The Complex Infrared Dust Continuum Emission of NGC 1068: Ground-based N- and Q-band Spectroscopy and New Radiative Transfer Models

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Abstract

Thanks to ground-based infrared and submillimeter observations the study of the dusty torus of nearby active galactic nuclei has greatly advanced in the last years. With the aim of further investigating the nuclear mid-infrared emission of the archetypal Seyfert 2 galaxy NGC 1068, here we present a fitting to the N- and Q-band Michelle/Gemini spectra. We initially test several available spectral energy distribution (SED) libraries, including smooth, clumpy and two-phase torus models, and a clumpy disk+wind model. We find that the spectra of NGC 1068 cannot be reproduced with any of these models. Although, the smooth torus models describe the spectra of NGC 1068 if we allow variation of some model parameters among the two spectral bands. Motivated by this result, we produced new SEDs using the radiative transfer code SKIRT. We use two concentric tori that allow us to test a more complex geometry. We test different values for the inner and outer radii, half-opening angle, radial, and polar exponent of the power-law density profile, opacity, and viewing angle. Furthermore, we also test the dust grains’ size and different optical and calorimetric properties of silicate grains. The best-fitting model consists of two concentric components with outer radii of 1.8 and 28 pc, respectively. We find that the size and the optical and calorimetric properties of graphite and silicate grains in the dust structure are key to reproducing the spectra of NGC 1068. A maximum grain size of 1 μm leads to a significant improvement in the fit. We conclude that the dust in NGC 1068 reaches different scales, where the highest contribution to the mid-infrared is given by a central and compact component. A less dense and extended component is present, which can be either part of the same torus (conform a flared disk) or can represent the emission of a polar dust component, as already suggested from interferometric observations.

Unified Astronomy Thesaurus concepts: Active galactic nuclei (16); Dust continuum emission (412); Infrared astronomy (786); Seyfert galaxies (1447)

1. Introduction

According to the unified model of active galactic nuclei (AGN; Antonucci 1993; Urry & Padovani 1995), a dust structure surrounding the central engine and causing obscuration is the angular stone to explain the different types of AGN observed. This structure, commonly called the dusty torus, is located a few parsecs from the supermassive black hole (SMBH). However, the physical details of this structure, such as the dust characteristics (both in terms of chemical composition and grain size distribution) and its geometrical distribution, are still quite poorly understood (see Ramos Almeida & Ricci 2017, for a review).

One way to study the dusty torus in AGN is throughout the fitting of the spectral energy distribution (SED) to dust models using different distributions and/or chemical compositions. Initially, for the sake of simplicity, most authors have used smooth dust distributions using radial and vertical density profiles (Pier & Krolik 1992; Granato & Danese 1994; Efstathiou & Rowan-Robinson 1995; van Bemmel & Dullemen 2003; Schartmann et al. 2005). Other authors have developed radiative transfer models to reproduce geometries where the dust is distributed in clouds (Nenkova et al. 2008a, 2008b; Höing & Kishimoto 2010). This is the so-called clumpy distribution. A mix of smooth and clumpy distributions has also been proposed (Stalevski et al. 2012; Siebenmorgen et al. 2015). More recently, a more complex scenario has been proposed to explain the infrared nuclear emission of Seyfert galaxies. Höing & Kishimoto (2017) produced a model that includes a compact, geometrically thin disk in the equatorial region of the AGN, and an extended, elongated polar structure (see also Stalevski et al. 2019). The interpretation of high spatial resolution spectra, achieved by means of SED fitting techniques exploiting theoretical emission models, is the key to an unbiased study of the dust properties in AGN, limiting the effect of the host galaxy emission (Ramos Almeida et al. 2009, 2011; Alonso-Herrero et al. 2011; González-Martín et al. 2019a).

NGC 1068 ($D = 10.58$ Mpc; we used the average distance independent of redshift reported in NED) is considered to be the...
prototype Seyfert 2 galaxy (Bland-Hawthorn et al. 1997) showing broad lines using polarized light (Miller & Antonucci 1983; Antonucci & Miller 1985), where the central source is obscured by dust. Although NGC 1068 is probably one of the best explored AGN at all wavelengths, there is still controversy on the geometry of the obscurer (e.g., Gravity Collaboration et al. 2020, and references therein). This torus has been studied in a large number of works.

Works at submillimeter wavelengths are particularly relevant because they have observed the nuclear molecular gas and dust with unprecedented spatial resolution. García-Burillo et al. (2016) used the Atacama Large Millimeter Array (ALMA) to map the molecular and continuum emission from the circum-nuclear disk of NGC 1068 and resolve its dusty torus with a size of ∼4 pc. Imanishi et al. (2018) found sizes of 13 × 4 pc and 12 × 5 pc for the molecular torus as seen by HCN J = 3–2 and HCO+ J = 3–2, respectively. Lopez-Rodriguez et al. (2020) detected the polarization signature of the torus by means of magnetically aligned dust grain emission. They find that the torus is inhomogeneous and turbulent. Through the HCN (J = 3–2) transition, Impellizzeri et al. (2019) identified two disk counter-rotating, an inner disk spanning 0.5 ≤ r ≤ 1.2 pc, and an outer disk extending up to ∼7 pc. Indeed, the inner disk seems to be linked to the kinematics of the maser spots, which are located in a rotating disk with inner radius of ∼0.65 pc and outer radius of ∼1.1 pc (Greenhill & Gwinn 1997), which traces the outer, colder part of the accretion disk. García-Burillo et al. (2019) also found that the molecular torus has a radial stratification extending over a range of 10–30 pc, since different tracers show different sizes: the HCO+ (4 – 3), CO(2–1), and CO(3–2) with a full size of 11, 26, and 28 pc, respectively.

