MODELLING THE PAN-SPectRAL ENERGY DISTRIBUTION OF STARBURST GALAXIES: III. EMISSION LINE DIAGNOSTICS OF ENSEMBLES OF EVOLVING H II REGIONS

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ABSTRACT

We build, as far as theory will permit, self consistent model H II regions around central clusters of aging stars. These produce strong emission line diagnostics applicable to either individual H II regions in galaxies, or to the integrated emission line spectra of disk or starburst galaxies. The models assume that the expansion and internal pressure of individual H II regions is driven by the net input of mechanical energy from the central cluster, be it through winds or supernova events. This eliminates the ionization parameter as a free variable, replacing it with a parameter which depends on the ratio of the cluster mass to the pressure in the surrounding interstellar medium. These models explain why H II regions with low abundances have high excitation, and demonstrate that at least part of the warm ionized medium is the result of overlapping faint, old, large, and low pressure H II regions. We present line ratios (at both optical and IR wavelengths) which provide reliable abundance diagnostics for both single H II regions or for integrated galaxy spectra, and we find a number that can be used to estimate the mean age of the cluster stars exciting individual H II regions.

Subject headings: galaxies: general – galaxies: star formation rates – galaxies: abundances – galaxies: starburst – ISM: H II – ISM: abundances

1. INTRODUCTION

Much of what we have learnt about the chemical evolution of the Universe, or of individual galaxies throughout cosmic time has been gleaned from the study of the spatially unresolved emission line spectra of distant galaxies (Steidel et al. 1996; Kobulnicky, Kennicutt & Pizagno 1999; Kobulnicky & Zaritsky 1999; Kewley & Kobulnicky 2005). This emission line spectrum arises from the ensemble average of H II regions within the galaxy, characterized by a wide range of physical parameters.

For example, in disk galaxies, the chemical abundance of heavy elements falls continuously from centre to edge. In like manner, both the pressure and density of the interstellar medium in the disk drops exponentially with radius. For a given input of mechanical energy by the central star cluster, this means that the outermost H II regions expand more rapidly, and are both larger and have lower internal pressure at a given age. However, the properties of the central cluster of a given mass change systematically with chemical abundance. Massive stars with higher chemical abundances lose more mass prior to supernova explosion, have stronger stellar winds, evolve more rapidly, and have lower effective temperatures while they are on the Main Sequence.

Finally, the temporal evolution of individual H II regions is extremely important in determining the integrated emission line spectrum. Leitherer, Gruenwald & Schmutz (1992) demonstrated the importance of aging of the OB stars in lowering the number of ionizing photons as the most massive stars evolve away from the Zero Age Main Sequence (ZAMS) to become supergiants. Later, these stars enjoy a brief resurgence in their ionizing photon and mechanical energy production as they become Wolf-Rayet stars.
With so many temporal and physical variables, it is perhaps not surprising that the nebular modelling community (ourselves included) have in the past been reduced to making severe, even gross, oversimplifications in attempts to model the integrated strong emission line spectra of galaxies. Indeed, frequently only a single line ratio has been used to determine the metallicity of extragalactic H II regions or even whole galaxies. This is the famous R_{23} ratio; \((\text{[O III]} \lambda \lambda 4959,5007)/\text{H}\beta\).

This ratio was first proposed by Pagel et al. (1979). The logic for its use is impeccable, since it uses the two strongest lines of the strongest coolant of H II regions, and it should therefore be sensitive to the total oxygen abundance. By using two stages of ionization, it accounts for the emission in the bulk of the ionized nebular volume. However, the calibration of this ratio in terms of the abundance has proved to be very difficult and many different and often contradictory calibrations of R_{23} are available, including Pagel et al. (1979); Pagel, Edmunds & Smith (1980); Edmunds & Pagel (1984); McCall, Rybski & Shields (85); Dopita & Evans (1986); Torres-Peimbert, Peimbert & Fierro (1989); Skillman, Kennicutt & Hodge (1989); McGaugh (1991); Zaritsky, Kennicutt & Huchra (1994); Pilyugin (2000); Kewley et al. (2002b).

The basic cause of this difficulty in calibrating the R_{23} ratio is common to many ratios formed from the flux of optical forbidden line divided by the flux of a recombination line of hydrogen. Initially, as \(Z\) is increased, the forbidden line increases in flux, and the line ratio increases. However, as the abundance increases further, the cooling by forbidden lines lowers the electron temperature making it more difficult to collisionally excite the optical forbidden lines. Eventually there comes a point at which an increase in abundance is matched by a decrease in collisional excitation and the line ratio reaches its maximum. Any further increase in \(Z\) then leads to a decrease in the relative strength of the forbidden line. R_{23}, like other optical diagnostics is therefore a two-valued function of \(Z\). Because infrared lines have lower thresholds for collisional excitation, they remain monotonically functions of \(Z\) up to much higher metallicities. Recognizing this physics, the S_{23} ratio; \((\text{[S II]} \lambda \lambda 6717,6731+\text{[S III]} \lambda \lambda 9069,9532)/\text{H}\beta\), or even more complex ratios, have been used either in the place of or to supplement the R_{23} ratio (Dennefeld & Stasinska 1983; Kennicutt & Garnett 1996; Oey et al. 2000).

The calibration problems of the R_{23} ratio are made worse by the scatter, at fixed R_{23} and within each given branch, both between models and observational data, and amongst different models. The observational material is affected by uncertainty in the reddening correction applying to the [O II] \(\lambda \lambda 3727,29\)A, since classical extinction laws are usually used, rather than the attenuation laws which more correctly apply to extended objects (Fischera, Dopita & Sutherland 2003; Fischera & Dopita 2005). This point will be discussed more fully below. As far as the theoretical models are concerned, scatter in the relationship is easily generated, since the stellar atmospheres used for single stars can show very wide differences in the number of ionizing photons produced per unit frequency (Morisset et al. 2004).

Moving beyond the use of single line ratios, a more sophisticated analysis is made possible by the understanding that the strong line emission spectrum of an individual H II region is controlled by three physical parameters (Dopita & Evans 1986). These parameters are, the effective temperature of the exciting stars, the chemical abundance set (or “metallicity”, \(Z\) and the ionization parameter, defined either as the ratio of the mean ionizing photon flux to the mean atom density, \(q/c\). Thus, for a given stellar input spectrum a \(U:Z\) grid of models should provide the ideal means of interpreting the observational data (Kewley et al. 2002b).

This analysis leaves open the issue of the age distribution of the exciting stars. The metallicity and the age of the exciting stars determines the energy distribution of the EUV photons. In the modelling hitherto, this problem is usually treated in two limits; the instantaneous burst approximation (for which zero age is often, but not universally assumed) or the continuous star formation approximation in which stars are assumed to be born continually within the ionized region (see Kewley et al. (2001), and references therein). All this modeling effectively assumes a single H II region of a given metallicity and ionization parameter. Whilst such an approach is acceptable in attempts to understand the emission line spectrum of individual H II regions, it is certainly inadequate in attempts to interpret the integrated spectrum of a whole galaxy, or even of a complex of many H II regions.

The advent of the Starburst 99 v.5 (Leitherer et al. 1999) stellar spectral synthesis code finally allowed the construction of fully self-consistent models for H II regions. For a given stellar initial mass function (IMF), this code delivers not only the pan-spectral distribution of photons, including ionizing photons as a function of age, but also provides tables of the time-dependent mechanical energy input of the stars including OB-star stellar winds, red giant winds, Wolf-Rayet winds and the energy input from supernova explosions.

In the first paper of this series (Dopita et al. (2005), hereinafter referred to as Paper I), we computed the (one dimensional) evolution of H II regions around clusters of a single mass. We demonstrated how the size : age relationship is essentially determined by the density (or pressure) in the surrounding interstellar medium (ISM). This in turn determines the dust ‘temperature’ described by the wavelength of the peak of the far-IR dust re-emission feature.

In the second paper of this series, Dopita et al. (2006), in press, hereinafter referred to as Paper II), we investigated the role of metallicity and of the cluster mass function in controlling the excitation of the populations of H II regions in galaxies, be they disk or starburst.

We demonstrated that the ionization parameter of H II regions, previously treated as a free variable, is determined at any time by the instantaneous ratio of the ionizing photon flux to the mechanical energy flux of the central stars. This is because the HII region is evolving as a mass-loss bubble pressurized by the combined ram pressure of the stellar wind and supernova explosions, so HII region density and HII region radius are closely coupled. Although this conclusion was obtained using a simple 1-D spherical evolution model for the H II region,
it should remain valid in more complex geometries, since wherever un-ionized or molecular inclusions exist, these will be pressure confined by the hot shocked stellar wind gas, and this gas pressure is coupled with the overall size of the H II region, which itself determines the dilution of the radiation field of the central stars.

Because the effective temperature of the exciting stars increases as metallicity is lowered, but the mechanical energy flux in the stellar winds decreases towards to lower metallicity, low abundance HII regions are characterized by higher ionization parameters, a fact that had been frequently noted by observers, but which had not previously been explained in a satisfactory manner.

