_{\text{rot}}$ there appears to be a remarkably sharp divide between galaxies that contain dust lanes and those that do not at around $V_{\text{rot}} \approx 120\text{km s}^{-1}$, with no abrupt change in the stellar or H\textsc{i} surface densities. They attribute this sharp divide to the onset of radial instabilities in galactic disks causing the vertical collapse of the ISM when perturbed by spiral structure.

The stability of the cold gas disk can be estimated from the $Q$ (Toomre, 1964) values where

$$Q = \frac{\kappa \sigma}{\pi G \Sigma}$$

and $\kappa$ is the epicyclic frequency, $\sigma$ the velocity dispersion, $G$ the gravitational constant and $\Sigma$ the mass surface density. This stability measure is an estimate of a local region’s ability to collapse under self-gravity before shearing can disrupt it. Several parameterizations exist to calculate the $Q$ values from observable quantities (Jog & Solomon, 1984; Rafikov, 2001; Elmegreen, 2011) but they generally all require an estimate of the epicyclic frequency ($\kappa$), velocity dispersion ($\sigma$) and the mass surface density ($\Sigma$).

If the disk is unstable the collapse leads to a higher gas density in the central galaxy having the effect of increasing the star formation rate and surface brightness. The increased gas density also causes a corresponding increase in the dust density in the galactic mid-plane which, when viewed edge-on, will produce the pronounced dust lanes observed. From Table 4.1 it can be seen that all three of the LSB galaxies have $V_{\text{rot}} < 120\text{km s}^{-1}$ and so from the results of Dalcanton et al. (2004) would be expected to be stable across most of their disks. This result suggests that as the disks are stable the gas and dust disk should have a scale height comparable to or larger than the stellar value, which is what has been found from modeling of the optical, NIR and FIR data.

In the case of the LSB galaxies studied here an alternative explanation for the comparable scale heights of the dust and stellar disks is that the scale height of the stellar disk is comparatively smaller than that found in HSB galaxies, contributing to the thin appearance of the galaxies. In this case the dust and gas disk scale height may be comparable to more massive galaxies but a drop in stellar scale height has concentrated the stars within the dusty ISM.
4.6. Discussion

Bizyaev & Kajsin (2004) have observed that stellar disks appear to become thinner as the $R$ band central surface brightness dims, which provides evidence that we may indeed be seeing a reduced stellar scale height in the LSB galaxies studied here. This effect may be due to the inefficiency of processes that contribute to the vertical heating of the stellar component such as scattering by giant molecular clouds, the effects of bar formation and a lack of gravitational interactions with neighboring galaxies.

Alternatively the effects observed may be a combination of both the processes mentioned above. An increase in the dust disk scale height caused by the stability of the ISM, coupled with a relative flattening of the stellar disk. Both effects combined would then result in comparable scale heights of the dust and stellar distributions.

Previous works have suggested that the dust scale length in galaxies may range from being only slightly larger than the stellar scale length (Muñoz-Mateos et al., 2009) to being moderately extended (Xilouris et al., 1999; Tempel et al. 2010) or even up to an order of magnitude larger (Holwerda et al., 2005). The average value of dust scale length found here is $R_d = 2.3 \pm 0.24 R_s$, which is slightly larger than previous values based on FIR and optical extinction modeling but significantly smaller than the value estimated by Holwerda et al. (2005) from background galaxy counts.

The low SFRs observed in LSB galaxies are likely caused by the vertically and radially extended gas distributions leading to low surface and volume densities that inhibit star formation via the formation of cold, dense clouds. van der Hulst et al. (1993) find a mean peak H\textsc{i} surface density, in a sample of LSB disk galaxies, of $4.6 \pm 1.4 \, M_\odot \, pc^{-2}$. This value is around a factor $\sim 2$ lower than that found by Cayatte et al. (1994) for HSB Sd galaxies. Although the low density of LSB galaxy disks leads to gravitational stability and prevents global star formation driven by spiral density waves, star formation still occurs in localized high density regions. H\textalpha imaging suggests that this does not occur in the same pattern in all LSB disk galaxies. UGC 7321 shows H\textalpha emission concentrated in a thin layer (Matthews et al. 1999) while IC 2233 and NGC 4244 show more vertically extended emission and large star forming complexes in the outer disk (Hoopes et al. 1999; Matthews & Uson, 2008). These differences in the morphology of the current star formation suggest that there may be differences in the clumpy ISM structure. This may indicate a more gradual transition in the ISM structure across galaxies with decreasing $V_{\text{rot}}$ rather than simply an abrupt change at a given galactic mass.
4.6.1.1 Recent Results

Recently NGC 4244 has been observed by the Herschel satellite at FIR and sub-mm wavelengths. Herschel has a greater angular resolution than Spitzer and is able to provide observations further in to the sub-mm, providing information about the cold dust. Even with the increased resolution the galaxy is only resolved in the radial direction by Herschel and remains unresolved vertically. Holwerda et al. (2012b) have presented the Herschel data along with radiation transfer models of the UV/optical - sub-mm SED. Their results confirm that the dust scale height in NGC 4244 is comparable to the stellar scale height. Moreover they also find that the sub-mm observations are under predicted by the models presented here due to a lack of cold dust emission, which is not observable with the Spitzer data. They find that in addition to the increased dust scale heights an increase in the dust scale length is also necessary to fit the data. The flatter distribution of dust results in an increase of the dust mass required by their models compared to that used here. The observations of Holwerda et al. (2012b) are part of a larger galaxy sample being observed by Herschel under the NHEMESES project (Holwerda et al., 2012a) that should provide a wealth of new data on a number of low mass disk galaxies and allow a greater understanding of the processes shaping the dusty ISM.

4.6.1.2 Attenuation Inclination Relation

The attenuation inclination relation shows the reduction in the observed intensity for a galaxy when it is viewed at inclinations from face-on ($\theta = 0^\circ$) to edge-on ($\theta = 90^\circ$). The attenuation in magnitudes is defined as

$$A_\lambda = -2.5 \log[f_\lambda(esc)]$$

(4.3)

where $f_\lambda(esc)$ is the escape fraction in the direction of the observer

$$f_\lambda(esc) = \frac{\text{observed total intensity}}{\text{unextinguished total intensity}}.$$  \hspace{1cm} (4.4)

Figure 4.15 shows the attenuation inclination relations calculated for disks with central face-on, B band optical depths of 0.1, 1.0, and 5.0. The black lines show the relation for a “standard” type galaxy with a thick and thin dust disk as calculated by Tuffs et al. (2004). The LSB attenuation inclination relation shows a different shape to the standard galaxy relation at all optical depths. The LSB disk shows a higher face-on attenuation due to the better mixing of the dust and stars but at high inclinations the standard galaxy attenuation increases to a higher level than the LSB disk. This increase is due to the thin dust disk included in the
4.6. Discussion

Figure 4.15: The calculated attenuation inclination relations for a standard galactic dust disk (black) and the LSB type disk (red). The three sets of curves are calculated for, from top to bottom, central face-on, B band optical depths of 0.1, 1.0 and 5.0.

standard model which is associated with star formation regions.

The shape of the attenuation curve is different for both dust distributions and suggests that the LSB type distribution is able to produce higher internal attenuation values for a face-on galaxy but lower values for an edge on galaxy. This result may complicate the interpretation of observational data on the attenuation inclination relation (e.g. Driver et al., 2007) and will add to uncertainties which can be caused by inhomogeneous dust distributions.

