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SMITH, Robin <http://orcid.org/0000-0002-9671-8599>, BISHOP, Jack, WHELDON, Carl and KOKALOVA, Tzany

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Theoretical approaches to the 3α break-up of ^{12}C

Robin Smith^{1†}, Jack Bishop^{2}, Carl Wheldon^{3}, Tzany Kokalova^{3}

^{1}Faculty of Science, Technology & Arts, Sheffield Hallam University, Sheffield, S1 1WB, UK
^{2}Department of Physics & Astronomy and Cyclotron Institute, Texas A&M University, College Station, TX 77843, USA
^{3}School of Physics & Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK

E-mail: †`robin.smith@shu.ac.uk`

Abstract. Two recent experiments have indicated that the break-up of the ^{12}C Hoyle state is dominated by the sequential ^{8}Be(g.s.) $+ \alpha$ decay channel. The rare direct 3α decay was found to contribute with a branching ratio of less than 0.047% (95% C.L.). However, the ability of experimentalists to successfully disentangle these two competing decay channels relies on accurate theoretical predictions of how they each manifest in phase space distribution of the three break-up α-particles. The following paper reviews the current theoretical approaches to calculating the break-up of the Hoyle state and introduces a semi-classical WKB approach, which adequately reproduces the results of more sophisticated calculations. It is proposed that a more accurate upper limit on this branching ratio may be obtained if these new theoretical results are taken into account when analysing experimental data.

1. Introduction
There has recently been a renewed interest in studying the decay modes of the Hoyle state in ^{12}C [1, 2]. In astrophysics, the Hoyle state is crucial for the synthesis of carbon in the helium burning phase of main sequence stars. The presence of a 0^{+} resonance near to the 3α threshold was first predicted by Fred Hoyle to boost the triple-α capture process by seven orders of magnitude [3]. The prediction was successfully verified experimentally and this famous state bears Hoyle's name. Due to the way the Hoyle state resonance is synthesised in nature, it was proposed that this state is an excellent candidate for the presence of α-clustering, a feature of nuclei that has been discussed throughout the history of nuclear physics [4]. If we assume the ^{12}C nucleus to be made up of three α-particles, it leads to the question of what configuration they take within the nucleus.

The U(7) algebraic cluster model (ACM), which assumes an equilateral triangle 3α structure with $\mathcal{D}_{3h}$ point symmetry, well reproduces the low energy portion of the ^{12}C excitation spectrum [5]. In this model, the ground state is a compact 3α structure and the Hoyle state has a larger average separation of the α-clusters, as illustrated in figure 1. Contrastingly, an *ab initio* lattice approach using chiral effective field theory has predicted the state to have a 'bent-arm' configuration. Furthermore, other *ab initio* fermionic molecular dynamics (FMD) and antisymmetrized molecular dynamics (AMD) calculations predict a clear $\alpha + ^{8}$Be configuration in the intrinsic frame [6]. It has been suggested that the energy distribution of the three α-particles emitted during the decay of ^{12}C may provide some indication of the initial configuration