Using these insights, in this third paper of the series, we proceed to the next stage of sophistication in modeling – the construction of time-dependent photoionization models of individual H II regions, and the construction of ensemble averages of aging H II regions to provide galaxy-wide averaged spectra at a given metallicity. Such models applied to individual H II regions make it possible to estimate the ages of the exciting stars from the positions of the observations on theoretical H II region isochrones. Previously, this could not be done, since the ionization parameter and the effective temperature of the cluster (determined by the ageing of its stars) can both produce similar effects on the emitted spectrum. This degeneracy is raised thanks to the self-consistent geometry that we have developed, which includes a dynamical evolution of the H II region consistent with the properties of the stellar wind generated by the central cluster.

In this paper, we apply these new techniques to produce line ratio diagnostics which enable the independent determination of both the stellar ages and metallicities of the exciting clusters for individual H II regions. These should prove useful in the analysis of abundance gradients in resolved disk galaxies. More importantly, we develop line ratio diagnostics for the determination of abundances in ensembles of H II regions in starburst and normal galaxies. This should greatly assist in analyses of the strong emission lines of the more distant and un-resolved galaxies, observed either at optical wavelengths or in the IR.

2. MODELS

2.1. Codes

We have used the Starburst 99 v.5 code in its latest (2005) version to compute the pan-spectral distribution of clusters of stars with a piece-wise fit to a Miller-Scalo initial mass function (IMF) Miller & Scalo (1979) between 0.1 and 120 M⊙. The parameters of this fit are the same as given in Miller & Scalo (1979) and were also tabulated by us in Paper II. Either the use of a Miller-Scalo IMF or of a Salpeter IMF would not noticeably affect the line ratio diagnostics presented in this paper, since the slopes of the IMF are almost identical above 10 M⊙. However, the choice of the IMF has a much larger effect on the total mass of the cluster, since this is determined by the choice of the power law below 10 M⊙.

Stellar atmosphere models for stars with plane parallel atmospheres are based on the Kurucz (1992) models as compiled by Lejeune (1997). The fully line-blanketed Wolf-Rayet atmosphere models of Hillier & Miller (1998) and the non-LTE O-star atmospheres of Pauldrach, Hoffman, & Lennon (2001) have been incorporated into Starburst 99 v.5 as described in Smith, Norris & Crowther (2002). The flux distributions following from these atmospheres are coupled to the stellar evolution models by the Geneva group. We used the so-called "high-mass-loss" tracks, which provide the best match to the observed stellar inventory in the Hertzsprung-Russell diagram (Leitherer et al. 1999).

For the Initial Mass Function (IMF) we used piece-wise power-law fits to the Miller & Scalo (1979) mass function, although we note that their paper, Miller & Scalo (1979) represented their IMF as a truncated lognormal distribution (with its maximum at zero). However, they also represented it as a three-segment broken power law, which is the form of the IMF which Starburst 99 currently accepts. The logarithmic slopes of the piecewise power-law fits, Γ, and the mass range applicable to each segment were given in Table I of Paper II.

For a given cluster mass, we used the stellar wind and supernova power output, as tabulated by the Starburst 99 v.5 code, to solve for the radius of the H II regions as a function of time given the pressure or, equivalently, the mean density in the ISM. This requires a Runge-Kutta integration of the equation of motion of the swept-up shell, as was done and described in both Paper I and Paper II.

The pressure in the H II region is the same as in the shocked stellar wind gas. This is given by the classical Castor, McCray (1975) theory:

\[ P(t) = \frac{7}{(3850\pi)^{2/5}} \left( \frac{250}{308\pi} \right)^{4/15} \left( \frac{L_{\text{mech}}(t)}{\mu m_H n} \right)^{2/3} \frac{r(t)^{1/3}}{n(t)_{\text{HII}}} \]

(1)

where \( L_{\text{mech}}(t) \) is the instantaneous production of mechanical energy by the cluster stars, \( r(t) \) is the radius, \( n_0 \) is the mean atom density in the surrounding ISM and \( n \) is the mean atom density in the ionized gas and \( \delta(t) = n(n_0) \) is the instantaneous ratio of the density interior to the bubble to the density in the surrounding ISM.

In Paper II, we showed that the ionization parameter at the contact discontinuity in the swept-up shell of ISM, which can be treated as the inner boundary of the H II region depends largely on the instantaneous properties of the exciting cluster stars:

\[ q(t) \propto \delta(t)^{3/2} S_\star(t)/L_{\text{mech}}(t). \]

(2)

where \( S_\star(t) \) is the instantaneous flux of ionizing photons from the central cluster.

The presence of the \( \delta(t) \) factor in the above equation provides a weak coupling between the ionization parameter and both the pressure in the ISM, \( P_0 \), and the mass of the central cluster, \( M_\text{cl} \). Together, these determine the strength of the outer shock of the mass-loss bubble and therefore the compression factor through it. The appropriate scaling factors are \( q \propto P_0^{-1/5} \) and \( q \propto M_\text{cl}^{1/5} \). Thus, once \( P_0 \) and \( q \propto M_\text{cl}^{1/5} \) are fixed, the ionization parameter is determined.

Using this dynamical model to derive the instantaneous size and ionization parameter of the H II region, the latest version of our code Mappings IIIr (Sutherland & Dopita 1993; Dopita et al. 2002; Groves, Dopita & Sutherland 2004) with the physical parameters defined in Paper I was used to compute photoionization models. The resulting model isobaric dusty H II regions were
used to produce a table of emission lines, described in
the Appendix, and given fully the Electronic version of
the paper. These enable us to compute the line ratio
diagnostics described in this paper.

2.2. Metallicities & Depletion Factors

The solar abundance set adopted here is taken from
Asplund, Grevesse & Sauval (2005). This incorporates
the results of many papers which together have provided
a self-consistent re-calibration of the solar abundance.
In many cases, these abundances are nearly a factor of
two lower than those used previously (Anders & Grevesse
1989). The corresponding logarithmic abundance ratios
of the elements with respect to Hydrogen are given in ta-
table 1. For the purposes of the modeling, when we refer to
solar metallicity, $Z_\odot$, we are using this set of abundances.

We note here that as a consequence of the re-scaling
of the solar abundances (which is not yet reflected in
the stellar models), the Starburst 99 “solar” abundance set
is inconsistent with the new Asplund, Grevesse & Sauval
(2005) abundance set. The Starburst 99 code uses ab-
solute metallicities of $Z = 0.001, 0.004, 0.008, 0.02 and
0.04$, which makes the Starburst 99 “solar” metallicity,$Z = 0.02$, higher than the Asplund, Grevesse & Sauval
(2005) “solar metallicity”. $Z = 0.016$. Whilst this matter
very little in terms of the number of ionizing photons
emitted by the stars, it will mean that the computed stellar
UV photon field will slightly softer than it should be,
given the nebular abundance set.

The depletion factors from the gaseous phase deter-
mine the composition of the dust in the models. For these
we have took the measured gas-phase abundances in the
local interstellar cloud by Kimura, Mann & Jessberger
(2003), and used these to infer a set of local depletion
factors consistent with the Asplund, Grevesse & Sauval
(2005) abundance set. The adopted depletion set is also
given in table 1. For models with non-solar abundances,
the depletion factors were held constant at solar values.
This is equivalent to taking the dust:gas ratio to be propor-
tional to metallicity.

Three elements do not scale simply with the metallic-
ity. First, because of its high initial abundance as a result
of nuclear burning in the Big Bang, He then scales only
weakly with metallicity. For this element, we assume a
primary nucleosynthesis component in addition to its pri-
mordial value. From Russell & Dopita (1992) and Pagel
et al. (1992) we infer the empirical relationship:

$$\text{He}/H = 0.0737 + 0.024 \times Z/Z_\odot. \quad (3)$$

For both Nitrogen and Carbon there is clear evidence
that these are both a primary nucleosynthetic element,
dominant at low metallicity, and a secondary nucleosyn-
thetic element once higher abundances are reached. Al-
ternatively, both are produced in part by dredge-up in
intermediate mass stars, causing a delay in the onset of
enrichment of these elements from this source. For Nitro-
gen we have used a modified version of the form proposed
by Groves, Dopita & Sutherland (2004):

$$N/H = 1.1 \times 10^{-5} Z/Z_\odot + 4.9 \times 10^{-5} Z/Z_\odot^2. \quad (4)$$

For Carbon, we have used the HST data on the Carbon
abundances of H II regions as compiled by Garnett et al.
(1999). This provides a fit of the same mathematical

| Element | $\log [N_X/n_H]$ | $\log (D)$ |
|---------|-----------------|-----------|
| H       | 0.00            | 0.00      |
| He      | -1.01           | 0.00      |
| C       | -3.59           | 0.15      |
| N       | -4.22           | 0.23      |
| O       | -3.34           | 0.21      |
| Ne      | -3.91           | 0.00      |
| Mg      | -4.47           | 1.08      |
| Si      | -4.49           | 0.81      |
| S       | -4.79           | 0.08      |
| Ar      | -5.20           | 0.00      |
| Ca      | -5.64           | 2.52      |
| Fe      | -4.55           | -1.31     |

form as for N:

$$C/H = 6.0 \times 10^{-5} Z/Z_\odot + 2.0 \times 10^{-4} Z/Z_\odot^2. \quad (5)$$

The fit to the observations is shown in figure 1.