It can also be seen from Tables 4.3 and 4.1 that in order to model the FIR emission of UGC 7321 and NGC 4244, which are known to contain molecular hydrogen in the nuclear regions of their disks, it has been necessary to include a larger fraction of emission from our template of embedded compact star forming regions. IC 2233 on the other hand has not been detected in CO emission and, indeed, is shown to require a much lower amount of emission to originate from compact sources with a warmer dust emission peak. This result is not surprising when one examines high angular resolution optical imaging of UGC 7321 and NGC 4244 (Figure 113).
4.3) in which dark clouds suggestive of molecular gas are observed. IC 2233 shows some dark clouds in its central regions but less than the other two galaxies studied, reinforcing the suggestion that it is the galaxy poorest in interstellar molecular gas.

From the total dust masses (Table 4.3) and the H\textsuperscript{I} and molecular hydrogen masses from the literature (Table 4.1) the global gas-to-dust ratios can be calculated. After accounting for the contribution of Helium (assuming $Y = 0.25$) global gas-to-dust ratios of $\sim 666$ (UGC 7321), 734 (NGC 4244) and 1266 (IC 2233) are found. These values are significantly higher than the Galactic value of $\sim 140$ Whittet (1992). The gas-to-dust ratios of UGC 7321 and NGC 4244 fall between those found for the Large Magellanic Cloud (Koornneef, 1982) and the Small Magellanic Cloud (SMC) (Bouchet et al., 1985) while the value for IC 2233 is consistent with that of the SMC.

4.6.2 Model Limitations and Future Prospects

It is somewhat unclear what effect the adoption of a clumpy dust and emissivity distribution would have on the FIR emission of our galaxy sample. Matthews & Wood (2001) found that in order to reproduce the optical appearance of UGC 7321 it was necessary to allocate approximately 50% of the dust mass to a clumpy component. The effect that such a two phase diffuse dust distribution may have on the FIR emission would depend on the associated emissivity distributions. Such dense clumps could be “quiescent” and represent over-dense regions of the ISM illuminated only by the diffuse ISRF, but recent evidence suggests that such clouds are optically thin and will contribute little to the attenuation and dust emission (Molinari et al., 2010). However, if the dark clouds seen in HST imaging are star forming molecular clouds then they will be illuminated by both the ISRF and by young stars embedded within them. It is thought that in the case of LSB galaxies the optical depths of the clumps are similar to those found for diffuse molecular clouds in the Milky Way (Matthews & Wood, 2001). In this case the clumpy component may provide a significant contribution to the FIR emission reducing the need to have a radially extended dust disk as is found using smooth density distributions.

It has also been shown by Indebetouw et al. (2006) that the observed SED of young stellar objects (YSOs) that are embedded in clumpy circumstellar material can have a strong dependence on the observer’s viewing angle (azimuth) and inclination. The observed MIR flux was found to vary by up to two orders of magnitude for the same highly embedded

\[^{9}\text{In the case of IC 2233 we use the upper limit H\textsubscript{2} mass of } 1.4 \times 10^{6}M_{\odot}\]
system viewed along a different sightline. The effects are more severe at shorter wavelengths. Although the case of YSOs is very different to the galactic environment studied here it should be noted that the effects of a clumpy galactic ISM containing optically thick clouds may cause viewing angle and inclination dependent effects on the MIR SEDs that are not accounted for in our smooth, axisymmetric models.

4.7 Summary

I have utilized multi-wavelength imaging and photometry in conjunction with sophisticated Monte Carlo radiation transfer codes to investigate the structure of three edge-on, LSB disk galaxies. The galaxies have been chosen to span a range in central optical surface brightness and molecular hydrogen masses.

I have been able to reproduce the global, optical appearance of all three galaxies using smooth emissivity and dust distributions. We find that the composition and size distribution of dust grains adopted, which are based on Milky Way extinction, provide a good match to the observed properties in our sample of LSB disk galaxies. The models also reproduce the total emission at 70 and 160\(\mu\)m for all three galaxies. However, the FIR morphology of the models appears more centrally concentrated than the more diffuse distribution suggested by the data and the models fail to predict recently obtained sub-mm data. Due to the treatment of PAH/VSGs the models also over predict the FUV emission and under predict the NIR and MIR emission slightly. There are also differences I find that the dust mass appears to be distributed in an exponential disk with a scale height comparable to or exceeding that of the stellar disk. This is in contrast to the findings for HSB galaxies where the dust disk is found to have a vertical scale height of approximately half the stellar disk (Xilouris et al., 1999). The comparable scale heights in the dust and stellar disks is likely associated with the increased stability of the ISM in LSB disks against vertical collapse (Dalcanton et al., 2004) and the thin nature of the stellar disks, which suggests minimal dynamical heating.

The dust masses and distributions derived suggest dust masses in the range \(1.16 - 2.38 \times 10^6 M_\odot\) corresponding to face on, V band, optical depths between \(\tau_{face} = 0.034 - 0.106\).

In future work I would like to re-perform the model fitting procedure taking account of the recent sub-mm data in order to further constrain the structure of these galaxies. I also hope to develop our radiation transfer models to include small scale non-axisymmetric structures which may shed further light on the structure of the ISM and star formation processes in LSB disk galaxies. The inclusion of radial variations in the dust disk scale heights, associated with
a flaring gas disk, could also prove important.
Active galactic nuclei (AGN) are a striking class of objects seen in observations of both the nearby and distant universe ($z = 0.002 – 7$). They often possess very high luminosities and some can outshining their parent galaxies, but their emission appears to originate from intrinsically very small volumes (~few pc$^3$). They are observed to emit their energy at a huge range in frequency, from X-ray to radio, and show spectra with emission lines that are broadened by velocities of thousands of $km s^{-1}$. Although still numerous in the local universe they appear to have been many times more abundant in the past (Croom et al., 2004), indicating that AGN are associated with the early phases of galaxy evolution. Due to their high intrinsic luminosity AGN can be observed in the distant universe and may be used as lighthouses providing insight into the conditions of the earlier universe. AGN activity and black hole (BH) mass are seen to correlate with galaxy stellar bulge mass and velocity dispersion (Marconi & Hunt, 2003; Gebhardt et al., 2000) which suggests that feedback from AGN can play an important part in galaxy evolution.

Observationally AGN are generally associated with small angular size, high luminosity and often short period variability on timescales of hours. The small size of AGN compared with
Figure 5.1: Composite image of the galaxy NGC 4051 which has been classified as a Seyfert 1 galaxy. The nucleus is obvious as the very bright point in the center of the galaxy.

their host galaxy means that they often appear as point like sources at the centre of the galaxy. At radio wavelengths some AGN show jets of material being expelled while other show little or no radio emission.

AGN luminosities are observed to range between $\sim 10^{43} - 10^{47}\text{ergs}^{-1}$ (Krolik 1999) which takes them from a few percent of the characteristic luminosity of field galaxies to thousands of times higher. These luminosities may be misleading, however, as there is evidence that some AGN may beam their output into only a small angle, rather than emit isotropically (Urry & Shafer 1984; Urry et al. 1991). It is clear, however, that they are a powerful energy source.