At mid-infrared (MIR) wavelengths several studies have also tried to infer the properties of the dust in NGC 1068. Early works already showed a complex and extended morphology at MIR (Cameron et al. 1993; Bock et al. 2000), which were later on confirmed by interferometry (Wittkowski et al. 2004; Jaffe et al. 2004; López-Gonzaga et al. 2014) and spectroscopy (Mason et al. 2006; Raban et al. 2009). SED fitting including MIR emission has also been very useful. For instance, Lopez-Rodriguez et al. (2018) used Stratospheric Observatory for Infrared Astronomy (SOFIA), infrared and submillimeter observations in order to characterize the emission and distribution of the dust in NGC 1068, which was first studied by Alonso-Herrero et al. (2011). They found that a clumpy torus is able to reproduce the observed emission, although with some discrepancies mainly at short wavelengths. More recently Pasetto et al. (2019) fitted the SED of NGC 1068 to MIR spectra (N and Q bands) using a smooth torus model finding that the torus has a more complex structure, since they are not able to fit both spectral bands with the same values for the parameters of the torus model. Note that in these works only one or two torus models were used for the SED fitting.

The aim of this work is to reproduce the 7–23 μm MIR spectra of NGC 1068 (divided into N- and Q-band spectra at 7–13 and 18–23 μm, respectively). This kind of work can only be done for NGC 1068 because it is the only AGN with both N- and Q-band ground-based observations, and therefore, with enough spatial resolution to isolate the nuclear dust continuum emission from other dust contributors. Future James Web Space Telescope (JWST) observations will allow these types of studies for dozen of nearby AGN. Thus, this work also aims to refine the SED fitting technique in preparation for oncoming JWST observations. For that purpose, we explore here available models and create new SEDs. In particular, we test four different torus models to reproduce the SED of NGC 1068: the smooth torus model by Fritz et al. (2006), the clumpy torus model by Nenkova et al. (2008b), the two-phase torus model by Stalevski et al. (2016), and the clumpy disk+wind model by Höning & Kishimoto (2017). We confirm the complex dust distribution needed to reproduce the MIR spectra by producing new synthetic SEDs using the 3D Monte Carlo radiative transfer code SKIRT.9

The paper is organized as follows. Section 2 gives a brief summary of the available dusty models used in this paper. Section 3 describes the spectral fitting of the data to existing models. We explore the dust properties using the radiative transfer code SKIRT in Section 4 and a discussion of these results is in Section 5. Finally, in Section 6 we summarize our main results.

2. Torus Models

Here, we give a brief summary of the four AGN dust models tested in this paper. The parameters and a sketch of the dust distribution for each model are included in Table 1 and in Figure 9, respectively (see also González-Martín et al. 2019a, and references therein):

1. Smooth torus model by Fritz et al. (2006): They use a toroidal geometry, consisting of a flared disk that can be represented as two concentric spheres, delimiting, respectively, the inner and the outer torus radius, having the polar cones removed (see the top-left panel in Figure 9). For the composition of dust, they consider a typical silicate and graphite grain size with radius 0.025–0.25 and 0.005–0.25 μm, respectively, in almost equal percentages (52.9% silicate and 47.1% graphite).

2. Clumpy torus model by Nenkova et al. (2008b): They use a formalism that accounts for the concentration of dust in clouds, forming a torus-like structure (see the top-right panel in Figure 9). They assume spherical dust grains and a standard Galactic mix of 53% silicate and 47% graphite grains.

3. Two-phase torus model by Stalevski et al. (2016): They model the dust in a toroidal geometry with a two-phase medium, consisting of high-density clumps embedded in a smooth dusty component of low density (see the bottom-left panel in Figure 9). The dust chemical composition is set to a mixture of silicate and graphite grains. The fraction of total dust mass in clumps compared to the total dust mass is set to 0.97.

4. Clumpy disk and outflow model by Höning & Kishimoto (2017): They model the dust in a clumpy disk-like geometry and a polar hollow cone (see the bottom-right panel in Figure 9). The dust chemical composition is set to only large graphites (0.1–1 μm) in the outflow. For the disk, the dust composition consists of graphites of 0.1–1 μm in the inner part, and a mixture of graphites and silicates of 0.025–0.25 μm in the rest of the disk.

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9 https://www.skirt.ugent.be
Table 1  
Summary of Used Dusty Models Described in Section 2

| Model                  | Parameter                                                                 | Dust Distribution       | Dust Composition          | Grain Size (μm) |
|------------------------|---------------------------------------------------------------------------|-------------------------|---------------------------|-----------------|
| Fritz et al. (2006)    | Viewing angle toward the torus, i                                        | Smooth torus            | Silicate and graphite     | Silicate: 0.025–0.25 Graphite: 0.005–0.25 |
|                        | Half-opening angle of the torus, σ                                        |                         |                           |                 |
|                        | Index of the logarithmic azimuthal density distribution, Γ                  |                         |                           |                 |
|                        | Index of the logarithmic radial density distribution, β                   |                         |                           |                 |
|                        | Ratio between the external and internal radius, Y                         |                         |                           |                 |
|                        | Edge-on optical depth at 9.7 μm, τν, 9.7 μm                                |                         |                           |                 |
| Nenkova et al. (2008b) | Viewing angle toward the torus, i                                        | Clumpy torus            | Standard ISM              | Silicate: 0.025–0.25 Graphite: 0.005–0.25 |
|                        | Number of clouds in the equatorial plane, N                               |                         |                           |                 |
|                        | Half-opening angle of the torus, σ                                        |                         |                           |                 |
|                        | Ratio between the external and internal radius, Y                         |                         |                           |                 |
|                        | Slope of the radial density distribution of clouds, q                     |                         |                           |                 |
|                        | Optical depth of the individual clouds, τν                               |                         |                           |                 |
| Stalevski et al. (2016)| Viewing angle toward the torus, i                                        | Smooth and clumpy torus | Silicate and graphite     | Silicate: 0.025–0.25 Graphite: 0.005–0.25 |
|                        | Half-opening angle of the torus, σ                                        |                         |                           |                 |
|                        | Index of the logarithmic azimuthal density distribution, p                 |                         |                           |                 |
|                        | Index of the logarithmic radial density distribution, q                   |                         |                           |                 |
|                        | Ratio between the external and internal radius, Y                         |                         |                           |                 |
|                        | Edge-on optical depth at 9.7 μm, τν, 9.7 μm                                |                         |                           |                 |
| Höning & Kishimoto (2017)| Viewing angle toward the torus, i                                           | Clumpy disk and outflow | Standard ISM              | Standard: 0.025–0.25 Large: 0.1–1 |
|                        | Number of clouds in the equatorial plane, N                               |                         |                           |                 |
|                        | Index of the radial distribution of clouds, a                             |                         |                           |                 |
|                        | Half-opening angle of the wind, θ                                         |                         |                           |                 |
|                        | Angular width of the walls of the cone, σ                                |                         |                           |                 |
|                        | Power-law index for dust cloud distribution along the wind, a_w            |                         |                           |                 |
|                        | Wind-to-disk ratio, f_w                                                  |                         |                           |                 |
|                        | Optical depth of individual clouds, τcl (fixed)                           |                         |                           |                 |