of those α-particles before the decay, meaning that precise break-up measurements could be a powerful structural probe.
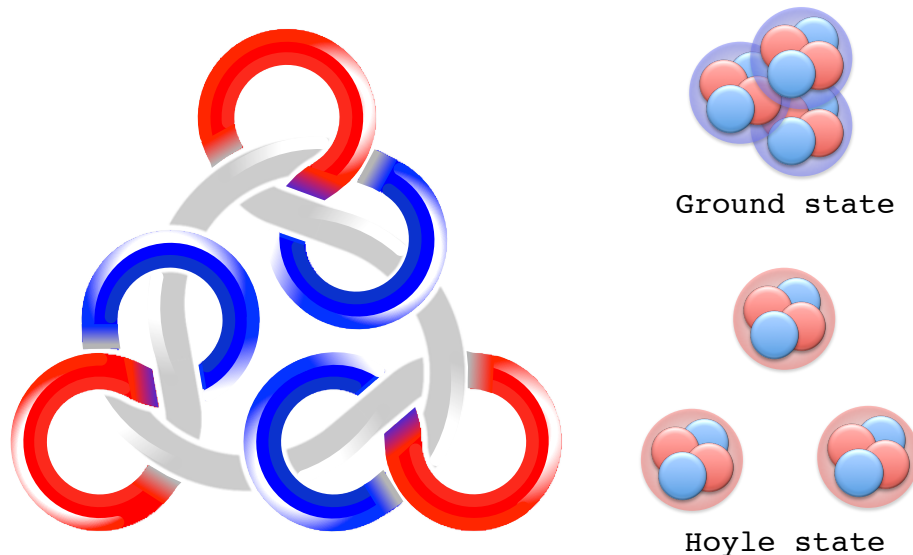
Figure 1. (Colour online) Traditional Celtic knot design illustrating the 3α structures in ^{12}C. The dark (blue) loops represent the compact ground state and the lighter (red) loops represent the excited Hoyle state, which possesses a large radius. The two structures are linked by a single knot, alluding to the fact that these two manifestations are both part of the same nucleus.

One particular theory for the structure arises from the idea that the bosonic nature of the α-particle could dominate the dynamics of this nuclear state. In agreement with the predictions of the ACM, the charge form factor for inelastic electron excitation from the ground state to the Hoyle state indicates that the Hoyle state has a large radius and hence a larger average separation of the alpha clusters [7]. This feature is illustrated in figure 1. Under this assumption, the important degrees of freedom could then be considered bosonic rather than fermionic, producing the nuclear analogue of an atomic Bose Einstein Condensation (BEC) [8]. Under these conditions there should be no structural preference for either a sequential, ^{8}Be $+ \alpha$, or a direct 3α decay and so the branching ratio should depend only on the available phase space and penetrabilities through the decay barrier [9]. The present experimental upper limits on the direct decay mode cannot exclude this possibility due to theoretical uncertainties [10], so more experimental work is needed to further constrain the direct decay branching ratio.

Until recently, when comparing experimental decay data to theoretical predictions, simple phenomenological models for sequential and direct 3α break-up were used. For the sequential case, a narrow intermediate ^{8}Be ground state resonance at 92 keV was modelled. However, the possible enhancement of this resonance at higher excitations in the form of its *ghost* was not considered in detail. Further, the direct decay mode has historically been modelled purely phenomenologically. Uniform decays to the available phase space, equal α-particle energies, and collinear cases have been compared with data, but none of these have any firm theoretical grounding.

One of the most recent studies made a more accurate theoretical description of the direct decay phase space distribution using the WKB method in hyperspherical coordinates. Using this model, an improved upper limit of 0.035% was placed on the direct decay branching ratio [10].

A description of this theoretical methodology and the `PeTA` code used in the calculations is the focus on this paper. Later, other theoretical approaches to describing the direct decay are discussed and compared with the semi-classical approximation. These calculations indicate that some of the data in experiments that are labelled as *direct* decay, may in fact be a different manifestation of the *sequential* decay. It is argued that a reanalysis of the latest experimental data is needed.

2. A semi-classical WKB approach to 3α decay

2.1. Sequential decay

The semi-classical approach presented in reference [11] was extended in order to examine the energy distribution of α-particles emitted during the direct decay of the Hoyle state. The present section builds on the work of reference [10]. The WKB approximation is a method for obtaining an approximate solution to the time-independent Schrödinger equation in one-dimension. In this case, it is used to calculate 3-body tunnelling rates through Coulomb potential barriers.