It is widely believed that the source of AGN activity is a central supermassive BH and an accretion disk of material surrounding it (Lynden-Bell 1969; Shakura & Sunyaev 1973). As
5.1. Thermal reprocessing by the accretion disk

In the above picture the central portion of an AGN is composed of a BH and an optically thick accretion disk of material. The disk is heated by the dissipation of viscous torques and irradiation by high energy photons produced close to the BH. Under the paradigm of thermal reprocessing, variations in the UV/optical flux can be explained by reprocessing of high energy ionizing photons and subsequent re-emission at wavelengths determined by the local surface temperature of the disk. This relationship should be observable in a correlation between the X-ray and UV/optical light-curves and also in the inter-band lags between the UV and optical light-curves.

Wanders et al. (1997) were able to identify time lag between the variations in the UV bands in the Seyfert 1 galaxy NGC 7469. The 1485, 1740, and 1825 Å bands were found to lag the 1315 Å band with delays between 0.25 – 0.35 days. The delays were found to be consistent with the UV continuum variations being produced within a thin accretion disk.

Figure 5.2: Optical spectra of the Seyfert galaxy UGC 1597 from the SDSS DR8 (Aihara et al., 2011). The broad hydrogen emission lines can be seen along with narrow emission lines from ionized oxygen. The BH attracts and captures gas from the central galaxy, an accretion disk of material forms around it. Viscous dissipation of energy within the disk heats the gas to temperatures where it becomes bright at UV/optical wavelengths.
Figure 5.3: Above is a plot from Wanders et al. (1997) showing the cross correlation function for various continuum bands and emission lines. Each has been correlated with the 1315Å band. The UV continuum bands show a small lag while the emission lines show a much longer lag suggesting that they are produced at a greater distance from the central engine.
5.1. Thermal reprocessing by the accretion disk

Collier et al. (1998) found that the optical continuum in the galaxy NGC 7469 lagged the UV with delays of $1.0 \pm 0.3$ days (4865Å) and $1.5 \pm 0.7$ days (6962Å), which is consistent with an irradiated accretion disk. In a sample of 14 AGN, Sergeev et al. (2005) found that there was a delay between the variations in the $V, R$ and $I$ bands compared to the $B$ band with the delay being increased at longer wavelengths. In addition it was found that the delays were systematically larger for higher luminosities ($\tau \propto L^b$ where $b = 0.4 - 0.5$) which is again consistent with UV/optical emission originating in an accretion disk. A correlation between the X-ray and optical variations in NGC 4051 has been observed by Breedt et al. (2010) with the optical variations lagging the X-ray by 1.2 days. Interestingly the same authors also observe a second peak in the cross correlation function at $\sim 39$ days which they attribute to scattering/and or thermal emission from dust just outside the dust sublimation radius. Lira et al. (2011) find correlations between the optical and near-IR light curves of two nearby AGN that are well represented by an accretion disk reprocessing model. Together these results present a strong case for the UV/optical/near-IR variations in AGN originating in the surface of an accretion disk.

However, there are some observations which suggest that the simple picture of disk reprocessing may not be able to explain the data obtained for all AGN. Maoz et al. (2002) found that there appeared to be no correlation between the X-ray and UV/optical continuum in NGC 3516, in monitoring over a timescale of years. Doroshenko et al. (2009) collected X-ray and optical data for the Seyfert galaxy 3C 120 and found that while the lags between the optical bands were consistent with a re-processing paradigm it appeared at times that the optical variations were leading the X-ray variations (negative lags) which is hard to resolve in a purely re-processing scenario (but see section 5.11.2.1). Other authors have suggested that the interplay between the X-ray and the UV/optical continuum variations may be more complex and consist of several processes including feedback effects from the UV to X-ray (Gaskell, 2008; Nandra et al., 2000). Cackett et al. (2007) fitted the optical SEDs and time delays in 14 AGN using an accretion disk reprocessing method and found that while it was possible to obtain good fits the results indicated distances for the AGN which gave very low values of $H_0$ (the Hubble constant). They attributed the discrepancy to likely effects produced by the simple thin disk, black body model used.
Chapter 5. Echo Mapping of Accretion Disks

5.2 Echo Mapping

Echo mapping (or reverberation mapping) \cite{Blandford1982, Peterson1993} provides a tool to extract a picture of the geometry of the reprocessing region within the accretion disk. The basic principle of echo mapping is that a system will respond to an input of ionizing luminosity in a certain way that is characterized by the geometry of the system and the location of the source of ionizing luminosity. We assume that the delay of the response compared to the input is purely determined by the distance that the photons must travel as they all travel at the same speed, namely $c$. We do not include the possible effects of the strong gravitational field found close to the central black hole. The shape and size of the reprocessing region can be estimated using the delays and we can determine structure on small scales that would be impossible to observe directly.

A simple example is to imagine that you are located at a source of ionizing photons and are surrounded, at a distance $r$, by a spherical shell of gas. If a $\delta$ function burst of photons is emitted isotropically then it will take a time $t_1 = r/c$ for the photons to reach the gas. The photons are absorbed and their energy instantaneously re-emitted, as emission line photons, isotropically by the gas. The return journey takes the same amount of time as the outward journey i.e., $t_2 = t_1 = r/c$ and at a time $t = t_1 + t_2 = 2r/c$ you would observe the response at your location. From the delay and the known velocity of the photons you would be able to estimate the distance to the shell, using only the delay. The situation becomes more complex when the observer is no longer at the source and the geometry of the system is more complex but the basic principle of echo mapping remains.

For this treatment to be accurate we have to assume that the time taken to reprocess the ionizing luminosity into line (or continuum) photons is much smaller than the light travel time in the system and this is certainly true for emission lines \cite{Peterson1993}.

The emission line or continuum flux that we observe can then be described as

$$L(t) = \int_{-\infty}^{\infty} \Psi(\tau)C(t - \tau)d\tau,$$

where $L(t)$ is the observed response, $C(t)$ is the driving ionizing light curve and $\Psi(\tau)$ is the transfer function of the system. The transfer function represents the response of the system as a function of delay ($\tau$) to a $\delta$ function burst. The transfer function encodes information about the shape and size of the reprocessing region so we may use it to gain information on
5.3 The “lamp post” model

In order to calculate the time-dependent variation in the X-ray and optical continuum a Monte Carlo radiation transfer code has been used. The “lamp-post” model has been adopted in which the X-ray source is assumed to be a point-like source at a height $H_x$ above the origin in the z-direction. Initially all photons are emitted isotropically at X-ray energies from the source located above the BH at a height $h_x$ which emits X-ray photons isotropically. A fraction of these impact the accretion disk where they can be scattered or absorbed. Photons A and B are both seen by a distant observer at a very similar delay as both have almost the same path length. Photon A will be observed as an X-ray as it has been scattered at the disk surface, while photon B has been absorbed and its energy re-emitted at UV wavelengths. At a later time photon C is observed in the optical as it interacted with the disk at a larger distance from the central source, where the temperature was lower.

Observationally it is possible to estimate the transfer function of a given object by collecting time series data that represent both the driving ionizing luminosity and the line or continuum emission that result. The problem is then to interpret the transfer function in terms of the geometry of the system which is responsible for producing it. For instance a flat accretion disk will produce a different signature to one which is highly flared due to heating or warped due to the misalignment of inflowing material. Hence there is a need to estimate the theoretical transfer functions of various geometries to help interpret observational results.