Note. We show the parameters in Column 2, dusty distribution in Column 3, dust chemical composition in Column 4, and grain size in Column 5.

3. Data and Spectral Fitting

We use the N-band (7–13 μm) and Q-band (17–23 μm) spectra obtained with Michelle spectrometer located in the 8.1 m Gemini-North Telescope. This data set was processed for a previous analysis by Alonso-Herrero et al. (2011). They scale the spectra to the corresponding 0′4 photometric points in order to match the angular resolutions of the imaging and spectroscopic data. The spectra were extracted as point-like sources, following the center and the trace of the standard star. Point-spread function (PSF) and slit-loss corrections were applied to the spectrum. Further details are included in Alonso-Herrero et al. (2011). In Figure 1, we show the N- and Q-band spectra of NGC 1068. We include the photometric points reported by Tomono et al. (2001) using a circular aperture of 0′4 diameter (similar to the spatial resolution achieved by the ground-based spectra), and the photometric point used in Lopez-Rodriguez et al. (2018) estimated by using their PSF-scaling method. Note that all but two photometric points (at 9.69 and 10.38 μm) agree with the spectra. A similar figure is shown in Alonso-Herrero et al. (2011). This comparison ensures proper flux calibration of the N- and Q-band spectra.

We used the four dust models presented in Section 2 in order to fit the N- and Q-band spectra. Spectral fitting is performed using the XSPEC\(^{10}\) fitting package, which is a command-driven, interactive, spectral-fitting program within the HEASOFT\(^{11}\) software. XSPEC (Arnaud 1996) already includes a large number of incorporated models but new models can be uploaded using the additive table, using the ATABLE task. We converted the spectra to XSPEC format in order to upload and fit them to the dust models within XSPEC. In order to assess

\(^{10}\) http://heasarc.gsfc.nasa.gov/docs/xanadu/xspec/

\(^{11}\) https://heasarc.gsfc.nasa.gov

Figure 1. N- and Q-band spectra of NGC 1068 (black lines). The green circles and orange square symbols are the photometry of Tomono et al. (2001) and Lopez-Rodriguez et al. (2018), respectively.
the goodness of fit for each model, we used the reduced $\chi^2$ statistics value.

We first test whether both $N$- and $Q$-spectra could be fitted with a single SED dust model (Section 3.1), then we tested more complex SEDs by allowing some parameters to vary among the two bands (Section 3.2.)

### 3.1. Single SED Dust Model

This initial attempt assumes that a single SED is able to simultaneously fit the $N$ and $Q$ bands. This is the same approximation done in previous works (e.g., Alonso-Herrero et al. 2011; García-Bernete et al. 2019). Figure 2 shows the best fit for the four dust models tested. All the models provide unacceptable fits with reduced $\chi^2, \chi^2 = \chi^2 / \text{dof} > 4$. Among them, the best fit is obtained with the disk+wind clumpy model by Hönig & Kishimoto (2017) ($\chi^2 = 4.41$), followed by the smooth torus model by Fritz et al. (2006) ($\chi^2 = 4.98$). The other two models provide $\chi^2 > 10$. Tables 5–8 (Column 2) in Appendix B show the values obtained for each parameter and the goodness of the fit throughout the $\chi^2 / \text{dof}$. In general, all models overestimate the $Q$-band flux and they struggle to reproduce the 10 $\mu$m silicate absorption feature. A clear flux deficit at short wavelengths (below 9 $\mu$m) is also visible irrespective of the model used.

### 3.2. Two SED Dust Model

Due to the poor fits obtained with the one-SED models, which tend to overpredict the $Q$-band flux compared with observed spectrum, and show poor agreement in the 10 $\mu$m silicate absorption profiles, we propose that a combination of models might provide a better fit, allowing complex dust geometries. Note that this is not an attempt to obtain a physically motivated fit but to explore the complexity that can achieve a better match to the data. In Section 4, we then use these results to explore new SEDs using the radiative transfer code SKIRT, which produces physically motivated SEDs. Therefore, this exploration of complex models is needed to obtain the initial guess for the parameters in the radiative transfer modeling. This was already explored by Pasetto et al. (2019) by unlinking the slope of the azimuthal distribution of dust, $\gamma$, and the edge-on optical depth at 9.7 $\mu$m, $\tau_{9.7}$, for the smooth model presented by Fritz et al. (2006). This provided a much better fit in Pasetto et al. (2019). Here, we perform a systematic analysis using the four AGN dust models described in Section 2.