2.3. Parameters of the Photoionization Models

The Starburst 99 v.5 code allows us to study line
ratios at five (fixed) absolute metallicities of $Z = 0.001, 0.004, 0.008, 0.02 and 0.04$. For each of these abundance
sets we have computed several families of H II region models with ages 0.2, 0.5, and 1.0 Myr and in
further 0.5 Myr steps up to a maximum age of 6.5 Myr.
By this time, more than 96% of ionizing photons
have been emitted, the H II regions have faded by factors of
between 5 and 12 from their peak luminosity, and their
surface brightnesses will have faded by much greater fac-
tors than these.

The ionization parameter is not a free variable in these
models. The geometry of the gas with respect to the
ionizing stars is instead determined by the equation of
motion of the expanding H II region under the driving
pressure of the stellar mass-loss and supernova explo-
sions. This pressure also determines the density of the

\[ \frac{\log C/O}{\log O/H} \]
ionized plasma. As was shown in Paper II, the equation of motion and the pressure together lead us to infer that there is a weak coupling between the ionization parameter and both the pressure in the ISM, \( P_0 \), and the mass of the central cluster, \( M_{cl} \). Together, these determine the strength of the outer shock of the mass-loss bubble and therefore the compression factor through it. The appropriate scaling factors are \( q \propto P_0^{-1/5} \) and \( q \propto M_{cl}^{1/5} \).

The ratio, \( R = (M_{cl}/M_\odot)/(P_0/k) \), with \( P_0/k \), measured in cgs units (cm\(^{-3}\)K), uniquely determines the run of ionization parameter with time. It is this variable that replaces the ionization parameter and other geometrical considerations in our models. In figure 2 we show the run of the computed ionization parameter \( q \) as a function of time and ISM pressure for a solar abundance cluster with \( M_{cl} = 3 \times 10^5 M_\odot \) and having a Miller-Scalo IMF. The (dimensional) ionization parameter \( q \) is related to the more frequently used (dimensionless) ionization parameter \( U \) by \( U = q/c \).

The run of \( q \) with time is computed using the Starburst 99 output, and solving for the time dependent radius and internal pressure of the mass-loss bubble as described above. In the early phases (\( t < 2 \) Myr) the ratio of ionizing photon flux to mechanical energy flux is almost constant, and the changes in \( q \) mostly reflect the size evolution of the mass-loss bubble. After 2 Myr, the ionizing photon flux rapidly decreases as massive stars evolve to red supergiants, and then the mechanical energy flux increases as a result of Wolf-Rayet stellar winds. Both of these lead to a strong decline in \( q \). At around 3.5 Myr, supernova explosions add to the internal pressure of the bubble, sharply decreasing the \( q \) in the ionized gas and re-accelerating the expansion of the mass-loss bubble. At later times, the progressive death of the high-mass stars leads to further declines in the ionizing photon flux, but the decline in \( q \) is slower because the internal pressure of the mass-loss bubble also declines, partially offsetting the decline in ionizing photon flux.

The theoretical ionization parameter rather strongly dependent upon the chemical abundance. It is driven by two factors. First, at higher abundance, the stellar wind has a higher opacity and therefore absorbs a greater fraction of the ionizing photons, reducing the \( q \) in the surrounding H II region. Second, the atmosphere scatters the photons emitted from the photosphere more efficiently when the atmospheric abundances are higher, leading to a greater conversion efficiency from luminous energy flux to mechanical energy flux in the stellar wind base region. This also leads to a diminution of \( q \) in the surrounding H II region. These factors acting together provide a sensitivity to metallicity of \( q \propto Z^{-0.8} \), approximately.

As described above at any age \( t \), the instantaneous ionization parameter - which determines the excitation of the H II region - is governed by the ratio of the mass of the cluster and the pressure in the surrounding ISM. Since cluster masses may vary between \( \sim 100 M_\odot \) and \( 10^6 M_\odot \), and the likely range of ISM pressures are between \( 10^4 < P_0/k < 10^7 \) cm\(^{-3}\) K it follows that reasonable values for \( R \) fall within the range \(-6 < \log R < +2 \). We have therefore computed, for each metallicity, an age sequence of model H II regions having \( \log R = -6, -4, -2, 0 \) and +2. For a given metallicity, the instantaneous value of the ionization parameter depends on \( R^{1/5} \), as we have shown in Paper II. Note that a particular choice of \( R \) is not tied to any particular cluster mass. Thus, a cluster of \( 10^5 M_\odot \) would be characterized by \( \log R \sim 0.6 \) in the solar vicinity, and \( \log R \sim -1.0 \) in a high-pressure starburst environment.

It is worth noting at this point that this parameterization of the problem of evolving H II regions only remains valid for as long as stochastic variation in the cluster membership may be ignored. This means that the exciting cluster has to be massive enough that the upper IMF is adequately populated with stars so as to avoid stochastic variations in either the mass to light ratio or the effective temperature of the cluster stars. This effectively limits the cluster mass for which these models are valid, \( M_{cl} \geq 10^3 M_\odot \).

Together, the two parameters \( Z/Z_\odot \) and \( \log R \) define a unique H II region spectrum, with one caveat, namely, that if the density of the ionized gas becomes too high, then collisional de-excitations of forbidden lines will alter the emergent spectrum. This only becomes a concern at the very highest values of ISM pressure either within ultra-compact H II regions (as computed by Doppital et al. 2006a) or else in starburst environments with \( P_0/k > 10^7 \) cm\(^{-3}\) K. For the current purposes, we have computed the particular case of \( P_0/k = 10^6 \) cm\(^{-3}\) K, which constrains the electron density in the H II region below \( \sim 100\) cm\(^{-3}\) except at very earliest times and in the models of highest metallicities, where it may reach \( \sim 10^6 \) cm\(^{-3}\).

For each model, we have prepared tabular data for all the strong lines between the Lyman Limit and 88\textmu m, from which we form H\beta flux weighted time averaged spec-

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**Figure 2.** The computed run of ionization parameter at the inner edge of the H II region as a function of time and ISM pressure \( \log P_0/k \) (cm\(^{-3}\)K) for a cluster having a mass of \( 3 \times 10^5 M_\odot \) and assuming a Miller-Scalo IMF. A given choice of the variable \( R = (M_{cl}/M_\odot)/(P_0/k) \) defines a unique run of the ionization parameter with time.
tra to represent the integrated spectrum for a given $Z/Z_\odot$ and $\log R$. The set of strong spectral line intensities with respect to H$\beta$ are available on-line. The form of the tables is given in the Appendix, Tables 2 - 7. The code also returns the intensities of very many more fainter lines, which are not listed here.

3. **H II Region Emission Line Diagnostics**

3.1. Optical Lines

3.1.1. Veilleux & Osterbrook Diagnostics

The diagnostics that have been most frequently used in the classification of the nature of nebular excitation are those proposed by Veilleux & Osterbrook (1987) (hereinafter V&O). In these, the [N II] $\lambda 6584$/H$\alpha$ the [S II] $\lambda \lambda 6717,31$/H$\alpha$ or the [O III] $\lambda 4959$/H$\alpha$ are plotted against the [O III] $\lambda 5007$/H$\beta$ ratio.

These V&O ratios have the virtue of only using lines which are close together in wavelength in forming the ratio, so errors due to uncertain reddening corrections are avoided. These plots also nicely separate H II regions from regions excited by active galactic nuclei (Seyfert or LINER nuclei) and from shock-excited objects. The H II regions form an extremely tight sequence, particularly in the diagram using the [N II] $\lambda 6584$/H$\alpha$ ratio.

The results of our modelling for the [N II] $\lambda 6584$/H$\alpha$ vs. the [O III]/H$\beta$ ratio is shown in figure 3. Because of the difficulty of representing so many theoretical models on the same figure, this is presented here in color, and in four panels. The first panel shows models of all ages for each metallicity, color coded for clarity. The model series corresponding to $\log R = -2$ is drawn bold, since this is our best guess of the most likely value of $\log R$ in disk galaxies ($10^2 \leq M_\odot/M_\odot \leq 10^4$ and $10^4 \leq P/k \leq 10^6$ cm$^{-3}$K). The remaining three panels show the complete grid of models for $\log R = 0, -2$ and -4, respectively. Isochrones are plotted for 0.2, 1.0, 2.0, 3.0 and 4.0 Myr.

In this figure, the observational datasets for individual H II regions are presented as crosses. The data are drawn from van Zee et al. (1998); Kennicutt & Garnett (1996); Dennefeld & Stasinska (1983); Walsh & Roy (1997); Roy & Walsh (1997) and the extension of the data set to low abundances is from Pagel et al. (1992).