In this work I have focussed on estimating the transfer function for continuum emission driven by X-rays in an AGN accretion disk. As the different radii of the disk are at different temperatures the transfer function is a function of both time and wavelength.
X-ray source. They are propagated and allowed to interact with the dense material in the disk. Interactions can be scatterings, in which case the X-ray continues to propagate, or absorption. In response to the absorption of the X-ray energy there will be a response in the thermal continuum radiation of the inner accretion disk in the UV/optical. This is modeled by immediately releasing the energy at a wavelength appropriate for blackbody emission at the disk’s local surface temperature. This optical/UV photon is then followed in the same way as before. If an optical photon is absorbed then it is terminated and the next X-ray photon is emitted from the X-ray source. A simple illustration is given in figure 5.4.

The travel time for each energy packet to reach the observing plane is calculated simply by \( t = d/c \), where \( d \) is the cumulative distance travelled and \( c \) is the speed of light. Optical photons emitted from the disk retain the cumulative travel time of the X-ray photon which drove the emission and in this way the relative time delays between the X-ray and optical/UV continuum emission can be determined. This method assumes that the response time of the disk is small compared to the light travel times.

Photons that escape the system are binned in time and angle, for X-ray and additionally frequency in the case of the reprocessed optical photons. Images are also produced of the accretion disk at a specified viewing location as a function of time.

### 5.4 Density Structure

For the density structure of the accretion disk a flared disk geometry is adopted. The inner disk radius is set to be

\[
R_{in} = 3R_s = \frac{6GM}{c^2}, \quad (5.2)
\]

the last stable orbit of the accretion disk. The mid plane density is taken to be constant with radius and the variation with height out of the mid plane follows

\[
\rho = \rho_0 \exp\left(-\frac{1}{2} \left( \frac{z}{h(r)} \right)^2 \right) \quad (5.3)
\]

where \( \rho_0 \) is the mid plane density and \( h(r) \) is the disk vertical scale height. This is the equation of a thin disk in hydrostatic equilibrium (Frank et al., 1992). The scale height \( h(r) \) is determined by the relation:

\[
h(r) = h_0 \left( \frac{r}{r_0} \right)^\beta \quad (5.4)
\]
5.5 Temperature structure

The surface temperature of the disk is estimated from a combination of the expected viscous heating as well as a contribution from heating by X-rays from the central source. Pure viscous heating (Frank et al., 1992) is combined with a simple approximation for the irradiation by X-rays:

\[
T(r) = \left[ \left( \frac{3GM\dot{M}}{8\pi R^3\sigma} \left( 1 - \left(\frac{R}{R_{in}}\right)^{0.5} \right) \right) + \left( \frac{(1-A)L_X}{4\pi\sigma R_X^2} \right) \sin(\alpha) \right]^{1/4}.
\]

Here \( M \) is the BH mass, \( \dot{M} \) the accretion rate, \( R \) the cylindrical radius, \( A \) the disk X-ray albedo, \( L_X \) the X-ray luminosity, \( R_X \) the distance from the X-ray source to the disk surface and \( \alpha \) the angle between the disk surface and the incident radiation. The X-ray albedo (A) of the disk is assumed to be 0 and all of the incident X-ray flux is locally absorbed as results show that the X-ray albedo for neutral matter is generally low (Colbert et al., 2002; George & Fabian, 1991).

The X-ray luminosity is calculated from the accretion rate by:

\[
L_X = \eta\dot{M}c^2,
\]

where \( \eta \) is the radiative efficiency and \( c \) the speed of light. A radiative efficiency of \( \eta = 0.05 \) is used and this is lower than the usual adopted value of \( \eta = 0.1 \) as we are converting to X-ray luminosity rather than bolometric luminosity. Often due to the uncertain nature of the X-ray generation mechanism the factor \( (1-A)L_X \) from equation 5.5 is used as a free parameter when fitting observational data (Lira et al., 2011).

The angle \( \alpha \) is approximated as

\[
\alpha = \arcsin \left( \frac{H_X}{R_X} \right) + \left( \frac{dH}{dR} \cdot \frac{H}{R} \right)
\]

where the first term represents the “lamp-post” illumination of a flat disk by source (see figure 5.5) and the second corrects the angle for the effects of flaring in the outer regions (Armitage, 2009). Flaring of the outer disk can allow the disk surface to intercept a larger fraction of the X-ray flux and leads to a warmer outer disk than expected if the disk was flat (Kenyon & Hartmann, 1987). In figure 5.7 the surface temperature distribution of a disk around a
10^7 M_⊙ BH with an accretion rate of 0.1M_⊙ yr^{-1} is plotted. The pure viscous temperature is shown by a solid black line, the temperature of a flat disk is shown in blue and the effects of a slightly flared disk (β=1.2) is plotted in red. The inner disk (R < 5AU) is dominated by the viscous heating of the disk. Then at larger radii the irradiation heating by X-rays becomes an important source of heating. The effects of the flared disk on the temperature only become apparent at larger radii (R ≥ 500AU).

5.6 Properties of disk Material

5.6.1 X-rays

The photo-electric cross-sections of Morrison & McCammon (1983) calculated for solar abundances are used to estimate the X-ray disk properties. The cross section per hydrogen atom as a function of energy can be seen in figure 5.8 and is a strong function of energy.

The X-rays of interest are treated as having an energy E < 10keV and the scattering cross section as the classical Thompson cross-section in this case. The adopted X-ray photoelectric cross section is the median in the range 0.2 – 10keV, calculated from figure 5.8 as \( \sigma_X^{abs} = 4.22 \times 10^{-24} \text{cm}^2\text{H}^{-1} \). Assuming the composition of (Morrison & McCammon, 1983) then the X-ray absorption cross opacity is \( \kappa_X^{abs} = 1.77 \text{cm}^2\text{g}^{-1} \).

For energies E > few keV electrons bound to atoms can be treated as free (George & Fabian, 1991) and in this case the majority of the electrons are provided by H and He leading to \( N_e = 1.2N_H \) for a hydrogen to helium ratio of 0.1. The scattering cross-section is then

\[
\sigma_X^{scatter} = n_e \sigma_T.
\]

which based on the electron number density mentioned previously gives an electron scattering
5.6. Properties of disk Material

Figure 5.6: The geometry of the outer disk \((H > H_X)\). The illumination angle \(\alpha\) is the angle between the tangent to the local disk surface and the incoming radiation of the source.

Figure 5.7: The disk surface temperature as a function of radius for a central black hole mass of \(M_{bh} = 10^7 M_\odot\) and an accretion rate of \(M = 0.1 M_\odot yr^{-1}\).
Figure 5.8: The absorption cross section per hydrogen atom for the elemental abundances of Morrison & McCammon (1983).
5.7. Standard re-processing from an accretion disk

Cross section of $\sigma_{\text{scatter}} = 0.4 \text{cm}^2 \text{g}^{-1}$. The albedo is defined as

$$\text{albedo} = \frac{\sigma_T}{\sigma_T + \sigma_a}$$

and this can then be directly calculated from the values of the photo-electric and electron scattering cross sections, leading to a value of $\text{albedo} = 0.18$.

5.6.2 Optical

For the optical opacity we adopt the frequency averaged opacity law of Bell & Lin (1994) which gives a maximum value for the absorption cross section of $\kappa_{\text{abs}} = 1.5 \times 10^{-1} \text{cm}^2 \text{g}^{-1}$ for temperatures exceeding $10^3 \text{K}$, excluding scattering by free electrons. This value is dependent on the assumed temperature and density of the disk material and the density has been taken to be the mid plane density and the maximum opacity in the temperature range of interest has been adopted. There is no reprocessing of optical photons and once an optical photon is absorbed it is terminated.