Using the best fit from each model (Section 3.1), we separately fit the $N$- and $Q$-band spectra, allowing just one parameter to vary between the two fits. In other words, we kept all the parameters fixed during the fit, except for one of them. We found that changing the parameters does not always result in an improvement of the fit. Tables 5–8 (Column 3 onward) in
Appendix B show the values obtained and the best statistics (i.e., $\chi^2$/dof) when each parameter of the model is untied between bands. In order to study if the fit improved by allowing to vary one of the parameters, we used the f-statistic test (f-test). For the smooth torus model by Fritz et al. (2006), the fit improves by untying any parameter. For the clumpy torus by Nenkova et al. (2008b), the two-phase torus by Stalevski et al. (2016), and the clumpy disk+wind by Höning & Kishimoto (2017), we obtain improved spectral fits by untying any parameter except for $Y$, $p$, and $i$, respectively. However, the improvement is not enough to obtain $\chi^2 < 2$ for the clumpy torus by Nenkova et al. (2008b) and clumpy disk+wind by Höning & Kishimoto (2017). For two-phase torus by Stalevski et al. (2016), the fit improves with $\chi^2 < 2$ only by untying the half-opening angle of the torus $\sigma$; and for the smooth torus model by Fritz et al. (2006), the fit improves significantly by untying any parameter except for the viewing angle, $i$ ($\chi^2 = 2.17$). Thus, unlinking almost any parameter improves the final fit, pointing to the complex nature of the source.

We then test if untying two parameters significantly improves the resulting fit. We discard the subsequent analysis of clumpy torus by Nenkova et al. (2008b) and clumpy disk +wind by Höning & Kishimoto (2017) due to the poor spectral fit obtained so far. In general, we consider those parameters that produce a statistical improvement (see above). For the smooth torus model by Fritz et al. (2006), we discard the model obtained by untying viewing angle, $i$, because we do not expect two different values for the viewing angle of the torus. In the case of the two-phase torus by Stalevski et al. (2016), we only consider the model obtained by untying the half-opening angle, $\sigma$, because untying the other parameters does not produce a significant improvement.

We show in Table 2 the results for the smooth torus model by Fritz et al. (2006) obtained by untying two parameters between the $N$ and $Q$ bands. We have 10 possible combinations of the parameters. We discard six of them because they do not provide physically plausible scenarios (e.g., due to the better resolution of the $N$ band compared to the $Q$ band, values for $Y$ in the $N$ band larger than the $Q$ band are not expected). We have four scenarios that significantly improved the fits by untying: (1) $\sigma$ and $\gamma$; (2) $\sigma$ and $\beta$; (3) $\gamma$ and $\tau$; and (4) $\beta$ and $\tau$. Figure 3 shows the best fit obtained for these four scenarios. For the two-phase torus model by Stalevski et al. (2016), we discard the combination untying $\sigma$ with any other parameter because any of them results in a physically plausible scenario, since the half-opening angle of the torus related to the $N$ band (with better resolution) is bigger than that related to the $Q$ band (with worse resolution). Table 9 in Appendix B shows the results of combining the half-opening angle, $\sigma$, with the other parameters for the two-phase torus model by Stalevski et al. (2016).

### 4. SED Simulations with SKIRT

In order to better explore the complex torus structure of NGC 1068, we produced synthetic SEDs based on the results from the previous section. For this, we used the 3D Monte Carlo radiative SED transfer code SKIRT (Baes et al. 2003, 2011). SKIRT offers state-of-the-art software for simulating radiative transfer in dusty astrophysical systems. We created grids of the parameters based on the smooth torus geometry used by Fritz et al. (2006), which provides the best-fit statistics. We remark that clumpy distributions were not tested to be consistent with the results obtained using the available SED models (see Section 3).

We fitted the NGC 1068 $N$- and $Q$-band spectra including the foreground extinction using the extinction law described by Calzetti et al. (2000). We assumed a ratio of total to selective extinction $R_V = 3.1$ and an optical extinction in the range of $A_V = [0–10]$ magnitudes. This extinction is applied to each SED to test if additional foreground extinction improves the final fit.

In order to determine the best synthetic SED, we used the $\chi^2$ statistics through the standard $\chi^2 = \chi^2$/dof, where dof is the total number of data bins in the spectrum. We also use the Bayes factor (see Appendix C for details) to evaluate to what extent a model is better than another one. When the Bayes factor is $\leq 0.01$, the first model is preferred. The second model is preferred when the Bayes factor is $\geq 100$.

We initially used a mix of graphite and silicate grains from Li & Draine (2001) (already available within SKIRT), hereafter identified as Graph$_{35}$ and Sil$_{18}$, respectively. We also selected a smooth distribution of the dust particles covering a minimum grain size of size(min) = 0.005 and a maximum grain size of size(max) = 0.25 $\mu$m. Moreover, we assume a percentage within the dust mix of 49% and 51% for the graphite and silicate grains, respectively, close to the dust mix used by Fritz et al. (2006). Geometry, grain size, composition, and optical depth are further explored in Sections 4.1–4.3.

#### 4.1. Grids A and B: Geometry and Optical Depth

Following the results found in Section 3.2, we constructed a dust geometry conformed by two tori coexisting in the same plane and we explore the parameters of each of the two tori. We varied the radial power-law exponent, $p$, the polar index, $q$, the half-opening angle, $\sigma$, the maximum/outer radius, $R_{max}$, the edge-on optical depth and $\tau$ between the two tori for this first grid. Note that the symbols of the parameters are according to the SKIRT notation. In order to cover a large range of values and to optimize the computational time (roughly 2–3 days per simulation using up to 30 GB of RAM and 12 cores) we impose the following physical restrictions. First, the outer radius should be smaller in one of the tori. Moreover, the radial power-law exponent, $q$, the polar index, $\gamma$, and the equatorial optical depth, $\tau_{9.7\,\mu m}$ must be different for each torus. Finally, the viewing angle of the system, $i$, is the same for both tori. These restrictions allowed reducing the number of SEDs produced by focusing in meaningful scenarios. All together we produce a total of 2376 synthetic SEDs. We call this set of models Grid A. The set of parameters tested are included in Column 2 of Table 3.

The best-fit parameters are given in Column 3 of Table 3. Note that suffixes 1 and 2 are used to discriminate between the two tori. Although the best fit shows a poor statistic ($\chi^2 = 5.27$), it is as good as a single SED from the smooth torus by Fritz et al. (2006) and the clumpy disk-wind model by Höning & Kishimoto (2017), and already better than the two-phase torus by Stalevski et al. (2016) and the clumpy torus model by Nenkova et al. (2008b). Figure 4 (top panel) shows the best fit for Grid A. The center of the silicate absorption feature appears at shorter wavelengths compared to the data and the slope between the $N$ and $Q$ bands also fails to be reproduced by this SED.