The reason why the observed H II regions on a [N II]/H$\alpha$ vs. [O III]/H$\beta$ form such a narrow sequence is quite evident. First, to be bright, and therefore selected for observation, observed H II regions should have an age less than $\sim$ 3 Myr. In this age range, the isochrones of all models of different abundances fall into the very narrow strip defined by the observations. Although it depends somewhat on the assumed value of $\log R$, it is clear that no observed H II region has an age greater than 3 - 4 Myr, consistent with the presumption of strong observational selection against old H II regions.

This figure should be compared with Figure 2 of Dopita et al. (2000), in which a grid of models in $Z/Z_\odot$ and $q$, the ionization parameter were presented. It is clear that, in order to have a low metallicity H II region with a low ionization parameter, the H II region has to be faint and old, and would therefore not have been observed in these surveys. For metallicities greater than about $Z/Z_\odot \sim 0.5$, the models are highly degenerate in terms of both the metallicity and the cluster age. This accounts for the very tight distribution of observed points in the region of the plot where $\log ([O III]/H$β$) < 0.0$.

Since the models of Dopita et al. (2000) were run, the EUV field predicted by the Starburst 99 v.5 code has softened, thanks to improvements in the treatment of extended atmospheres. This leads both to the reduction in the limiting [N II]/H$\alpha$ ratio seen in figure 3, which improves the fit with the observations, and the decrease in the limiting [O III]/H$\beta$ ratio, which tends to make the fit somewhat worse at the low metallicity end.

Note that the aging tracks make a sharp zig-zag causing the 3 Myr isochrone to lie above the 2 Myr isochrone for metallicities above solar. This is particularly visible in panel (c) of figure 3, and is the result of the appearance of the Wolf-Rayet stars at ages $\sim$ 3 Myr, which briefly harden the overall stellar radiation field before they themselves explode as Type II supernovae.

The fit between theory and observation is much poorer when we consider the second of the Veilleux & Osterbrock diagrams which plots the [S II] $\lambda \lambda 6717,31$/H$\alpha$ ratio vs. the [O III] $\lambda 5007$/H$\beta$ ratio. This is shown in figure 4. In general, the predicted [S II] lines are weaker than observed, by as much as a factor of two. A similar effect was seen in our earlier modeling, see figure 3 of Dopita et al. (2000), and is not fully understood.

The [S II] $\lambda \lambda 6717,31$/H$\alpha$ ratio is more ambiguous than the [N II] $\lambda 6584$/H$\alpha$ ratio if we wanted to use it as an abundance indicator, particularly at high metallicity. However, the 0.2 - 3 Myr isochrones still define a narrow range in line ratio space, albeit not exactly coincident with the observations. The reasons for such a discrepancy between theory and observation in this, as well as in other line ratio plots will be discussed in section 5.

3.1.2. The BPT Diagram

Baldwin, Phillips & Terlevich (1981) (hereinafter BPT) first proposed the use of the [O III] $\lambda 5007$/[O II] $\lambda 3727,29$ ratio vs the [O III] $\lambda 5007$/H$\beta$ line ratio as a diagnostic both to separate active nuclei from H II regions and also to provide an excitation sequence for H II regions. Our results for this line ratio are shown in figure 5. The [O III]/[O II] ratio is an excitation sensitive ratio, sensitive to the ionization parameter in the nebula. Because of their higher ionization parameters and their central stars with higher effective temperatures at a given age, the low-metallicity H II regions are characterized by systematically higher [O III]/[O II] ratios. Like all other ratios of optical forbidden lines to recombination lines, for a given stellar age, the [O III] $\lambda 5007$/H$\beta$ ratio starts off low at low metallicity, reaches a maximum at a certain metallicity, and then declines swiftly at higher metallicities. The reason for this was explained in the introduction in the context of the $R_{[O II]}$ ratio. As a consequence, the BPT diagram is highly degenerate in metallicity in the range 0.2 $\leq Z/Z_\odot \leq 2$, explaining the tightness of the observed H II region sequence. This means, however, that the [O III]/H$\beta$ ratio is of little use as an abundance diagnostic except when $Z/Z_\odot < 0.2$. Even then it requires the observation of the [O III]/[O II] ratio before an Oxygen abundance can be derived from it.
Although the theoretical sequence has much the same form as defined by the observations, it is notable that, for all values of the \([\text{O III}]/\text{[O II]}\) ratio, the maximum of the \([\text{O III}]/\text{H}\beta\) lies below the maximum defined by the observations. Furthermore, even for the highest value of \(\log R\), the zero-age models do not reach to the maximum \([\text{O III}]/\text{[O II]}\) ratio defined by the observations. As discussed in section 5, below, both of these discrepancies can be ascribed to a single source, namely that the input spectrum we are using in the models is somewhat ‘softer’ than the EUV spectrum found in real H II regions.

3.1.3. The \(R_{23}\) Ratio

As described in the introduction, the \(R_{23}\) ratio has had a long and checkered history as a metallicity indicator. However, the sensitivity of the \([\text{O III}]\ \lambda 5007\text{Å}/\text{H}\beta\) ratio to the cluster age shown in figure 4 suggests that we should plot the \(R_{23}\) ratio against the \([\text{O III}]/\text{[O II]}\) ratio in order to be able to investigate the age sensitivity of the \(R_{23}\) ratio. This diagnostic is shown in figure 5.

For this diagnostic the fit between theory and observation is quite poor, due mainly to the fact that the \(R_{23}\) ratio is systematically underestimated in the models. The
effect is larger than that seen in the [O III]/Hβ ratio (see figure 5), showing that predicted strengths of the [O III] but especially the [O II] lines weaker than observations suggest. This will be discussed in the Discussion section, below. Points with low R$_{23}$ would be explained as having metallicities greater than twice solar.

This diagnostic plot shows immediately why the calibration of the R$_{23}$ ratio in terms of metallicity has been so difficult. Not only is the range of R$_{23}$ rather restricted, but it degenerate in terms of metallicity over a rather generous range, 0.2 ≤ Z/Z$_\odot$ ≤ 1.5, approximately. Not only that, but the ratio is fairly sensitive to excitation, as measured by the [O III]/[O II] ratio. Because low metallicity H II regions are characterized by high ionization parameters, the low metallicity points tend to occur in the upper right of this plot, while, from the form of the isochrones at high metallicity, the spray of points towards the bottom left of this diagnostic can only be due to very high metallicity (Z/Z$_\odot$ > 2) H II regions with ages of 1–3 Myr.

Based on these problems, we are constrained to conclude that R$_{23}$ is not a good abundance diagnostic. We will return to this point in Section 5, below.

3.1.4. Dopita et al. (2000) Diagnostics

Dopita et al. (2000) introduced two new abundance
diagnostics, based on the [N II]/[O II] line ratio. This ratio was favoured for two reasons which make it very sensitive to abundance. The first is that, over much of the range of interest, nitrogen is a secondary nucleosynthesis element, or at least has a large secondary component. Thus the ratio [N II]/[O II] will systematically increase with abundance. The second is connected with the fact that the [O II] λ3727,29Å lines are found in the near UV part of the spectrum, whereas the [N II] λ6584Å is in the red part of the spectrum. This might be construed as a disadvantage in the use of the [N II]/[O II] ratio, since the reddening corrections are large, and correspondingly more uncertain. However, this problem is more than offset by the fact that the mean temperatures of H II regions are a strongly decreasing function of metallicity and at high abundances, the mean thermal energy of the electrons becomes too low to excite transitions with large electron excitation energy. Thus transitions such as the [O II] λ3727,29Å lines are quenched, while the lower threshold energy [N II] λ6584Å continue to be excited. For this reason as well, the [N II]/[O II] line ratio falls with increasing abundance.

The systematic decrease in the electron temperature with increasing metallicity may also affect the
Fig. 6.—As figure 3 but for the R$_{23}$—ratio vs. the [O III] $\lambda 5007$/[O II] $\lambda\lambda 3727,29$ ratio. In panels (b) to (d) the solar metallicity track has been omitted for clarity. This shows that the traditional R$_{23}$ ratio is not a good abundance diagnostic in the range $0.2 \leq Z/Z_\odot \leq 1.5$, approximately, and that it is quite sensitive to the nebular excitation. The theoretical tracks are, however, a rather poor fit to the observations. This is because the models have [O III] $\lambda\lambda 4959,5007$ and, even more so, [O II] $\lambda\lambda 3727,29$ weaker than those observed. By itself, this would induce an increase in the [O III]/[O II] ratio with metallicity. However, this is more than offset by two factors. Firstly, the mean effective temperature of the exciting stars falls with metallicity, and secondly, the mean ionization parameter is itself a decreasing function of metallicity. Both of these lead to a net decrease in the [O III]/[O II] line ratio with metallicity. Nonetheless, the [O III]/[O II] line ratio remains a sensitive indicator of the ionization parameter, which is strongly age dependent. Therefore, a plot of [N II] $\lambda 6584$/[O II] $\lambda 3727,29$ against the [O III] $\lambda 5007$/[O II] $\lambda\lambda 3727,29$ ratio should separate stellar age from stellar abundance. This is illustrated in figure 7.