5.7 Standard re-processing from an accretion disk

Figure 5.9 shows the calculated shape of the transfer function for a thin disk with the driving source located at a distance of 0.1 light days (ld) above the origin along the z-axis. The BH mass is $10^8 M_\odot$ and the accretion rate $1 M_\odot \text{yr}^{-1}$ and along with $h_X$ they determine the temperature profile of the disk (see figure 5.7) and hence the regions of the disk bright in each wavelength. The small initial delay is caused by the light travel time from the driving source to the disk surface. The value of $\beta$ is kept constant at $\beta = 1.2$ appropriate for a thin accretion disk (Shakura & Sunyaev, 1973). As we are interested in the shape of the transfer function we have normalized the model transfer functions throughout this work to peak values of 1.

It can be seen that the $U$ band transfer function has a fairly sharp initial peak followed by a steady decay with time. For the $V$ and $I$ bands the peak of the transfer function is shifted slightly to a longer delay time, as is expected. The decay of the transfer function is also shallower for the longer wavelength bands and at delays greater than about 3 and a half days most of the reprocessed light is actually being emitted in the $I$ band. The hollow circles show the position of the centroid of the transfer function for each wavelength. The centroid shows a wavelength dependent shift to longer delays which is expected as the centroid should measure the luminosity weighted radius of the reprocessing region (Koratkar & Gaskell, 1991; Cackett...
Figure 5.9: The transfer function of a standard thin disk for a BH mass of $10^8 M_\odot$ and an accretion rate $\dot{M} = 1 M_\odot \text{yr}^{-1}$. Curves show the transfer function at $U$ (solid line), $V$ (dashed line) and $I$ (dotted line) bands as well as the Kepler band (solid red line). The centroids of the transfer function are plotted as hollow circles. The driving source is located 0.1 ld (17.6 AU) above the origin along the z-axis. 

Figure 5.10 shows the transfer function for an accretion disk with the same parameters are figure 5.9 but with an accretion rate of $0.1 M_\odot \text{yr}^{-1}$. The transfer functions at all wavelengths have sharper peaks and decay much faster in time than the previous case. The changes are caused by the differences in the surface temperature brought on by the decreased accretion rate. The outer disk is now cooler and so reprocesses fewer optical photons at large delays.

5.8 Observational Motivation

The data motivating an extension to the standard transfer functions were obtained from observations of the Seyfert 1 galaxy Zw229 – 15 (Proust, 1990; Falco et al., 1999). Seyfert galaxies are marked by emission line spectra of both permitted and forbidden lines. The permitted lines are often those of Hydrogen ($H\alpha, H\beta$) and those of neutral and singly ionized
Figure 5.10: The transfer function of a standard thin disk for a BH mass of $10^8 M_\odot$ and an accretion rate $\dot{M} = 0.1 M_\odot \text{yr}^{-1}$. Curves show the transfer function at $U$ (solid line), $V$ (dashed line) and $I$ (dotted line) bands as well as the Kepler band (solid red line). The centroids of the transfer function are plotted as hollow circles. The driving source is located 0.1 ld (17.6 AU) above the origin along the z-axis.
Helium and single ionized Iron. Forbidden lines such as O\textsc{iii}, O\textsc{ii} and Ne\textsc{iii} are also observed. In Seyfert type 1 galaxies the permitted lines have very broad wings at FWHM corresponding to $v = 1 - 10000 \text{km/s}$. The forbidden lines on the other hand are much narrower corresponding to velocities up to $\sim 1000 \text{km/s}$. This is suggestive that the two types of emission lines are being produced in two different locations within the AGN. Seyfert type 2 galaxies have both permitted and forbidden lines with similar widths corresponding to $v \sim 1000 \text{km/s}$.

A V band image from Barth et al. (2011) can be seen in figure 5.11 showing the galaxy and its surroundings. We can see the nucleus of the AGN as a bright point source in the center of the galaxy and also the more extended galactic disk component surrounding it. Figure 5.12 shows the optical spectra obtained by Barth et al. (2011) for the galaxy. We can see the broad Hydrogen emission lines in the optical as well as the much narrower forbidden lines of O\textsc{iii} that are typical of Seyfert type 1 galaxies.

Barth et al. (2011) were able to use multiple V band observations over a length of time along with coincident spectral observations to obtain an estimate of the lag between variations in the V band continuum emission and the H$\beta$ emission. By cross-correlating the two measurements they found that the lag between the peaks of the two was $\tau_{peak} = 3.5^{+0.5}_{-0.75}$ days. This estimate, along with the H$\beta$ velocity width, allowed them to calculate the mass of the central BH at $M_{BH} = 1.00^{+0.19}_{-0.24} \times 10^7 \text{M}_\odot$. An estimate of the Eddington ratio, determining the accretion rate, was also possible from their data leading to a ratio $L/L_{edd} = 0.05$.

Zw229 – 15 is one of the brightest AGN within the Kepler field and has been monitored with good time coverage over several quarters. The Kepler optical photometry have better time sampling and lower errors than almost any ground based observations of AGN made to date. Over a period of a few weeks Zw229-15 was monitored in X-rays by the Swift and Suzaku X-ray observatories as well as by Kepler in the optical (the Kepler band pass is centered at $\sim 6000 \text{\AA}$). In the lower panel of figure 5.13 the X-ray data can be seen and in the upper-right panel the optical data for the same time period is shown. The X-ray data have different time sampling at different times due to a switch from one X-ray observatory to the other. It can be seen from the data that Kepler provides much denser time sampling than is available with current X-ray observatories. The MEMECHO code (Horne, 1994) has been used to estimate the transfer function from the X-ray and optical observations and can be seen in the upper-left panel of figure 5.13 and plotted in figure 5.14. It can be seen that the transfer function does
Figure 5.11: A V band image of Zw229-15 showing the galaxy and surrounding field taken from Barth et al. (2011). The numbered stars are the photometric comparison stars used by the authors for monitoring.
Chapter 5. Echo Mapping of Accretion Disks

Figure 5.12: An optical spectra of Zw229-15 taken from Barth et al. (2011). Labeled are some of the broad Hydrogen emission lines as well as the more obvious forbidden lines of O\textsc{[III]}.
not follow a purely smooth decay with time as we would expect from a thin disk (see figure 5.9). Starting at around $\sim 2.5$ days there is a “bump” in the transfer function that is suggestive of additional structure present in the accretion disk.
Figure 5.14: The transfer function estimated from the optical and X-ray data using the MEMECHO package. The bump in the transfer function beginning at a delay of $\sim 3$ days is not consistent with a standard thin accretion disk.
5.8. Observational Motivation

5.8.1 Beyond a simple thin disk

The transfer function that is extracted from the observations gives information as to the distribution of matter within the region around the BH. It appears from figure 5.14 that the simplest picture we can imagine with a uniform, thin accretion disk surrounding the BH, may not be able to fully account for the observations in this case. A simple extension to this picture is to assume that the flaring of the accretion disk is not constant with radius. If instead of the case outlined in equation 5.4 with a constant value of $\beta$ at all radii the encountered situation may be:

$$\beta = \begin{cases} 
\beta_1 & R \leq R_0 \\
\beta_2 & \text{otherwise.}
\end{cases}$$

(5.10)

Physically this means that there is a change in the flaring of the disk at a given transition radius, $R_0$ (see section 5.10). This leads to the area subtended by the disk, as viewed from the driving source, changing at that radius. If the flaring parameter increases then the area subtended by the disk will increase at the radius $R_0$, leading to a greater fraction of the X-ray luminosity being absorbed by the disk beyond that point, compared to $\beta$ remaining constant. Hence the transfer function will show a wavelength dependent change in shape at at delay corresponding to the light travel time to a distance $R_0$. The change will be wavelength dependent as the temperature of the disk is also a function of radius. A change in the flaring of the disk will also alter the irradiation temperature of the disk surface, as a more flared disk is able to intercept a greater fraction of the flux at a given distance. If the change occurs at a small radii it will be more noticeable in the short wavelength continuum as this will primarily be produced in the high temperature inner disk. Conversely a large value of $R_0$ will lead to a larger change in the long wavelength transfer function.