We then create a new grid with the best values obtained previously and a larger range of values for the outer radius of
Table 2

Values of the Parameters and Statistics Obtained with the Smooth Torus model by Fritz et al. (2006) When Two Parameters are Unlinked at the $Q$ band Compared to the $N$ band

| Param | Band | $\sigma/\gamma$ | $\sigma/\beta$ | $\sigma/Y$ | $\sigma/\tau$ | $\gamma/\beta$ | $\gamma/Y$ | $\gamma/\tau$ | $\beta/Y$ | $\beta/\tau$ | $Y/\tau$ |
|-------|------|-----------------|----------------|-----------|----------------|----------------|-----------|----------------|-----------|----------------|---------|
| $i$   | $N$  | $40 \pm 0.5$    | $>0.01$        | $>0.01$   | $>0.01$       | $>0.01$       | $>0.01$   | $>0.01$       | $>0.01$   | $>0.01$       | $>0.01$ |
| $Q$   | $N$  | $25.49^{+0.69}_{-0.51}$ | $>20$           | $33.89^{+0.47}_{-0.77}$ | $>20$       | $>20$         | $>20$     | $>20$         | $>20$     | $>20$         | $>20$   |
| $\gamma$ | $N$  | $0.02 \pm 0.01$ | $0.17 \pm 0.6$ | $0.05^{+0.03}_{-0.02}$ | $2.0^{+0.5}_{-0.3}$ | $0.05^{+0.05}_{-0.01}$ | $>0.01$ | $0.18^{+0.11}_{-0.13}$ | $2.0^{+0.08}_{-0.01}$ | $1.99^{+0.13}_{-0.02}$ |
| $Y$   | $N$  | $>10$           | $>10$          | $>10$     | $13.26^{+0.75}_{-0.84}$ | $>10$          | $>10$     | $113.45^{+7.94}_{-7.76}$ | $134.89^{+1.98}_{-1.76}$ | $137.0^{+3.3}_{-3.3}$ |
| $\tau_{9.7\,\mu m}$ | $N$  | $2.0^{+0.07}_{-0.06}$ | $2.0^{+0.08}_{-0.05}$ | $1.87^{+0.03}_{-0.01}$ | $1.84^{+0.04}_{-0.01}$ | $2.0^{+0.01}_{-0.01}$ | $1.84^{+0.01}_{-0.01}$ | $1.8^{+0.1}_{-0.1}$ | $1.93^{+0.02}_{-0.02}$ | $5.98^{+0.03}_{-0.02}$ | $5.73^{+0.02}_{-0.02}$ |

$\chi^2$/dof | $94.04/258$ | $151.45/258$ | $77.76/258$ | $67.37/258$ | $89.16/258$ | $67.75/258$ | $68.88/258$ | $101.66/258$ | $83.82/258$ | $68.54/258$ |

Note. Note that the viewing angle is measured with respect to the equatorial plane.
Figure 3. Spectral fit to the smooth torus model by Fritz et al. (2006) with two parameters unlinked: $\sigma/\tau$ (top left), $\gamma/\beta$ (top right), $\gamma/\tau$ (bottom left), and $\beta/\tau$ (bottom right). The description is the same as that given in Figure 2.

Table 3

| Parameters Tested in the Grids Described in Sections 4.1 and 4.2 |
|---------------------------------------------------------------|
| Geometry and Optical Depth (Section 4.1)                     |
| Grid | Param     | Grid A Best Fit | Grid B Best Fit | Grid A Best Fit | Grid B Best Fit |
|------|-----------|-----------------|-----------------|-----------------|-----------------|
| $i$  | [60, 75, 90]$^\circ$ | 60  | [60$^\circ$, 75$^\circ$, 90$^\circ$] | 60  | [50$^\circ$–75$^\circ$] | 55  | [50$^\circ$–75$^\circ$] | 60  |
| $\sigma_1$ | [20, 40, 60]$^\circ$ | 40$^\circ$ | 40$^\circ$ | … | 40$^\circ$ | … | 40$^\circ$ | … |
| $\sigma_2$ | [20, 40, 60]$^\circ$ | 60$^\circ$ | 60$^\circ$ | … | 60$^\circ$ | … | 60$^\circ$ | … |
| $p_1$ | [0, 1] | 0 | 0 | … | 0 | … | 0 | … |
| $p_2$ | [0, 1] | 1 | 1 | … | 1 | … | 1 | … |
| $q_1$ | [0, 3, 6] | 3 | 3 | … | 3 | … | 3 | … |
| $q_2$ | [0, 3, 6] | 6 | 6 | … | 6 | … | 6 | … |
| $R_{\text{max,1}}$ | [2, 20] | 2 | [1–4] | 2 | 2 | … | 2 | … |
| $R_{\text{max,2}}$ | [2, 20] | 20 | [1–5, 10, 20, 30] | 30 | 30 | … | 30 | … |
| $\tau_1$ | [2, 20] | 20 | 20 | … | 20 | … | 20 | … |
| $\tau_2$ | [2, 20] | 2 | 2 | … | 2 | … | 2 | … |
| $\lambda_{\text{c}}$ | [0–10] | 0 | [0–10] | 1 | [0–10] | 6 | [0–10] | 3 |
| Silicate | $\text{Sil}_1$ | … | $\text{Sil}_1$ | … | $\text{Sil}_1$ | $\text{Sil}_M$ | $\text{Sil}_M$ | … |
| Graphite | $\text{Graph}_1$ | … | $\text{Graph}_1$ | … | $\text{Graph}_1$ | $\text{Graph}_M$ | $\text{Graph}_M$ | … |
| log(size(min)) | $-2.3$ | … | $-2.3$ | … | $-2.3$ | … | $-2.3$ | … |
| size(max / min) | 5 | … | 5 | … | 5 | … | 5 | … |
| $N_{\text{SED}}$ | 2376 | 726 | 2376 | 726 | 2376 | 726 | 2376 | 726 |
| $\chi^2$/dof | 5.27 | 3.74 | 4.09 | 1.33 | 1.32 | |