It is clear that the [O III] $\lambda 5007$/[O II] $\lambda\lambda 3727,29$ ratio is an excellent diagnostic of both the stellar age and the nebular abundance. According to the theoretical tracks, all the observed H II regions have ages between 0 and roughly 4 Myr, with most lying in the age range 1–3 Myr. The division into abundance bins by use of the [N II] $\lambda 6584$/[O II] $\lambda\lambda 3727,29$ is very clean. Provided that the calibration is correct, then the abundance can be
obtained using only the [N II]/[O II] ratio to a precision of roughly 0.15 dex.

The [O III] $\lambda 5007\text{Å}/$H$\beta$ line ratio can be substituted for the [O III]/[O II] ratio, since both are sensitive to ionization parameter and therefore to the age of the cluster. However, the separation into age classes is not so sharp using this ratio, as can be seen in figure 8. Furthermore, we have seen in figure 5 that the models tend to systematically underestimate the [O III] $\lambda 5007\text{Å}/$H$\beta$ ratio, so therefore it follows that the age of the H II regions inferred using this diagnostic is also likely to be an underestimate of the true age.

The third Dopita et al. (2000) diagnostic which utilizes the [N II] $\lambda 6584\text{Å}/$[O II] $\lambda 3727,29\text{Å}$ ratio is that which plots this ratio against the [O III] $\lambda 5007\text{Å}/$[N II] $\lambda 6584\text{Å}$ ratio. The [O III] $\lambda 4959,5007\text{Å}/$[N II] $\lambda 6548,84\text{Å}$ ratio was first proposed by Alloin et al. (1979) as a more convenient abundance diagnostic, which is similar to the one we are using here. The observations and theoretical curves on this diagnostic are shown in figure 9. As can be seen in the diagram, both axes are quite sensitive to abundance, but the Alloin et al. (1979) ratio, by its use of the [O III] $\lambda 5007\text{Å}$ in the place of the [O II] $\lambda 3727,29\text{Å}$ is also more sensitive to parameters other than the abun-
dence.

Pettini & Pagel (2004) have argued that the \( \text{[O III]} \lambda 5007\AA / \text{[N II]} \lambda 6584\AA \) ratio is of itself a sensitive abundance indicator suitable to be used in the analysis of abundances in high-redshift galaxies. This is a little too simplistic. Because the \( \text{[O III]} / \text{[N II]} \) ratio is strongly dependent upon the excitation of the nebula, it is also sensitive to both the ionization parameter, as shown by Dopita et al. (2000) and to the age of the cluster of exciting stars. These sensitivities are as great as the sensitivity to abundance alone. Nonetheless, the \( \text{[N II]} \lambda 6584\AA / \text{[O II]} \lambda 3727,29\AA \) vs. \( \text{[O III]} \lambda 5007\AA / \text{[N II]} \lambda 6584\AA \) diagnostic plot has great utility in separating abundance from cluster age, and the results that it gives are in broad agreement with figure 7. From these two plots we can conclude that most H II regions are observed in the age range 1–3 Myr with little sensitivity of this age range with abundance.

This is in full accord with expectations. As shown in Paper II, after an age of 3 Myr, the absolute luminosity of H II regions in the recombination lines drops sharply, and due to the expansion of the H II region, the surface brightness drops even more rapidly. Both of these militate strongly against the observation of old H II regions in extragalactic studies. Furthermore, very young H II regions tend to be dust obscured since they are still embedded in their placental molecular cloud complex. Such H II regions will not be bright at optical wavelengths. In Paper II we estimated the molecular cloud dissipation timescale for the molecular clouds to be about 1 Myr using the particular example of M17. The molecular cloud dissipation timescale was introduced in Paper I, and is the characteristic timescale \( \tau \) for the H II region to emerge from its compact or ultra-compact configuration, and is a measure of the solid angle (as measured at the exciting stars) which is intercepted by molecular clouds; \( \Omega(t) = \exp[-t/\tau] \). Clearly, the relative dearth of young H II regions between 0.2 and 1.0 Myr, evident in figures 7 and 9, is consistent with \( \tau \sim 1 \) Myr.

In conclusion, the \( \text{[N II]} \lambda 6584\AA / \text{[O II]} \lambda 3727,29\AA \) ratio vs. the \( \text{[O III]} \lambda 5007\AA / \text{[N II]} \lambda 6584\AA \) provides a good diagnostic of both metallicity and age of the exciting cluster. The \( \text{[O III]} \lambda 5007\AA / \text{[N II]} \lambda 6584\AA \) ratio can only be used by itself as an abundance indicator to the degree to which we can assume a (fairly restricted) characteristic age for the exciting clusters. Statistically, this may be valid, but the results of its use in single galaxies should be treated with caution.

3.1.5. \( \text{[N II]} / \text{H}\alpha \) vs. \( \text{[S II]} / \text{H}\alpha \)

Because they lie very close to each other in wavelength, and because we have seen that \( \text{[N II]} \) is very sensitive to abundance, the \( \text{[N II]} \lambda 6584\AA / \text{H}\alpha \) vs. \( \text{[S II]} \lambda 6717,31\AA / \text{H}\alpha \) plot offers some hope as an abundance diagnostic. This has recently been investigated by Moustakas & Kennicutt (2005), who were interested to find out whether integrated spectra of galaxies were different from single H II regions when plotted in this way. We would expect to find such a difference in principle, because the integrated spectra do not discriminate against the emission from old H II regions in the manner described in the previous section. The results of our modelling is shown in figure 10.

In Paper II, we found that the diffuse component due to old, evolved, large and faint H II regions could amount to 20–30% of the total H\( \alpha \) emission, and suggested that this could be identified with the Diffuse Ionized Medium (DIM) which is almost ubiquitously seen in disk galaxies (Hoopes, Waterbos & Greenwald 1996; Martin 1997; Wang, Heckman & Lehnert 1998, 1999). This is usually referred to as the “Reynolds Layer” in the context of our own Galaxy; see a recent review by Reynolds (2004). In the past, the excitation of the DIM has been usually ascribed to leakage of ionizing photons from young H II regions. However, the emission from large, faint, low pressure and evolved H II regions might provide a better explanation.

In figure 10, the models of old H II regions with metallicities \( Z/Z_\odot > 1.0 \) reach up to line ratios of \( \text{[S II]} \lambda 6717,31\AA / \text{H}\alpha \sim 1 \) and \( \text{[N II]} \lambda 6548,84\AA / \text{H}\alpha \sim 2/3 \), which is certainly consistent with observed line ratios encountered in the DIM. However, in our Galaxy, line ratios even greater than these are seen. To explain these, we would have to invoke an additional heating mechanism, such as shocks, or a harder EUV field possibly produced by old ex-nuclei of Planetary Nebulae, which are sufficiently numerous to produce an appreciable EUV field out of the plane of the Galaxy.

3.2. Infrared Line Diagnostics

The ISO satellite first demonstrated the utility of mid-IR line diagnostics in the analysis of H II region spectra. For normal galactic H II regions, Giveon et al. (2002) obtained extensive ISO spectroscopy, as did Peeters et al. (2002) in the context of Ultra-Compact (UC) H II regions. Later, Verma et al. (2003) measured integrated spectra for a number of famous Starburst galaxies. We will use these data here, although we note that both the high-resolution and low-resolution modes of the Infrared Spectrometer (IRS) (Houck et al. 2004) on the Spitzer Space Observatory are producing much new and excellent data on both individual H II regions as well as on spectroscopy of whole galaxies.

Within the spectral range of the IRS, such line ratios that can be constructed are primarily sensitive to the nebular excitation. Examples include the \( \text{[Ne III]} 15.5\mu m / \text{[Ne II]} 12.8\mu m \) ratio, the \( \text{[S IV]} 10.5\mu m / \text{[S III]} 18.7\mu m \) ratio, the \( \text{[S IV]} 10.5\mu m / \text{[Ar III]} 9.0\mu m \) ratio, and the \( \text{[Ne III]} 15.5\mu m / \text{[S III]} 18.7\mu m \) ratio. Unfortunately, these are of little use in measuring anything other than the hardness of the EUV radiation field. All of the strong lines accessible in this region of the spectrum are produced by \( \alpha \)-process elements, and therefore the abundance ratios stay approximately constant with abundance. All the lines have low energy thresholds for excitation, and therefore none of them are particularly sensitive to the electron temperature, which varies strongly with abundance. In figure 11 we present only one example to demonstrate how poor these line ratios are as abundance diagnostics when used alone.

Much of the data used in this plot refers to observations of ultra-compact H II regions, which are not exactly comparable to “normal” H II regions. In particular, they are extremely dense, most are excited by only a single OB star, and many of the ionizing photons from the exciting star are absorbed by dust rather than by the ionized plasma. This accounts for much of the offset between
Fig. 8.—As figure 3 but for the [N II] λ6584Å/[O II] λλ3727,29Å against the [O III] λ5007Å/Hβ ratio, as used by Dopita et al. (2000). This is also a good diagnostic of both metallicity and of stellar age. Given that the models tend to underestimate the [O III] λ5007Å/Hβ ratio, the age of the H II regions using this diagnostic is also likely to be an underestimate.