In the simple two-body $\alpha + {}^8\mathrm{Be}$ decay of ${}^{12}\mathrm{C}$, the Schrödinger equation can be easily solved for the relative motion of the two daughter nuclei and the Coulomb interaction between them. For a general 2-body decay, where the two daughters have charges Z_1 and Z_2, a separation of r, and a relative angular momentum of ℓ, the potential is given as the sum of the Coulomb and centrifugal terms by the equation

$$V_\ell(r) = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r} + \frac{\ell(\ell+1)}{2\mu r^2}, \tag{1}$$

where μ is the reduced mass of the two-particle system. The potential for the $\ell = 0$ $\alpha + {}^8\mathrm{Be}$ decay of the Hoyle state is shown in the left panel of figure 2. Using this potential, the tunnelling penetrability "T" may then be calculated using the WKB method as

$$T = \frac{1}{1+e^{2S}} \approx e^{-2S}, \quad \text{where} \quad S = \frac{1}{\hbar}\int_{r_0}^{r_1} dr\sqrt{2\mu(V_\ell(r) - E)}, \tag{2}$$

E is the energy of the system above the two-body decay threshold, r_0 is the matching radius and r_1 is the classical turning point. This method works well and calculates a penetrability for the $\alpha + {}^8\mathrm{Be}$ decay of the Hoyle state within 5% of the exact value calculated using the regular and irregular Coulomb wave functions evaluated at the channel radius [12].

2.2. Direct decay

Unlike in the simple sequential decay case, a direct decay into three α-particles permits a variety of different configurations. These vary from an extreme collinear decay, where two of the α-particles are emitted back-to-back, leaving the third stationary, all the way through to an equal energies case, where the α-particles are emitted at 120° to one another. These cases are pictured in the inset of the right panel of figure 2. Importantly, these different decay configurations possess different Coulomb barriers which are also shown in the right panel of figure 2. Therefore, even though a direct decay mechanism may uniformly sample the phase space for a given decay, certain 3α configurations are preferred, and these Coulomb effects will heavily influence the phase space distribution in a direct decay.

To model this kind of decay, we parameterise the system using a quantity called the hyperradius, ρ, which depends on the masses of each particle m_i and their separation r_{ik}. It is defined as
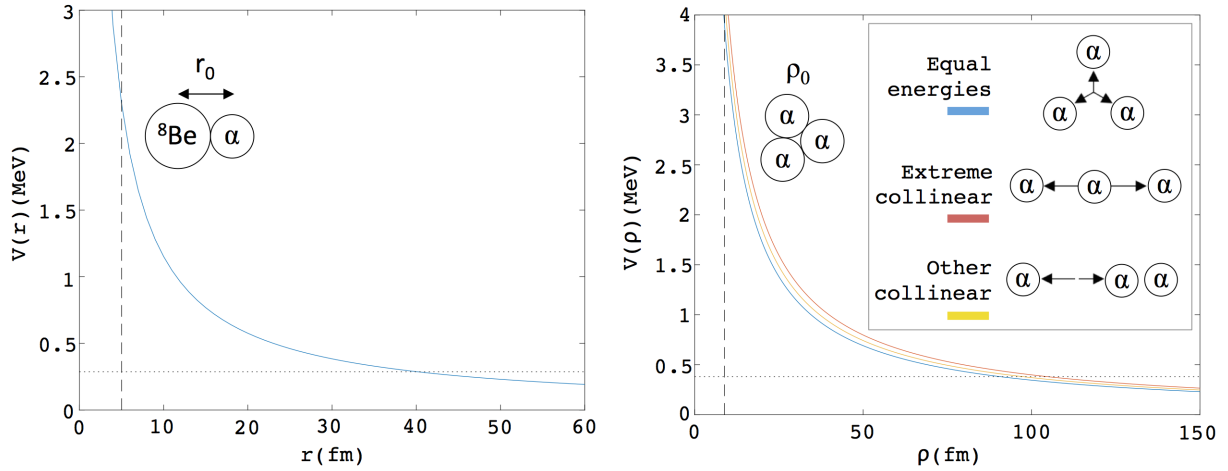
Figure 2. (Colour online) Left panel: the Coulomb potential for the $\alpha + {}^8\text{Be}$ decay of the Hoyle state. Right panel: the Coulomb potential as a function of the hyperradius for various direct 3α break-up configurations of the Hoyle state.