Note. Suffixes 1 and 2 are used to discriminate between the two tori. In the second grid, for those untested parameters, we use the values obtained with the best previous model. $\text{Sil}_1$ and $\text{Graph}_1$: Optical and calorimetric properties of the dust silicate and graphite grains reported by Li & Draine (2001). $\text{Graph}_M$: Optical and calorimetric properties of the dust graphite grains reported by Min et al. (2007) (see the text).
the structure, \( R_{\text{max}} \), referred to as Grid B in Table 3. We impose again that the outer radius of the structure is at least equal or larger in one of the torus. Notice that we do not explore outer radius greater than 30 pc since they would be spatially resolved with the current data, which is not the case. The total number of SEDs produced was 726, including three viewing angles. The best fit \( (\chi^2 = 3.74, \text{Figure 4, bottom panel}) \) is already better than any single SED fit reported in Section 3. The best fit from the second grid has a Bayes factor of \( 10^{80} \) compared to the previous one. However, the issues found for the first grid remain, i.e., the center of the silicate feature is displaced compared to the spectrum and slope between the \( N \) and the \( Q \) bands is not well recovered. We also explored a broad range for the viewing angle, although this did not yield better results. Thus, hereinafter we focus our analysis on viewing angles in the range of \( i = [50–75]^\circ \), which is also consistent with the type 2 nature of NGC 1068.

4.2. Grids C, D, and E: Dust Grain Size and Composition

As explained above, one of the main problems of our SED simulations is the spectral shape of the silicate absorption feature at \( \sim 9.7 \mu m \). This silicate feature is strongly dependent on the dust composition and size. In particular, grain size is expected to be different from that of the interstellar medium (ISM). The inner torus radius versus luminosity relation derived by dust reverberation in AGN requires an emission region more compact than expected. Having a smaller inner radius implies higher temperature than the silicate sublimation temperature, pointing to the existence of large graphite dust grain near AGN (Kishimoto et al. 2007). Indeed, large grains can survive close to the accretion disk, whereas small grains are more easily destroyed. Moreover, the dense environment of AGN promote dust aggregation, possibly making it more efficient for larger than average dust aggregates to form large dust particles.

Although silicate grains with various compositions display a spectral feature in the 10 \( \mu m \) region due to the Si–O stretching mode, there are differences in the spectral appearance (both the peak and shape) depending on the composition of the silicates (see Figure 4 by Min et al. 2007). Furthermore, the shape and position of the 10 \( \mu m \) silicate feature also has a strong dependence on grain shape. Indeed, the absorption spectrum caused by homogeneous spherical particles is very different from that caused by other particle shapes, being much larger than the differences due to various nonspherical particle shapes (Min et al. 2003). In general, the spectral extinction features caused by irregularly shaped particles are much broader and shifted toward the red with respect to those caused by homogeneous spherical particles (see Figure 3 by Min et al. 2007). In practice, both composition and particle shape affect the scattering and absorption efficiencies, increasing the impact on the resulting spectrum.

In the previous simulations, we used graphite and silicate grains reported by Li & Draine (2001) (referred to here as GraphB and SilL) and we assumed dust grains with sizes in the range of 0.005–0.25 \( \mu m \), consistent with most of the AGN dust SED libraries reported in the literature (e.g., Fritz et al. 2006). In order to explore the effect of the optical and calorimetric properties of the dust, we changed the silicate grains from Li & Draine (2001) to those reported by Min et al. (2007) and available in SKIRT (hereinafter SilH).

We initially explored only the effect on the new silicate by Min et al. (2007) keeping the size of the particles and the values of the parameters obtained with the best fit in Section 4.1 (Grid C in Table 3). The resulting fit shows a statistic of \( \chi^2 = 4.09 \), which is worse than the best fit obtained with silicates from Li & Draine (2001). However, the effect of the inclusion of these particles together with a change in grain size results in a significant improvement of the results. We therefore explored different dust grain sizes for both tori, fixing the minimum grain size and allowing to very the maximum grain size (Grid D in Table 3). We obtain a best fit with \( \chi^2 = 1.33 \). This fit has a Bayes factor of \( 1.8 \times 10^{46} \) compared to the previous one. Note that we also investigate if keeping the canonical grain size of 0.005–0.25 \( \mu m \) for the largest torus and allowing larger particle sizes of 0.005–1.0 \( \mu m \) only for the small torus improves the result. However, this SED produces a slightly worse fit than that of \( \text{size}_1 = \text{size}_2 = 0.005–1.0 \mu m \).

We also explored whether covering size ranges (i.e., from minimum to maximum grain size distributions) of one, two, and three orders of magnitude for the particles size have an impact on the final fit (Grid E in Table 3). The best statistical fit is found using dust grain sizes of \( \text{size}_1 = \text{size}_2 = 0.001–1 \mu m \), \( \text{size}_1 = \text{size}_2 = 0.01–1 \mu m \), and \( \text{size}_1 = \text{size}_2 = 0.1–1 \mu m \) with \( \chi^2 = 1.52, \chi^2 = 1.32, \) and \( \chi^2 = 2.07 \), respectively. Thus, in all the cases the best fit is found when the maximum particle grain size is \( \sim 1 \mu m \). Moreover, the preferred minimum grain size is in the range of 0.005–0.01 \( \mu m \). These minimum grain sizes are in the range of 0.005–0.01 \( \mu m \).
The Astrophysical Journal, 926:192 (19pp), 2022 February 20

Victoria-Ceballos et al.

Figure 5. Best model for using graphite by Li & Draine (2001), silicate by Min et al. (2007), and size1 = size2 = 0.005–1 μm (Grid E). The description in this figure is the same as that reported in Figure 4.

sizes have a Bayes factor of $8.8 \times 10^{-12}$ and $8.6 \times 10^{-44}$ compared to the fit obtained with 0.001 and 0.1 μm, respectively. Figure 5 shows the best resulting fit for Grid E.\footnote{Note that minimal differences are found between 0.005–1 μm and 0.01–1 μm.} It is clear how this fit better describes the silicate absorption feature and the slope between the $N$ and $Q$ bands at the same time.