5.8.2 The “standard” disk

To illustrate the effects of the various free parameters involved in a geometry with multiple flaring regimes a standard flared model is adopted. This standard model has the BH mass at $M_{BH} = 10^8 M_\odot$ and the accretion rate $\dot{M} = 1 M_\odot yr^{-1}$. The $\beta$ values are taken as $\beta_1 = 1.2$ and $\beta_2 = 1.4$ with $R_0 = 600 AU$. The driving source is located at ($h_x =$) 0.1 ld above the origin and the initial scale height, $h_0 = h_x$.

It is immediately clear from figure 5.15 that the inclusion of a change in the disk $\beta$ is able to produce features in the transfer function which bear a strong resemblance to those seen
Chapter 5. Echo Mapping of Accretion Disks

Figure 5.15: The transfer functions for a disk with $\beta_1 = 1.2$, $\beta_2 = 1.4$ and $R_0 = 600$AU. Here a BH mass of $10^8 M_\odot$ and an accretion rate of $1.0 M_\odot yr^{-1}$ have been used.
5.8. Observational Motivation

Figure 5.16: The transfer functions for a disk with $\beta_1 = 1.2$, $\beta_2 = 1.6$ and $R_0 = 600\text{AU}$. Here a BH mass of $10^8M_\odot$ and an accretion rate of $1.0M_\odot\text{yr}^{-1}$ have been used. The bump can be seen as a small feature in the $U$ band and becomes more prominent at longer wavelengths. At $I$ band the bump is more prominent than the initial peak of the transfer function at small delays. This is due to the transition radius ($R_0$) being located at a position in the disk which is bright in the $I$ band because of the local disk surface temperature.

As can be seen in figure 5.16 increasing $\beta_2$ to a slightly larger value significantly increases the size of the bump in the transfer function. The same progression of a more pronounced increase in the size of the bump is also seen as we move to longer wavelengths.

Inclination can also affect the observed properties of the transfer function. In figure 5.17 the effects of inclination on the Kepler band transfer function of a disk with: $\beta_1 = 1.2$, $\beta_2 = 1.6$ and $R_0 = 600\text{AU}$ are shown. At an inclination of $10^\circ$ the transfer function at small delays is mostly unaffected and is indistinguishable from the face-on disk. The bump in the transfer function appears around half a day sooner than the face-on case and peaks at a slightly smaller
value. The change is caused by the differing path lengths which photons from the transition radius in the disk now have to reach the observer. On the side of the disk which is effectively nearest the observer the light has a shorter path and so the response reaches the observer slightly earlier than before, causing the early appearance of the bump. On the far side of the disk the path length has increased and so the response is slightly delayed. The effects become more pronounced as the inclination is increased with the bump appearing to be stretched out over a longer time.

The effects of changing the radius, $R_0$, where the transition in $\beta$ takes place can also be investigated. Figure 5.18 shows the effect of varying $R_0$ between 200 and 1000AU on the Kepler band transfer functions. At $R_0 = 1000$AU there is a small feature in the transfer function peaking at a delay of around 6 days but the feature is small. At $R_0 = 600$AU as has been seen before the bump appears at a delay of just over 3 days and is an obvious feature in the transfer function. For $R_0 = 400$ and 600AU the bump becomes the most prominent
5.9. Comparison to the Data

Figure 5.18: The transfer function in the Kepler band for a disk with $\beta_1 = 1.2$, $\beta_2 = 1.4$ and a variety of values for $R_0$.

feature in the transfer functions. Because of the increased scale heights in the outer disk the light travel time is much reduced and the transfer function becomes much more compressed in time and in the case of the $R_0 = 200$AU disk there is very little response after around 4 days.

5.9 Comparison to the Data

It is now possible to try and interpret the features in the observationally derived transfer function in terms of a physical structure for the accretion disk. Here it will only be attempted to try and reproduce the general features of the transfer function rather than perform a full fit to the data. The BH parameters of Barth et al. (2011) (see section 5.8) of $M_{BH} = 10^7 M_\odot$ and $M = 0.015 M_\odot yr^{-1}$ are used as a starting point and the accretion rate varied in order to alter the temperature profile of the disk. The height of the X-ray source, $h_X$, is kept fixed at 0.1ld (17.6AU) and $h_0 = h_X$.

It has been found that a transition from a standard thin disk flaring of $\beta_1 = 1.2$ to a
value of $\beta_2 = 1.8$ with a transition radius of $R_0 = 600\text{AU}$ is able to reproduce the general shape of the observed transfer function if the disk is viewed slightly inclined ($i = 12^\circ$). It should be noted that while in this simple model it is the disk itself which flares at large radii the true picture may be more complex. An outflow or wind from the disk surface, if of sufficient density, would be capable of providing the signature observed. The model requires a significantly higher accretion rate than that suggested by Barth et al. (2011). An accretion rate of $\dot{M} = 0.2M_\odot\text{yr}^{-1}$ will reproduce the observed transfer function and this is an order of magnitude larger than that estimated by Barth et al. (2011) but is still below the Eddington luminosity for a $10^7M_\odot$ BH. Due to the uncertain nature of the X-ray production, and its true location, it is not unsurprising that the accretion rates are discrepant.

Due to the simplified nature of the model that has been adopted it has not been possible to account for the negative delays that have been inferred from the data but the model is
5.9. Comparison to the Data

Figure 5.20: Top panel: The disk scale height as a function of radius for the fitted transfer function (solid black line) with the filled circle showing the position of the X-ray source. The dashed line shows the disk scale height if there was no change in $\beta$. Lower panel: The variation of the ratio $H/R$ with radius. The value of $H/R$ remains low out to 2000AU, corresponding to a delay of $\sim 10$ days.

able to reproduce the general shape and position of the peak of the transfer function. The adoption of an increase in the disk flaring at large radii also appears to provide a reasonable approximation to the bump in the observed transfer function. The increased flaring in the outer disk also allows us to follow the decay in the tail of the transfer function out to a delay of $\sim 10$ days, this would not be possible without the additional irradiation heating caused by the increased flaring. It can be seen from the lower panel of figure 5.20 that the ratio $H/R$ remains low out to a delay of $\sim 10$ days (2000AU) and the disk may be classed as “thin” out to at least this radius. If the disk continued to flare with a value of $\beta=1.8$ then the ratio $H/R$ would increase to the point where it would no longer be considered a thin disk but that does not affect the results here.
Figure 5.21: UV spectrum of NGC 4151 from Kriss et al. (1995). Blue-shifted absorption can be seen in the CIV doublet (1548, 1551 Å) which is suggestive of outflowing ionized gas.