$$\rho^2 \equiv \frac{1}{mM} \sum_{i<k}^{3} m_i m_k r_{ik}^2, \tag{3}$$

where $M = \sum_{j}^{3} m_j$ and m is an arbitrary normalisation mass. If the particles are emitted during the decay with certain energies (velocities), as the decay progresses, the separation between the particles, and hence, the hyperradius of the system, will increase linearly. This only applies under the strict assumption that we ignore final-state Coulomb interactions. In reality, the Coulomb interactions between the particles during the decay will perturb their paths and hence the Coulomb barrier. Here, we assume the particles follow their initial trajectory, unperturbed, and hence tunnel through a constant potential barrier. The validity of this assumption is addressed in the approach presented in section 3.

A particular decay orientation is defined by positive scaling constants s_{ik}, which are a constant of the decay, and are calculated by normalising the relative distances between the particles by the hyperradius as

$$s_{ik}^2 \equiv \frac{r_{ik}^2}{\rho^2}. \tag{4}$$

The Coulomb potential, accounting for the interactions between all α-particles can be parameterised by the hyperradius and scaling constants as

$$V_C(\rho) = \sum_{i<k}^{3} \frac{Z_i Z_k e^2}{r_{ik}} = \frac{1}{\rho} \sum_{i<k}^{3} \frac{Z_i Z_k e^2}{s_{ik}}. \tag{5}$$

Although it is not needed for the decay of the 0^+ Hoyle state, a general 3-body decay must account for the centrifugal barrier term

$$V_K(\rho) = \frac{\hbar^2 (K + 3/2)(K + 5/2)}{2m\rho^2}, \tag{6}$$

where m is the normalisation mass and K is the hypermomentum quantum number. In this model it is assumed that only the lowest value partial wave contributes because it has the lowest barrier [11, 13]. In general, the total potential barrier, $V(\rho)$, is the sum of equations 5 and 6. This may be used in conjunction with equation 2 to give the tunnelling penetrability as

$$T = \frac{1}{1 + e^{2S}} \approx e^{-2S}, \quad \text{where} \quad S = \frac{1}{\hbar} \int_{\rho_0}^{\rho_1} d\rho \sqrt{2m\left(V(\rho) - E\right)}, \tag{7}$$

where ρ_0 corresponds to the hyperradius where all three α-particles are touching, shown in the right panel of figure 2 and ρ_1 is the classical turning point. The `PeTA` code utilises this result.

*2.3. Penetrability of Three Alphas (`PeTA`) code and results*
The Penetrability of Three Alphas (`PeTA`) code was used to determine a realistic distribution of the three α-particle energies during the direct decay of the Hoyle state. The `Matlab` source code may be obtained from reference [14]. It is a Monte-Carlo code which uniformly samples the available phase space for a given direct decay and generates the permitted non-relativistic 3α momenta subject to the constraints of energy and momentum conservation. To quantify the total phase space of an n-body decay, all of the kinematically-allowed configurations must be integrated over. The total phase space for an n-body decay into particles of mass m_i, with an energy over threshold of E, is given by the equation

$$W(E, n) = \left(\frac{1}{\sum_{b=1}^{n} m_b} \prod_{b=1}^{n} m_b\right)^{3/2} \frac{(2\pi)^{3(n-1)/2}}{\Gamma(3(n-1)/2)} E^{3n/2 - 5/2}, \tag{8}$$

where Γ is the Gamma function. The full derivation of this function is shown in reference [10]. From this alone, it is possible to estimate the direct 3α decay branching ratio as $W(E_3, 3)/W(E_2, 2) = 1.8 \times 10^{-3} = 0.18\%$.