4.3. Grids F, G, and H: Optical Depth and Dust Grain Size

In order to test the effect of the optical depth, which is sensitive to the other physical parameters, we created a new grid with 19,008 SEDs (Grid F in Table 4) exploring a range of values according to the latest best model. The test resulted in a best fit ($\chi^2 = 1.04$). This model has a Bayes factor of $8.7 \times 10^{59}$ compared to that obtained previously. Notice that we made these grids with grain sizes of 0.005–1 μm (one of the three combinations producing the best fit from the previous tests).

We then create a new grid of SEDs (Grid G in Table 4) exploring the optical extinction $\tau_{0.7}$ around the best values from the previous test. Moreover, we tested the best grain sizes obtained in the previous section. In total, 14,256 SEDs are created. We obtained the best fit with $\chi^2 = 0.48$ using grain sizes of 0.1–1.0 μm, which is significantly larger than those used in the currently available models. The best fit has a Bayes factor of $3.92 \times 10^{12}$ compared to that obtained in the previous test. Figure 6 shows the resulting best fit.

Finally, the best fit is expected to depend on the fine-tuning of the parameters. For that purpose we explore again a range of parameters around the best fit obtained so far (Grid H in Table 4).

The statistic for this fit is $\chi^2 = 0.4$. This fit has a Bayes factor $4.5 \times 10^4$ compared to that obtained previously. Figure 7 shows the final best fit obtained.

Figure 8 shows a sketch of the dusty distribution that we obtain through our best model. The smallest (purple) and largest (red) component are two concentric torus with inner radius of 0.2 pc (according with the dust sublimation radius) and line of sight $i = 71^\circ$. The ionization cone in NGC 1068 as seen in Hubble Space Telescope (HST) images is centered around PA = 10°, while modeling of HST spectra based on the kinematics of the gas indicates the ionization cone with an opening angle of 80° centered around PA = 30° (Das et al. 2006), roughly perpendicular to the maser spots. Using SED fitting, Lopez-Rodriguez et al. (2018) derived a viewing angle of $i = 75^\circ \pm 4^\circ$ while García-Burillo et al. (2016) found $i = 66^\circ \pm 9^\circ$. Gravity Collaboration et al. (2020) found an inclination angle of $70 \pm 5^\circ$ through image reconstruction of their interferometric observations of the near-infrared (NIR) emitting-dust. All of them are consistent with an almost edge-on orientation of the torus, as expected for the type 2 classification of NGC 1068, which agrees with the value reported in our work.

Some authors have found that the inclination parameter is very difficult to restrict. Ramos Almeida et al. (2014) concluded that the inclination of the torus is better restricted by using the combination of sub-arcsecond resolution NIR and MIR. However, at least for NGC 1068, the inclination angle can be restricted using only MIR spectra. This is due to the availability of spectroscopic data. Indeed, González-Martín et al. (2019a) found that the viewing angle can be well restricted using only MIR spectroscopy as long as the wavelength range covers at least between 5 and 25 μm. Alternatively, the use of combined X-ray and MIR spectra simultaneously has been demonstrated to allow to recover the viewing angle, at least for another type 2 AGN IC 5063 (Esparza-Arredondo et al. 2019).

5. Discussion

5.1. Geometry of the Dust Component

Early works in the infrared domain such as the one presented by Cameron et al. (1993) pointed out that complex structures must be present at small scales in NGC 1068 since the MIR continuum is extended within 1′. Using higher resolution data, Bock et al. (2000) showed there was a central core component (<0″2), which they associated with the AGN dust torus. However, this core was still not resolved within scales of tens of parsecs. Wittkowski et al. (2004) and Jaffe et al. (2004) presented spatially resolved images at NIR and MIR wavelengths using interferometric techniques. They favor a multi-component model for the dust distribution in NGC 1068, where part of the flux originates from a hot and small (<1 pc) component with also a large warm component (2.1 × 3.4 pc). Consistent with this result, Mason et al. (2006) found that the MIR emission originates in two distinct components. A compact bright source with radius <15 pc, which they identified with the obscuring torus, and a diffuse component with dust in the ionization cones. Mid-infrared interferometric instrument (MIDI) observations by Raban et al. (2009) found that the $N$-band MIR emission can be represented by two components. They identified the first component as the inner funnel of the torus, with 0.45 × 1.35 pc. The second component was identified with the cooler body of the torus, with a size of 3 × 4 pc.

From the analysis presented here we conclude that to obtain a good spectral fit using the available AGN dust models it is necessary to consider a two-phase composite geometry for the dusty torus. Indeed, none of the proposed models are able to explain the $N$- and $Q$-band spectral range simultaneously (see Section 3). Alonso-Herrero et al. (2011) attempted to simultaneously fit the $N$ and $Q$ spectra in addition to the NIR and MIR photometric points. They manage to produce a
reasonable fit, using an early version of the clumpy torus model by Nenkova et al. (2008b). The current version of this clumpy torus model did not produce good fits ($\chi^2 > 4$). Using the available models, we explored the possibility of adding complexity to them by untying one or two parameters between the fits of the two spectra. We found that the fit improves significantly from the statistical point of view. We interpret this as a signal of the complexity of the AGN dust torus in NGC 1068, consistent with early works.

Through MIR interferometry as well, López-Gonzaga et al. (2014) found that the emission of the core of NGC 1068 can be divided into two distinct regions. However, these two components are not concentric, with one consistent with a hot emission surrounded by warm dust and a large warm diffuse region approximately 7 pc away from the other. These two components could be associated with two different AGN, conforming a dual or binary AGN. Indeed, Wang et al. (2020) suggested that a binary SMBH could support the counter-rotating structures reported by Imanishi et al. (2018) and Impellizzeri et al. (2019) to explain the molecular gas observations of the torus of NGC 1068.