5.10 Physical interpretation

From an initial investigation the features observed in the transfer function appear to be caused by a change in the disk structure. The question still remains as to what physical process could lead to such a structure. As the accretion disk is a dynamic environment the structure could be a transient feature which we happen to observe before it is altered or destroyed as the disk returns to a more steady state configuration. In this case there may be no underlying cause other than the inhomogeneity of the material which makes up the accretion disk.

One interesting scenario is that the change in disk structure we see is associated with the emergence, or attempted emergence, of a disk wind. Here physical processes occurring in the disk and the central regions around the BH cause material to be accelerated close to the disk surface to high velocities. Evidence for disk winds comes from the blue-shifted absorption lines seen in some AGN spectra that have been proposed to show the existence of high velocity material along our line of sight (Krolik, 1999).
5.10.1 Driving a disk wind

5.10.1.1 Thermal winds

In order to drive a disk wind or outflow it is required that there to be a force (or forces) that can overcome gravity. Thermal pressure is one mechanism which may produce a disk wind. Here the low density gas near the disk surface is exposed to the output of the central source and the inner disk. For the low density gas the radiative heating and cooling processes will overcome the two-body cooling and the temperature of the gas will increase to a level determined by the radiation. This hot gas will have increased thermal velocities and the thermal velocity can exceed the escape velocity leading to an outflow or wind. In the inner regions of the disk where the escape velocity is high the result can be a corona of hot gas above the disk which may develop into a wind in the outer disk where the escape velocity is lower [Begelman et al., 1983].

5.10.1.2 Line driven winds

Disk winds may also be driven by local UV emission from the disk providing an acceleration on the UV lines of the gas. The acceleration that is provided on the material in the disk depends on the available flux radiated and the cross-section of the disk material itself. Radiative acceleration due to the continuum emission being scattering from free electrons can be written as:

$$a_{cont} = \frac{\sigma_e F}{c} = \frac{\sigma_e L}{4\pi r^2 c}, \quad (5.11)$$

where \(\sigma_e\) is the cross section for the electron, \(L\) is the source luminosity, \(r\) the distance from the source and \(c\) the speed of light. As well as free electrons in the gas, bound electrons are also able to interact with the photons and provide a source of acceleration. Castor et al. (1975) provided a parameterisation of the line driven acceleration due to radiation force on resonant lines

$$a_{lines} = \frac{\sigma_e F}{c} M(t) \quad (5.12)$$

where \(M(t)\) is the force multiplier giving the contribution of the lines. Here \(t\) is the optical depth for an outflowing wind (see Castor et al., 1975). The force multiplier is dependent on the number of lines available in the material, the line width, the optical depth of the line and the ionization. As large ionization fractions will remove electrons and reduce the number of available absorption lines line driving can be most effective at low temperatures and ionization levels. The ability of a disk to support a line driven wind is dependent on the ability of the
wind to shield itself from the X-ray emission from the central engine. This will act to ionize gas which rises from the disk plane and so remove the source of driving, causing a failure of the wind. It has been shown that with the aid of “hitch hiking” gas a line driven wind can form at a sufficient distance from the central source \cite{Murray1995, Proga2000}. An estimate of $\sim 10^{16}\,\text{cm} \approx 700\text{AU}$ for the emergence of a line driven wind \cite{Proga2000} is compatible with the $R_0$ value determined for the simple disk structure used here to model Zw-229. However, the numerical calculations were carried out for a $10^8\,\text{M}_\odot$ BH accreting at $1.8\,\text{M}_\odot\,\text{yr}^{-1}$ and complementary calculations for lower BH mass and accretion rate are not available. Even a failed wind can result in a puffed up disk \cite{Proga2004} and may be compatible with the increase in disk flaring used here.

5.10.1.3 Magnetic driving

Magnetic driving of a wind involves field lines which are frozen into the ionized gas in the disk and locked to the disk's rotation \cite{Blandford1982}. Gas needs to be loaded onto the field lines, perhaps by thermal or line driving, and it is then centrifugally accelerated above and away from the disk. Here the innermost radius is set by the transition of the disk becoming too neutral to support the locking of the magnetic field. \cite{Bottorff1997} adopt a value of $\sim 1$ light day but show that the radius is highly dependent on the adopted parameters of the BH and accretion disk, and \cite{Kato2002} suggest that even in sub-optimal conditions outflows along the disk surface can be produced. Hence it appears possible that a magnetic wind may be compatible with the distance of $R_0$ that we have used in our model for Zw-229.

5.10.2 Inhomogeneities in the disk structure

It is also possible that the signature that has been attributed to an increase in the flaring of the outer disk is caused by a clumpy or warped structure in the accretion disk. For simplicity it is assumed that the material in the disk is smooth but observations show that the material in the vicinity of the galactic center is highly structured \cite{Montero2009} and so it is highly likely that the accretion disk itself also harbors significant inhomogeneities. It is possible that such clumsiness could manifest in the observed transfer function as the bump that seen.
5.11 Limitations

5.11.1 Data

In the lower and top right panels in figure 5.13 the data points for both the X-ray and Kepler observations can be seen. While the Kepler data have a nearly uniform coverage at small time intervals the X-ray data are more complex. Between 10 and 20 days the time interval between the observations is much shorter than the rest of the period. This coincides with the period of maximum X-ray output and significant variability. However, the rest of the time period, which still shows significant variability, has a longer time sampling interval which may affect the robustness of the results obtained. Ideally X-ray data with a sampling rate which is comparable with the Kepler data would have been obtained allowing a more reliable estimate of the transfer function to be obtained. Unfortunately, there is currently no way to obtain such high quality X-ray data with the required time sampling.

5.11.2 Model

5.11.2.1 X-ray source

This model has been limited to the highly simplified scenario where the X-ray source is approximated by a single point source located above the central BH. In reality the source of X-rays is likely to be more complex and perhaps less spatially compact. The exact nature of the X-ray emitting region is not currently well understood. It is thought that in the case of super massive BH’s the emission may actually originate in the disk as thermal UV photons. These photons are inverse-Compton scattered to X-ray energies by a corona of hot, relativistic electrons that exist above the disk. Some of these photons are then able to rain back down on the disk producing a scattered X-ray component as well as the reprocessed UV/optical continuum emission studied here.

This generation method can have at least a couple of direct effects on the transfer functions that we observe. If the X-ray source is spatially extended above the accretion disk then it may affect the observed transfer function in the inner disk. In figure 5.22 the effect on the transfer function of a thin disk of the X-ray source being radially extended is shown. In all cases the height of the X-ray source above the disk is fixed at 0.1 ld. The point source is located directly above the central BH at $x_s = y_s = 0.0$. The extended source sees the X-ray photons emitted from a circular region with a radius of either $2R_{min}$ or $5R_{min}$ ($R_{min}$ is the last stable orbit as earlier). It is shown that when extended to $2R_{min}$ the transfer function is initially similar to
Figure 5.22: The *Kepler* band transfer function for a thin disk when the X-ray source is a point located above the origin (black solid line) and extended in a thin disk. The height above the disk is always a constant $h_\text{x}$ in all cases. The point source case but shows a slightly faster fall off beyond the peak but at large delays (> 8 days) the transfer functions are indistinguishable. When extended to $5R_{\text{min}}$ the transfer function shows a much sharper peak than the point source case and the peak is reached at a smaller delay. This is caused by the reduced light travel time to the regions of the disk which dominate the *Kepler* band from the outer parts of the extended X-ray sources.