The `PeTA` code generates a user-defined number of 3-body direct decay events within the allowed phase space (chosen here for illustration to be 10^6). For each event, the unique orientations of the α-particles result in a different Coulomb barrier, and the resulting penetrability is calculated using equation 7. The integral is calculated numerically using the trapezium rule. The decay amplitude for a particular orientation is weighted by this penetrability. A plot of the simulated events is shown in the right panel of figure 3 in the form of a Dalitz plot [15]. In contrast, uniform direct decays without any penetrability factor yield a uniform coverage of the Dalitz plot. For comparison, the sequential decay, where one of the α-particles carries away around half of the decay energy, is shown in the left panel of figure 3. This plot includes the effects of the experimental resolution. The coordinates of the Dalitz plots are written in terms of the fractional α-particle energies in the frame of the decaying ^{12}C, ϵ_i. The coordinates are defined as $x = \sqrt{3}(\epsilon_1 - \epsilon_3)$ and $y = 2\epsilon_2 - \epsilon_1 - \epsilon_3$.

Typically, when analysing experimental data, a uniform coverage of the Dalitz plot is used to model the direct decay. The more realistic direct decay profile peaks towards the centre of the Dalitz plot and has less overlap with sequential decays, which appear as a straight band. When considering this type of direct decay, named DDP^2 (Direct Decay + Phase space + Penetrability), an improved upper limit of the direct decay can be placed at 0.035%, compared with 0.047% when using the standard direct decay profile [10].
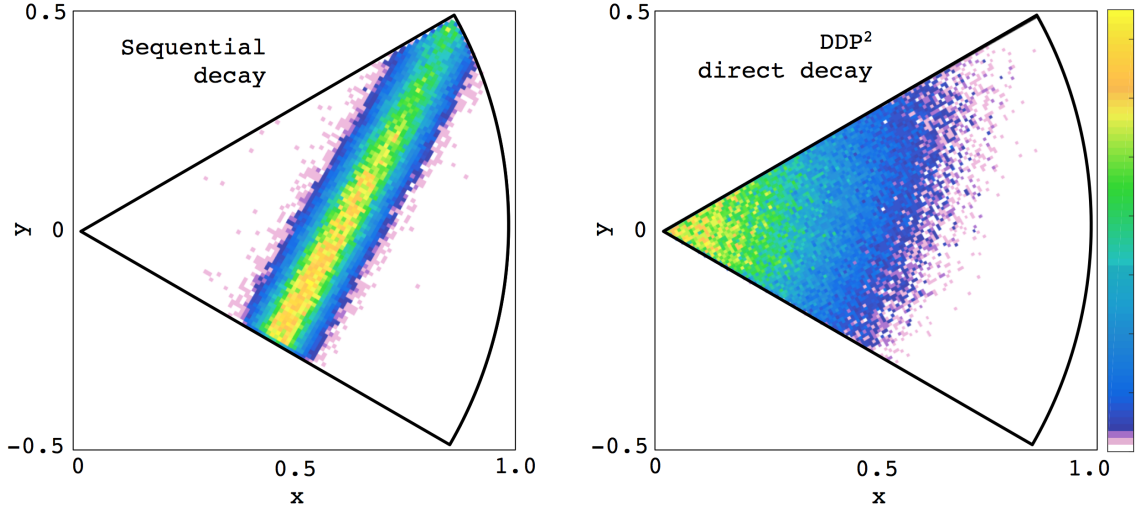
Figure 3. (Colour online) Left: Dalitz plot for sequential decays (including experimental resolution). Right: Weighted phase space distribution including the effects of the WKB 3-body penetrability (excluding experimental resolution). The coordinates are defined in the main text.