In order to form a line ratio that is sensitive to abundance, we need to use a ratio with a Hydrogen or Helium recombination line. Unfortunately, these are rather faint in the mid-IR. About the best line we have is Brα λ0.458µm. Alternatively, Pfund−α λ7.458µm might be useable, although it is often difficult to observe against the PAH features seen at this wavelength. In figure 12 we show one such diagnostic, the [Ne III] 15.5µm / [Ne II] 12.8µm ratio versus the [Ne III] 15.5µm / Brα λ4.051µm line ratio. This has the advantage that, at a given value of the excitation measured by the [Ne III] 15.5µm / [Ne II] 12.8µm ratio, the [Ne III] 15.5µm / Brα λ4.051µm line ratio is a monatonic function of abundance up to at least $Z \sim 2.0 \times Z_{\odot}$, and so it provides a clean abundance diagnostic, unlike the comparable optical line ratio shown in figure 5.

Currently, the uncertainties in the observational data are to large for this to provide a very accurate abundance diagnostic. However, we may note that the observations...
from Giveon et al. (2002) are consistent with abundances between 2.0 and 0.4 $Z_\odot$, and with ages between 0 and 2 Myr. This abundance range is exactly what we would expect to find for Galactic H II regions over the range of Galactocentric radii observed by him. It is interesting that the ages are lower than those derived for H II regions at optical wavelengths. This is consistent with the selection criteria for IR-bright, compact H II regions. This selects for young H II regions. Additionally, the use of mid-IR wavelengths allow the H II region emission to be seen almost unimpeded by the surrounding molecular material, so the molecular cloud dissipation timescale is not a relevant parameter here.

4. INTEGRATED SPECTRA

The diagnostics presented in the previous sections were designed to derive parameters for single H II regions. However, what we seek to do now is to develop a spectral synthesis by taking recombination line flux averaged spectra along an evolutionary track of an H II region with given parameters. This reduces the number of free parameters to two; $Z/Z_\odot$ and $\log R$. The observations can then be used to constrain the values $\log R$, allowing the...
Fig. 10.—As figure 3 but for the [N II] $\lambda$6584Å/H$\alpha$ vs. [S II] $\lambda\lambda$6717,31Å/H$\alpha$ diagnostic line ratios. As in Figure 3 the data for individual H II regions are shown as crosses, and the integrated spectra from Moustakas & Kennicutt (2005) are shown as points. Because these are both ratios of lines in the red portion of the spectrum, and because N is partially a secondary element, this diagnostic turns out to be a good abundance diagnostic for $Z/Z_\odot < 1.0$. The models of the older and more diffuse H II regions are located close to the right hand boundary of the observational points. This gas can be identified with the warm ionized medium (WIM) in galaxies.

extragalactic abundance sequence for ensemble averages of evolving H II regions to be derived. This technique opens the way to the accurate study of the metallicity evolution of both individual galaxies and the Universe.

The model we adopt assumes that clusters are formed continuously, and that any single cluster has all of its stars born coevally. As described above, the cluster mass function does not enter explicitly into the models, which are characterized by their $R$--values. The process of producing an integrated spectrum for any $Z$ is therefore simply to integrate the fluxes from a single H II model through time, until it has faded such that $\geq 96\%$ of all ionizing photons have been emitted. This limits the integration time to lie within the first $5-6.5$ Myr. Stochastic effects due finite sampling of the stellar IMF - important at low cluster masses - are not included. However, the form of the cluster initial mass function either as inferred in Paper II, or derived from stellar number counts is such that each logarithmic bin of cluster mass contributes a similar amount to the total flux. Massive clusters will
et al. (2002) are plotted as filled circles, UC H\ II \ [S \ IV] create as superb an example of theoretical spaghetti as anything these authors have seen.

The [Ne II] \[\lambda 6584, 31\] \AA/\Halpha provide a clean abundance determination which is monotonic over the full abundance range. The isochrones are given for the case log R = -2. This diagram is an infrared analog of fig 5, but is a much cleaner diagnostic because these IR line ratios are very insensitive to the nebular temperature.

therefore tend to wash out the stochastic effects of low-mass clusters.

On line ratio diagnostics, there is no simple relationship between the ensemble averaged line ratio and the line ratios in the individual H\ II regions which make up this average. For example, a high ionization line such as [O III] \[\lambda 5007\] \AA will be mostly produced in the very youngest H\ II regions with the highest R-values. Low ionization lines such as the [S II] \[\lambda 6717,31\] \AA lines will have a much greater weighting from older evolved H\ II regions with low R-values. Indeed, for this line the majority of the line flux may come from regions lying outside the bright H II regions that would be normally selected for observation in studies of individual H\ II regions - in other words, from regions that form part of the 'warm ionized medium' (WIM).

Given these quite different selection biases, it is interesting to compare line ratio observations of the integrated line fluxes of galaxies with those of individual H\ II regions. Such a comparison helps us to quantify the importance of the WIM in determining the global line ratio. For this purpose, we have used the observations of individual H\ II regions listed and used above (3 and references in Section 3.1), and have drawn our sample of integrated line fluxes of galaxies from the Nearby Field Galaxy Survey (NFGS) (Jansen et al. 2000), and the recent survey by Moustakas & Kennicutt (2005).

In figure 13 we plot the main V&O diagnostic [N II] \[\lambda 6584\] \AA/\Halpha vs. [O III] \[\lambda 5007\] \AA/\Hbeta. This should be compared with figure 3. The models provide a good fit to the integrated spectra of galaxies. Indeed, the fit is better than that of the models of individual H\ II regions compared to data in figure 3. This is especially apparent at the low abundance end (where most observations are of relatively nearby dwarf irregular galaxies such as NGC6822, IC1613, IIZw40 and the like). This suggests that the observations of these low-abundance H\ II regions may be affected by aperture effects. This would be caused by observers picking out bright high-excitation sub-regions of the H\ II region from their long-slit spectra for analysis, rather than observing across the whole H\ II region to obtain an integrated spectrum of it. This would preferentially enhance the [O III] \[\lambda 5007\] \AA/\Hbeta ratio while at the same time depressing the [N II] \[\lambda 6584\] \AA/\Halpha ratio, moving the observed point in line ratio space towards the top and the left.

The fit with the second V&O diagnostic, the [S II] \[\lambda 6717,31\] \AA/\Halpha vs. [O III] \[\lambda 5007\] \AA/\Hbeta (figure 14) is less convincing. The integrated spectra are displaced to the right on the [S II] \[\lambda 6717,31\] \AA/\Halpha ratio compared with the spectra from individual H I regions, showing the importance of the contribution of the more diffuse ionized component. It is interesting to note that most of the highest points in terms of the [O III] \[\lambda 5007\] \AA/\Hbeta ratio are contributed by the Moustakas & Kennicutt (2005) data set. In this respect there are systematic differences between this data set and the NFGS survey. The reason for this is not apparent to us.

In the models, the [N II] \[\lambda 6584,84\] \AA are the major coolants in the outer parts of the H\ II regions. It is possible that the abundance of Nitrogen in the ionized gas is somewhat overestimated (by an underestimate of the depletion, for example), leading to saturation in the [N II] \[\lambda 6584\] \AA/\Halpha ratio, and a reduction in the [S II] \[\lambda 6717,31\] \AA/\Halpha ratio. The problem with the models in reproducing the observed [S II] \[\lambda 6717,31\] \AA/\Halpha ratios is systematic. Even with the old Starburst 99 v2
models, a similar problem was encountered by Dopita et al. (2000). This will be discussed further in the next section.

Let us now turn our attention to the BPT diagram, the \([\text{O} \text{III}] \lambda 5007/\text{H} \beta\) ratio vs. the \([\text{O} \text{III}] \lambda 5007/\text{H} \beta\) ratio (Baldwin, Phillips & Terlevich 1981). This is plotted in figure 15. Once again, the fit between the theory and observation is good, although on this diagnostic the data once again fall somewhat high relative to the theory in the \([\text{O} \text{III}] \lambda 5007/\text{H} \beta\) ratio at the low abundance end \(Z/Z_\odot < 0.4\).

We note that the \([\text{N} \text{II}] \lambda 6584/\text{H} \alpha\) ratio covers quite a large range and displays considerable sensitivity to abundance. However, the same is not true of the \([\text{O} \text{III}] \lambda 5007/\text{H} \beta\) ratio. Only two points in the NFGS survey lie below \(\log\,[\text{N} \text{II}] \lambda 6584/\text{H} \alpha = -1.5\), and since the \(Z/Z_\odot\) curve lies to the left of \(\log\,[\text{N} \text{II}] \lambda 6584/\text{H} \alpha = -1.5\), figure 13 suggests that the lower abundance bound to the NFGS survey is about \(Z/Z_\odot < 0.2\). This is also consistent with what would be implied from figure 15. Both figure 14 and figure 15 suggest that the upper bound is about \(Z/Z_\odot \sim 2\).