Recent work by Kara et al. (2013) has shown that there is evidence that the spatial extent, in both height above the plane and radius, of the X-ray corona can be variable. They found that when in a high flux, flaring, state the X-ray data showed evidence that the source was more extended while in a quiescent, low flux, state the evidence was suggestive of a more compact source. This result could complicate the calculation of the transfer function, both observationally and theoretically, as the source geometry then becomes a time variable element. It is not clear on what timescale the size of the X-ray emitting region can change on, hence the importance of the result is unclear.
The source of the X-ray photons may also provide additional problems for a simple picture of the transfer function. If a component of the X-ray photons are inverse Compton scattered UV seed photons then it follows that variability in the X-rays may be produced by variability in the UV continuum emission from the inner disk. Hence it is possible to imagine a scenario where UV continuum could be observed both leading and trailing the X-ray variability in time. A fraction of the UV photons are up-scattered to X-rays, which then impact the disk and produce a second contribution to the UV continuum, while the rest of the initial UV photons escape. Hence we can observe a UV emission leading the X-rays. This can be described by negative delays in the transfer function which cannot be produced by the emission mechanism adopted in the model.

5.12 Future work

It would be desirable to have such high quality in both the X-ray and optical, for a larger sample of AGN. There are at least four AGN that are being monitored by Kepler (Mushotzky et al., 2011) and so if additional simultaneous X-ray observations can be obtained then high quality observational transfer functions could be estimated. This would give an indication of whether the features of the transfer function seen in Zw-229 are seen in other systems and if so whether any correlations with the properties of the BH can be found (i.e. mass, luminosity). Additional data would also allow us to investigate whether the features in the transfer function are time variable. Unfortunately the Kepler data processing means that only preselected targets in the field are monitored, meaning there is little scope to find additional AGN in archival data.

Multi wavelength observations at a variety of optical wavelengths would provide the ability to substantiate the findings here that the bump is caused by an increase in the flaring. The transfer function is wavelength dependent and we have seen that it should have a different signature at different wavelengths. This data may allow a better determination of the true underlying structure.

In this work the continuum transfer function has been used but with the appropriate observations an emission line transfer function can be obtained. Emission lines encode information not only about the geometry but also about the velocity structure. The doppler shift of the emission lines gives the line of sight velocity of the emitting material and so provides another window to investigate the structure of the accretion disk and its surrounds. Within the Monte Carlo approach adopted here it would be a simple matter to encode a velocity structure into
the model and provide additional observables to be compared to data, however this would come at the cost of additional computation time.

In addition a very simple approach to the emission/absorption process is used here to obtain a first order approximation to the transfer function. Again, however, the utility of the Monte Carlo Radiative transfer approach means that it would be straight-forward to increase the complexity of the model to encompass more of the physical properties. For instance a disk structure from MHD simulations (Proga et al., 2000) could be used to self-consistently calculate the disk ionization structure, as well as including the effect of self illumination of the disk by inverse Compton scattered UV photons. Although this would vastly increase the time required for each simulation, and provide a larger number of free parameters, it may allow more insight into the physics of the accretion disk.

5.12.1 Summary
In this chapter I have investigated the continuum transfer function of a simple model for the accretion disks that are thought to surround and power AGN. Motivated by observations that differ from a simple flat accretion disk I look at the effect of flaring of the outer disk on the transfer function at a number of wavelengths. Results indicate that a change in the disk flaring parameter between the inner and outer disk can produce features in the transfer function that are qualitatively similar to those seen in the observations. I propose that the increase in the flaring could be a signature of the emergence of a disk wind or outflow as suggested by other authors.
Conclusions and Outlook

The work in this thesis has spanned around nine orders of magnitude in size, from 1 au to 10's kpc. Its overarching theme has been the use of radiation transfer models to uncover structure from observations which may otherwise have gone unnoticed and to probe the impact of radiation on its surroundings. I have investigated the use of time resolved MCRT models to help uncover the structure of the inner regions of the accretion disks around super-massive black holes. By adopting a simple model for the structure of the X-ray emitting regions and the accretion disk it illuminates, I have been able to discern clues to the shape of the outer accretion disk. The observations along with these models suggest that a wind or outflow may emerge from the surface of the disk and alter the shape of the transfer function in an obvious way.

I have also attempted to assess the impact of massive stars on the large scale star formation process. By coupling a Monte Carlo photoionization code to a series of snapshots of a realistic numerical simulation of a star forming cloud within a spiral galaxy, I have determined the impact of photoionization feedback on the star formation process. The method has been tested against an SPH implementation of photoionization feedback and although the method
is not able to account for the dynamical effects of the ionized gas in inhibiting or triggering further star formation it does provide a first order estimate of the reduction in star formation due to massive stars. PI feedback is able to reduce the mass accreted by stellar sinks by 38% under the assumptions made here with many stellar clusters unable to effectively accrete gas. The maximum mass attained by a stellar cluster is reduced to 53% of its original value when PI feedback is included. I have also highlighted the possible issues with SFRs estimated from indicators which are only sensitive to clusters containing massive stars, such as Hα emission, when applied to the entire star forming region. These can lead to the SFR being underestimated unless under sampling of the high mass end of the IMF is taken into account.

By utilizing observations covering a wide range in wavelength to evaluate the structure of the dusty ISM in three LSB disk galaxies I have studied the structure of the dusty ISM. The results indicate that the dusty ISM has a different global structure to that seen in normal higher mass disk galaxies, with scale heights equal to or exceeding the stellar scale heights. This suggests that the cold ISM of low mass, LSB galaxies may be stable against axisymmetric perturbations leading to conditions less favorable for high SFRs.

6.1 Outlook

The Monte Carlo methods used in this work are likely to become more and more powerful in the future. At their heart they require computations of very large numbers of simple calculations. The increasing power of even desktop computers is opening up new possibilities of the kind of problems which can be investigated. Increasing use of parallel and distributed computing can be naturally applied to many Monte Carlo problems. In addition to astronomy the field of medical science is also making increased use of Monte Carlo methods to produce new non-invasive diagnosis and measurement techniques. It is encouraging to think that methods developed to study distant astronomical phenomena can find applications able to provide a real benefit to people lives.

The integration of radiative transfer methods with numerical hydrodynamics codes provides an exciting opportunity to produce fully self consistent models with a wide range of observables. Star formation regions may be modeled with a full treatment of feedback from massive stars to produce multi-wavelength views from the UV to the sub-mm, allowing a greater understanding of the physical processes behind observations. Some progress in implementing radiative transfer in hydrodynamical codes has already been made (Dale & Bonnell 2011; Vazquez Semadeni et al. 2010; Nayakshin et al. 2009). Many such problems require
computations over many orders of magnitude in size and the use of techniques like adaptive mesh refinement will be required to make such computations manageable.

The introduction of new observatories and instruments will provide a wealth of new data to motivate and constrain new models. The *Herschel* archive along with new observations by the Atacama Large Millimeter Array (*ALMA*) and the Scuba-2 camera at the James Clark Maxwell Telescope will provide a wealth of data in the FIR and sub-mm. These data will allow further investigation of the dusty ISM in galaxies throughout the Universe providing clues to star formation processes and the impact of massive stars.
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