3. An R-matrix approach

In 2018, Refsgaard *et al.* developed a sequential R-matrix model to describe the Hoyle state break-up [15]. They noted that even in the $\alpha + {}^8\text{Be}$ sequential decay, some features that may resemble a direct 3α decay naturally appear in the phase space distribution of the α-particles. This arises due to an unusual feature of near-threshold resonances called the *ghost anomaly* [16]. The R-matrix line shape for an isolated single channel resonance is given by the equation

$$w(E) = \frac{1}{\pi} \frac{\Gamma_i/2}{[E_i - E - \gamma^2(S - B)]^2 + \Gamma_i^2/4},$$ (9)

where S and B are the shift function and boundary condition for the channel. Since the channel width Γ_i is energy dependent ($\Gamma_i(E) = 2P_\ell(E)\gamma_i$ where γ_i is the reduced channel width), as the energy above threshold increases, so does the decay penetrability through the Coulomb barrier, meaning that $\Gamma_i(E)$ also increases. This modifies the standard Breit-Wigner lineshape of the resonance and permits an extra yield above the main resonance peak. It is this extra yield that may be mistaken for direct decays in experimental data.

The theoretical intensity of the ghost anomaly is highly dependent on the channel radius; a free parameter in R-matrix theory. Using this method with sensible channel radii, the ghost anomaly is expected to appear with a strength ranging between 0.01% and 1%. This is approaching the levels of sensitivity seen in the latest experiments and hence must be factored in when attempting to evaluate any direct decay contribution in the data.

Another important feature of this R-matrix approach is to include a final-state Coulomb interaction (FSCI) between the three α-particles. The secondary break-up of ${}^8\text{Be}$ happens within the Coulomb field of the initial emitted α-particle. This is built into the model by replacing the penetrabilities of the $\alpha + {}^8\text{Be}$ pair by the product of penetrabilities for the $\alpha + \alpha_1$ and $\alpha + \alpha_2$ pairs (where α_1 and α_2 are the two α-particles resulting from the ${}^8\text{Be}$ decay) once the α

+ ^{8}Be pair have separated to some distance. This model nicely fits experimental data from the break-up of the 1^+ state at 12.71 MeV and it would be desirable to test this model against the latest high precision Hoyle state decay data [1, 2].

This approach models direct decay by approximating this as a sequential decay through a very broad resonance at high excitation. The results were seen to be quite insensitive to the energy and width of this resonance. The phase space distribution predicted by this model produces a Dalitz plot (right panel of figure 3 in reference [15]) very similar to that shown by the right panel of our figure 3, adding credibility to the semi-classical WKB approximation.

4. Full 3-body quantum mechanical calculations

Although Coulomb interactions between the α-particles modify their final state configuration, the decay barriers are significantly altered when including an attractive $\alpha - \alpha$ interaction. Hence, several attempts have been made to understand the decay and structure of the Hoyle state by performing full three-body quantum mechanical calculations.

Alvarez-Rodríguez *et al.*, calculated the 3α decays of states in ^{12}C using the hyperspherical adiabatic expansion method of the Faddeev equations [17]. The interaction term was chosen to vary only with the hyprerradius. This approach simultaneously describes all the possible interactions in a system of three particles in a fully quantum mechanical way. The angular part of the Schrödinger equation is solved and the full wave function is then expanded using a basis of angular wave functions [13]. This allows these components of the wave function to be examined at fixed hyperradii, as the system separates. It was found that the Hoyle state is dominated by the $n = 1$ angular basis function over all values of the hyperradius from $\rho = 0$ to 80 fm. This indicates that the angular wave function does not significantly change during the decay and that the final state distribution of α-particle energies may be a good reflection of the initial structure. The calculations also predict a direct decay branch of the Hoyle state at 1%; significantly larger than the best experimental upper limits.