The first of the Dopita et al. (2000) diagnostics is shown in figure 16. This plots the \([\text{N} \text{II}] \lambda 6584/[\text{O} \text{II}] \lambda 3727,29\) ratio against the \([\text{O} \text{III}] \lambda 5007/\text{H} \beta\) ratio, and should be compared with figure 7. There is very little distinction between the distribution of the integrated spectra from the NFGS survey and the observations of individual H II regions on this diagram. Essentially any value of \(\log R\) seems to be permitted, although the majority of the points are consistent with a range 0 to -4 in this parameter. This is consistent with what we might have expected, given that the parameters which enter into \(R\), \(M_\alpha\) and \(P/k\), cover at least the range \(100 < M_\alpha/M_\odot < 10^5\) and \(10^4 < P/k < 10^7\,\text{cm}^{-3}\,\text{K}\).

The abundance range of the NFGS survey suggested by this plot is broader than that given by the V&O or BPT diagnostics, since the theory implies the existence of some galaxies with very low abundances. However, we must beware once again of the observational problems which enter into plots like this. The \([\text{N} \text{II}] \lambda 6584\) line and the \([\text{O} \text{II}] \lambda 3727,29\) lines lie at opposite ends of the spectrum, and so there is a very large reddening correction applied to the data. Generally speaking a standard reddening law is used to do this. In the case of the NFGS survey, for example the Clayton, Cardelli & Mathis (1989) extinction curve was used. However, the foreground dust screen in front of an individual H II region (let alone a whole galaxy) has a complex fractal structure, and rather than using an extinction curve, an attenuation curve should be used instead, see Fischera, Dopita & Sutherland (2003); Fischera & Dopita (2005) and Paper I.

The effect of an attenuation law will be to cause the strengths of lines in the red to be underestimated, while UV lines such as the \([\text{O} \text{II}] \lambda 3727,29\) lines will be systematically overestimated. These effects will mean that the observations corrected using an extinction law will land systematically too far to the left and too low on this diagram, while on (almost) extinction-free diagnostics such as the V&O plots, the data will plot onto the correct position. If this effect is the cause of the displacement

**Fig. 13.** — The synthesised H II region spectra on the V&O diagnostic \([\text{N} \text{II}] \lambda 6584/\text{H} \alpha\) vs. \([\text{O} \text{III}] \lambda 5007/\text{H} \beta\) (c.f. figure 3). The integrated galaxy spectra from the Nearby Field Galaxy Survey (NFGS) (Jansen et al. 2000) are shown as filled circles, while the crosses are for individual H II regions drawn from the sources referenced above, to show the degree to which the integrated spectra differ from the single source spectra. Note the large disparity between the integrated spectra and the observations of individual H II regions at the low abundance end \((Z/Z_\odot < 0.4)\). Compared with earlier models, the theory provides a good fit to the integrated galaxy data providing that \(\log R > -4\), and emphasizes the degeneracy of this V&O diagnostic.

**Fig. 14.** — The synthesised H II region spectra on the V&O diagnostic \([\text{S} \text{II}] \lambda 6717,31/\text{H} \alpha\) vs. \([\text{O} \text{III}] \lambda 5007/\text{H} \beta\) (c.f. figure 5). The integrated galaxy spectra are shown as filled circles, and include both the NFGS data and the data from Moustakas & Kennicutt (2005). Both the \([\text{S} \text{II}] \lambda 6717,31\) and the \([\text{O} \text{III}] \lambda 5007\) lines seem to be a little weak in the models compared with the observations.
between theory and observation seen in figure 15, this suggests that the [O III] λ5007Å/[O II] λλ3727,29Å ratio may be systematically underestimated by ~ 0.3 dex. This would imply that the [N II] λ6584Å/[O II] λλ3727,29Å ratio may be underestimated by a similar amount, since the extinction is determined from the Hα/Hβ ratio which means that the observed [N II] λ6584Å/[O III] λ5007Å ratio must necessarily be correct. The effect of a correction of this magnitude is shown on figure 16 as an arrow marked ‘extinction’. With a correction of this magnitude, not only can the lower bound of the abundance in the NFGS survey be reconciled with that given by figure 13 (Z/Z⊙ ~ 0.2), but also with the upper bound indicated by figure 15 (Z/Z⊙ ~ 2). The inferred range on log R would then be 2 to -4.

A systematic overestimate of the [O II] λλ3727,29Å lines would also lead to a systematic overestimate of R23. This may well account for much of the discrepancy between theory and observation in figure 6.

A similar effect is seen in the second of the Dopita et al. (2000) diagnostics is shown in figure 17. This plots the [N II] λ6584Å/[O II] λλ3727,29Å ratio against the [O III] λ5007Å/Hβ ratio. Once again, a systematic extinction correction error of 0.3 dex would shift the observational points into a range which is consistent with the both the abundance and R bounds inferred above.

Finally, we plot the [S II] λλ6717,31Å/Hα ratio versus the [N II] λ6584Å/Hα line ratio in figure 18 (compare with figure 10). This shows, once again, the value of the [N II] λ6584Å/Hα line ratio as an abundance diagnostic in its own right. It also illustrates, once again, our difficulties with the [S II] λλ6717,31Å/Hα ratio, with the observations, particularly the Moustakas & Kennicutt (2005) data set falling to the right of the theoretical curves in this ratio.

Note how the integrated spectra on figure 18 are con-
centrated along the right-hand side of the region defined by the observations of single H II regions. This reflects the fact that integrated galaxy spectra include the diffuse component of the ISM, even when this has a low surface brightness, because the total flux in the diffuse component may be an appreciable portion of the total emission. Indeed, a recent study by Oey et al. (2006) suggests that the “diffuse” fraction may exceed 50% in nearby starburst galaxies.

5. DISCUSSION & CONCLUSIONS

It should now be clear that these models represent a significant advance in our understanding of the strong line spectra of H II regions. In particular, the models explicitly account for the dynamical evolution of the H II region controlled through the mechanical energy input by both the stellar winds and supernova explosions. Two factors largely control the excitation of the young H II regions, both of these dependent on the chemical abundance. These are:

- The effective temperature of the exciting stars, which increases with decreasing metallicity, and
- The control of the ionization parameter by the stellar winds in the expanding H II regions. This was shown in Paper II to increase with decreasing metallicity

Since both of these effects operate to increase the excitation of low abundance H II regions, we therefore find an abundance dependent excitation, which much improves the fit of the theory compared to models in which the ionization parameter is treated as a free variable. In our models the ionization parameter is replaced by the $R$ parameter, the ratio of the cluster mass in solar masses to the pressure in the ISM: $P/k$ (cm$^{-3}$K). This parameter is used because all models with a given $R$ have a unique relationship between their instantaneous ionization parameter and time. This allows us to construct evolutionary tracks for ensembles of H II regions.

With increasing age, the ionization parameter falls almost monotonically, and the H II region fades after reaching its maximum brightness in H$\alpha$ after 1-2 Myr. The presence of Wolf-Rayet stars after about 3.5 Myr causes the effective temperature of the cluster to briefly increase. This increases the excitation for a short time, causing the 3 Myr and the 4 Myr isochrones to cross over each other on diagnostic plots for the cases of high metallicity ($Z/Z_\odot > 0.5$, approximately).

In this paper, we have identified a number of useful diagnostics for deriving the abundance and either the age, in the case of isolated H II regions, or the $R$ parameter, in the case of integrated spectra of galaxies. Our diagnostics for the integrated spectra are the first which explicitly take into account the fact that when we observe a whole galaxy, we are observing an ensemble average of H II regions of all ages, sizes and central cluster masses. The simplification we have been able to make by using the $R$ parameter has rendered this problem tractable to a more simple analysis other than treating each H II region separately, and adding the whole lot together at the end.

In comparing the models to the observational data we have identified some potential problems with the way that observations of H II regions have been made and analyzed. In particular:

- Long-slit observations do not integrate over the whole of an H II region, particularly in the case of observations of nearby, low metallicity dwarf irregular galaxies. By picking out the brightest regions of such H II regions, we bias the data towards the high-excitation regions and the spectrum is not representative of the whole H II region (Luridiana & Peimbert 2001; Stasinska & Izotov 2003) and

- The use of a reddening correction using an extinction curve, rather than an attenuation curve (which is appropriate for spatially extended objects) will cause the line intensities of UV lines to be systematically overestimated, biasing the strong line diagnostics which use the [O II] $\lambda\lambda$3727,29 Å lines.

This second effect would reveal itself in the spectro-photometry as a failure to reproduce the correct intensities of the higher members of the Balmer Series, such as H$\delta$ or He, and so should be quite easy to check for in observational data sets. Such an effect would also influence the measurement of the strength of the [O III] $\lambda$4363Å line, again causing it to be overestimated. This could be part of the reason for the long-standing discrepancy between the abundances derived from the strong lines and those obtained from measurements of the electron temperature using ratios such as [O III] $\lambda$4363Å/[O III] $\lambda$5007Å, see Bresolin, Garnett & Kennicutt (2004) for a recent discussion. We expect that the major part of the discrepancy will turn out to be caused by temperature fluctuations. However, this could be easily corrected for by assuming the Case B recombination
line ratio between H$\beta$ and H$\gamma$, and measuring the forbidden line strengths relative to the nearest Balmer lines in the spectrum.