The method also permits the energy distributions of the final state α-particles to be calculated, but the results for the Hoyle state are not discussed in the work of Alvarez-Rodríguez *et al.* However, a theoretical study by Ishikawa predicted the direct 3α component of the decay of the Hoyle state [18] and at the same time calculated the 3α phase space distribution. In that work, the wave function for the reaction $\gamma + {}^{12}\text{C} \rightarrow 3\alpha$ was solved using the Faddeev three-body formalism. The α-particles were treated as bosons and their underlying fermionic structures were considered to be incorporated into the various $\alpha - \alpha$ interactions used.

The phase space distribution of the three α-particles during the decay [18] is shown as the right panel of figure 4. This is in remarkably good agreement with the R-matrix model of Refsgaard *et al.* [15] shown as the left panel of figure 4. The majority of events that may be considered as *direct decay* lie near to the sequential decay band and so could just be a manifestation of the ^{8}Be ghost anomaly. The regions of the Dalitz plot predicted by Ishikawa were split up as in figure 1 b) in reference [18], in order to approximate the "direct decay" branching ratio. This indicates that the direct decay should contribute at the total level of $\approx 0.1\%$, with DDE (equal energies) and DDL (collinear) direct decay contributions at the levels of 0.005% and 0.03% respectively.

5. Summary

There are numerous ways to examine the 3α decay of the Hoyle state; from the semi-classical WKB approximation through to a full three-body quantum mechanical approach. Certain predictions of each of these models overlap. It was seen that the phase space distributions
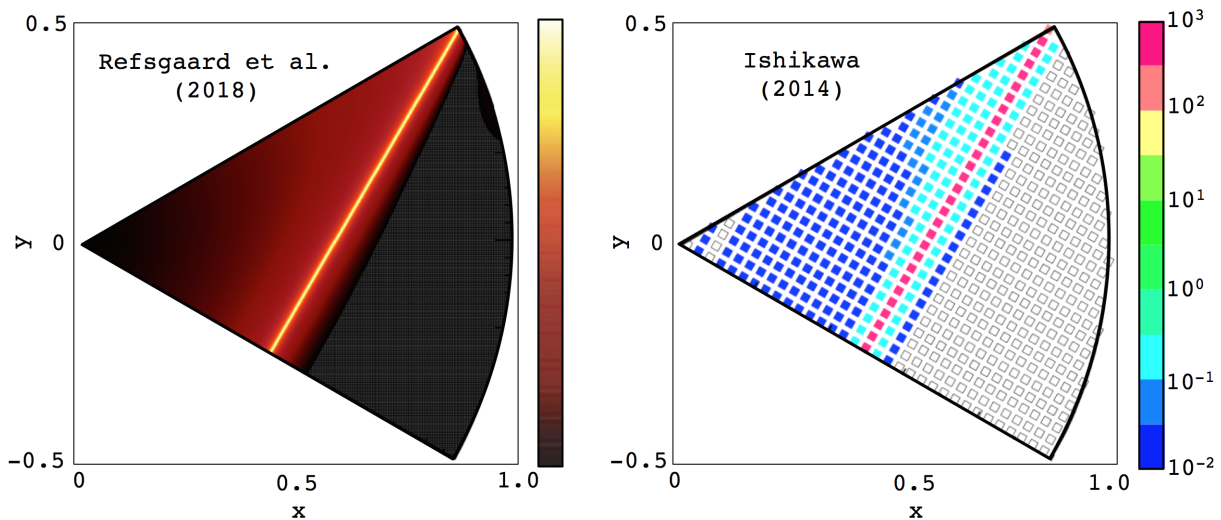
Figure 4. (Colour online) Theoretical Dalitz plot distributions by Refsgaard *et al.* [15] (left panel) and Ishikawa [18] (right panel). Both are plotted with a logarithmic colour scale.

for direct decay predicted by the WKB and *R*-matrix methods are very alike. Similarly, the distribution calculated using the Faddeev three-body formalism reproduces the main features of the *R*-matrix sequential model. The latest Hoyle state decay data need to be reanalysed and compared with these physically motivated α energy distributions, rather than the phenomenological models typically used.

6. Acknowledgements

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