There is clearly a need for integral field spectrophotometry on extragalactic H II regions. This would allow efficient construction of integrated spectra and assist in the removal of stellar flux from the spectrum. Such observations would not only help to remove the remaining discrepancies between theory and observation but also give insight into the use of theoretical integral spectra in the analysis of the chemical evolution history of the early Universe.

Our models have their deficiencies. In general, all the low ionization species are predicted weaker than observed. These include the [O I] $\lambda 6300\AA$, the [S II] $\lambda \lambda 6717,31\AA$, and the [O II] $\lambda \lambda 3727,29\AA$, although these lines are probably affected by the reddening corrections made to the observations.

What could enhance the [S II] $\lambda \lambda 6717,31\AA$/H$\alpha$ ratio or the [O I] $\lambda 6300\AA$/H$\alpha$ ratio? First, both the the O I and the S II ion are very much more sensitive than the N II ion to the diffuse radiation field in H II regions. They are therefore much enhanced in the vicinity of ionization fronts, and in shadow regions behind elephant trunk features, which are obscured from direct stellar radiation and illuminated only by the diffuse nebular radiation field. Second, both are much enhanced in shock regions. Indeed high [S II]/H$\alpha$ ratios are used as a means of identifying supernova remnants either embedded in H II regions or in the ISM at large, and [O I]/H$\alpha$ ratios reach 0.5 or higher in shock-excited regions. Neither of these effects are taken into account in the models.

In addition, the O I ion is locked by charge-exchange reactions to the concentration of H I. Furthermore, the collision strength of [O I] $\lambda 6300\AA$ increases with electron temperature. To produce a high [O I] $\lambda 6300\AA$/H$\alpha$ ratio in a purely photoionized region requires the presence of a hard radiation field. This could originate either as a thermal soft X-ray continuum from the shocked bubble of stellar wind material, or it could simply be an indication of a hotter sub-component in the global stellar radiation field.

If the radiation field produced by Starburst 99 v5 is too soft, this could be rectified in at least three ways. First, by the use of a flatter IMF in the upper mass ranges ($M/M_{\odot} > 10$). This could be possible because observationally we have very few constraints other than by use of the excitation of H II regions. Second, by adding another stellar component such as mass-exchange massive binaries to the stellar synthesis.

A third - and quite likely possibility is that the EUV spectrum of the massive stars used in Starburst 99 v5. may be in error. With previous versions of Starburst 99 based on the CoStar models (Schaefer & de Koter 1997), the EUV spectrum was, rather, too hard. However, Morisset et al. (2004) has demonstrated that the theoretical number of ionizing photons emitted by the central star and the shape of the ionizing spectrum is highly dependent upon the atmospheric model used. At one extreme are the CoStar models, at the other extreme are found the ‘classical’ Kurucz (Kurucz 1991, 1994) plane-parallel LTE line blanketed models used in Starburts99 v5. The Kurucz models display the softest EUV spectra and the lowest photoionizing flux, and are restricted to log $g = 3.0$ for the models with higher effective temperature, $T_{\text{eff}}$. In between these extremes are found three sets of models with fairly similar photoionizing flux predictions (Morisset et al. 2004), the TLUSTY models of Lanz & Hubeny (2003a,b), the WM-Basic models of Pauldrach, Hoffman, & Lennon (2001) and the CMFGEN models Hillier & Miller (1998). Of these, the TLUSTY models are plane-parallel hydrostatic, while the other two are spherical dynamic atmospheres. All of this offers plenty of potential for error in the estimation of the the hardness of the EUV spectrum for a given cluster mass and metallicity.

Given that the [O III] $\lambda 5007\AA$/H$\beta$ ratio of the models also appears to be on the low side, we believe that an increase in the stellar effective temperature, either by a flattening of the IMF or by some other means offers the best chance to more properly match the theory with the observations. The models are too weak in their forbidden line strengths overall. The Stoy (1993) method (Pottasch & Preite-Martinez 1983) of deriving the effective temperature of the exciting stars relies upon measuring the total flux cooling lines (which is a measure of the mean energy per photoionization) to a recombination line (which counts the number of photoionizations). Thus, if we want to increase the absolute strengths of the forbidden lines, we have to increase the stellar effective temperature. This increase would also strongly increase the [O I] $\lambda 6300\AA$/H$\alpha$ ratio by both increasing the extent of the partially-ionized zonr and by increasing the electron temperature within it.

A niggling uncertainty with the modeling is the mismatch between the Starburst 99 v5 abundance set and the abundance set given in table 1. The Starburst 99 v5 has to rely on the older stellar evolution models which use the old value of the solar abundances. In an attempt to quantify this effect, we ran a test model with a 0.4Z$_{\odot}$ spectral synthesis cluster model from Starburst 99 v5 embedded in a nebula with 1.0Z$_{\odot}$ (using the abundances given in table 1). This made surprisingly little difference, changing critical line ratios by 0.1 dex or less, except for the [O I] $\lambda 6300\AA$/H$\alpha$ ratio, which increased by 34%. We therefore conclude that the results presented in this paper are reasonably secure against any future adjustment of stellar atmospheric abundances.

In conclusion, the major advances in modelling made in this paper are:

- For individual HII regions, it becomes possible to estimate the ages of the exciting stars from the positions of the observations on HII region isochrones. Previously, this was not possible, since the ionization parameter and the effective temperature of the cluster (determined by the ageing of its stars) produce similar effects on the emitted spectrum. The self-consistent treatment we have developed which includes the dynamical evolution of the HII region consistent with the properties of the stellar wind generated by the central cluster, and which recognizes that the stellar wind determines the pressure in the HII region allows us to eliminate the use of arbitrary geometries.

- In addition, this work gives a methodology to construct much more “realistic” integrated spectra of
TABLE 2. LINE ID AND WAVELENGTH LIST

| Line ID # | Ion   | \(\lambda\) (Å) | Line ID # | Ion   | \(\lambda\) (Å) |
|-----------|-------|-----------------|-----------|-------|-----------------|
| 01        | H I   | 1215.7          | 27        | [S II] | 6716.3          |
| 02        | C III | 1909.1          | 28        | [S II] | 6730.7          |
| 03        | C III | 1911.2          | 29        | [Ar III] | 7751.0          |
| 04        | [C II] | 2325.2          | 30        | [S III] | 9069.3          |
| 05        | Mg II | 2767.9          | 31        | H I    | 10049.4         |
| 06        | [O II] | 3726.0          | 32        | H I    | 10049.4         |
| 07        | [O II] | 3728.7          | 33        | H I    | 10049.4         |
| 08        | H I   | 3797.9          | 34        | He I   | 10830.0         |
| 09        | H I   | 3835.4          | 35        | He I   | 10833.0         |
| 10        | [Ne III] | 3868.7      | 36        | H I    | 10938.1         |
| 11        | He I  | 3888.6          | 37        | H I    | 12818.1         |
| 12        | H I   | 3889.1          | 38        | H I    | 18751.0         |
| 13        | [Ne III] | 3967.4      | 39        | H I    | 26252.0         |
| 14        | H I   | 3970.1          | 40        | H I    | 40512.0         |
| 15        | H I   | 4104.7          | 41        | [Ar II] | 69832.8         |
| 16        | H I   | 4340.5          | 42        | [Ar III] | 89892.5       |
| 17        | He I  | 4471.5          | 43        | [S IV] | 105221          |
| 18        | H I   | 4861.3          | 44        | [Ne II] | 128115          |
| 19        | [O III] | 4958.8       | 45        | [Ne III] | 155513         |
| 20        | [O III] | 5006.8       | 46        | [S III] | 186821          |
| 21        | H I   | 5875.6          | 47        | [S III] | 336366          |
| 22        | [O I]  | 6300.2          | 48        | Si II  | 347941          |
| 23        | [N II] | 6548.0          | 49        | O III  | 517972          |
| 24        | H I   | 6562.8          | 50        | N III  | 573845          |
| 25        | [N II] | 6583.3          | 51        | O III  | 883017          |
| 26        | He I  | 6678.2          | ..        | ..     | ..              |

HII galaxies, something that has not been possible before in the approximations which assume that a whole galaxy can be represented by a single spherical HII region with a chosen abundance and ionization parameter.

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APPENDIX

Here we give a summary of the strong line flux ratios with respect to H\(\beta\) as computed in the photoionization models. The line identifications, the ionic species and the wavelengths of each line listed in the electronic version of this paper are given in Table 2.

In the electronic version of the paper, separate tables are given for each of the abundances computed; 0.05, 0.2, 0.4, 1.0 and 2.0 \(Z_{\odot}\), and in each of these tables, line fluxes with respect to H\(\beta\) = 1.0 are given for each of the 51 lines listed in Table 2. These spectral line intensities are given for each value of log \(R\) computed; +2, 0, -2, -4 and -6. The quantity \(R\) is that defined in the text of the paper:

\[
R = \left[ \frac{M_d}{M_{\odot}} \right] \left[ \frac{P/k}{10^4\text{cm}^{-3}\text{K}} \right]
\]

The electronic tables (Tables 3 through 7) will be available when the paper is published.

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