If the two AGN are far enough to not significantly influence the heating of dust associated to the other AGN, then the total SED should be reproduced with a combination of two AGN dust models. We tested this hypothesis using XSPEC spectral-fitting software as we did for the single models (i.e., dust+disk models). However, this test did not yield a good spectral fit ($\chi^2$/dof $\geq 5$). Instead, allowing the parameters of the models to vary independently for the $N$ and $Q$ bands produced a good fit, as already mentioned above.

Another possibility is that the two AGN are close enough to heat both AGN dust components. This scenario better matches the results by Wang et al. (2020) because they assume two

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Note. Suffixes 1 and 2 is used to discriminate between the two tori. For Grid F we vary the optical depth in steps of $\Delta(\tau_1) = 2$ and $\Delta(\tau_2) = 0.2$.
AGN with a separation of ~0.1 pc, which is a separation below the expected inner radius of the torus. However, note that this separation is not consistent with the 7 pc distance between the two dust components found by López-Gonzaga et al. (2014). In the SMBH binary case, the sum of two AGN dust models is not an accurate way to test this scenario and new radiative transfer models are needed including this complexity. We also tested this scenario by producing synthetic SEDs for two nonconcentric tori. Details on these new SEDs are reported in Appendix F. However, the best model obtained is \( \sim 1 \times 10^{12} \) times worse than the model with two concentric tori reported in our results. Note that the inner radius of the torus is larger than the binary AGN separation given by Wang et al. (2020) so this two concentric tori could virtually mimic the dual AGN claimed in their work. Thus, we do not rule out two nonconcentric tori associated with a binary SMBH with separations below the inner radius of the torus.

Studies at other wavelengths can also provide information about the complexity of torus. For example, through X-ray data, the reflection component can be used to probe the matter distribution of the gaseous (neutral and distant) torus (see Liu et al. 2016). Bauer et al. (2015) concluded that a complex reflector structure consisting of multiple components (two nuclear and one extended) is needed to fit the combined Nuclear Spectroscopic Telescope Array (NuSTAR), Chandra, X-ray Multi-Mirror Mission Newton (XMM-Newton), and Swift Burst Alert Telescope (Swift-BAT) spectra of NGC 1068. This is consistent with the two nuclear components shown in our work, although it is worth noting that the comparison between the X-ray gaseous torus and the MIR dusty torus might be very complex (Esparza-Arredondo et al. 2021).

Through radio-interferometry, molecular line and continuum observations are used for investigating the morphological structure of the torus (Imanishi et al. 2018). Although dust continuum from ALMA might have some issues due to jet contamination (Pasetto et al. 2019; García-Burillo et al. 2021), García-Burillo et al. (2019) inferred a size of 28 pc using the CO(3-2) line, which is in agreement with the large torus found in our work. This might be explained due to the fact that ALMA could be imaging the cooler (and therefore extended) dust, being the outer layer of the small torus found in our work. In support on the large torus, Lopez-Rodriguez et al. (2020) reproduced 860 μm polarimetric observations of NGC 1068, using synthetic polarimetric observations generated with the CLUMPY torus model by Nenkova et al. (2008b) with an outer radius higher than 9 pc. Furthermore, Gratadour et al. (2015) observed the core of NGC 1068 with the Spectro-Polarimetric High-contrast Exoplanet REsearch (SPHERE) instrument on the Very Large Telescope, using adaptive optics-assisted polarimetric observations in the NIR, finding evidence of an extended torus with \( 15 \times 27 \) pc. Very recently, using Very Large Telescope Interferometer/Multi AperTure mid-Infrared SpectroScopic Experiment (VLTI/MATISSE) observations, Gamez–Rosas et al. (2021) found that the torus of NGC1068 contains an optically thick ring on parsec scales and an optically less thick disk that extends to at least 10 pc, which is in agreement with our model where the smallest component is denser than the larger component.

The smallest torus with 1.8 pc (see Figure 8) has a high optical depth \( \tau_{0.7, \mu m} = 12 \); in the radial direction, the dust distribution is almost constant \( (\rho \sim r^{-0.2}) \), while in the polar direction it decays quickly \( (\rho \sim e^{-3.2(\cos\theta)}) \). The largest component has a smaller optical depth \( \tau = 0.3 \) compared with that of the smallest torus and the dust density decreases with \( r^{-1} \) and \( e^{-5.8(\cos\theta)} \) in the radial and polar directions, respectively. Our result might be interpreted as a complex distribution of dust rather than two distinctive components. Our components might be a simplification of a structure where the dust in the outskirts is geometrically thicker than the inner side and the opacity also abruptly falls toward the outskirts.

Alternatively, we could also think that the large torus is just the inner dust from the host galaxy or a polar contribution to the dust, as suggested for other nearby AGN (Hönig et al. 2013; López-Gonzaga et al. 2014; Asmus 2019) and also for NGC 1068 (Mason et al. 2006; Liu et al. 2019). This polar dust could produce mostly silicate emission features (Hönig & Kishimoto 2017). Although not included here, we also produce the SEDs of the two components alone. This polar dust resembles that of the large torus component modeled in this work due to its low opacity if the inner torus is not presented (although the inner torus gives the highest fraction contribution). Under this latter scenario, the complexity found for NGC 1068 might be the result of a more dynamic model, as is the case of the fountain model by Wada (2012). Under this model the radiation from the central source drives the onset of biconical outflows that start forming at the inner region and subsequently propagate outward. Most of this material becomes a truncated wind that backflows toward the disk plane forming a geometrically thick disk. The small torus found in this work could be related to the thick inner disk, which is the origin of the launching wind, while the large torus could be related to the failed wind producing the geometrically thick disk. García-Burillo et al. (2019) also found a kinematic model for the molecular torus, where the gas presents circular motions and a fraction of it, inside the torus, is launched as an outflow. In our two component model, the small torus could be related to the torus component in the model by García-Burillo et al. (2019), and the large torus could be related to the outflow component. As a final remark, in an attempt to find similarities
among other astronomical objects, our resulting geometry is not far from that proposed for protoplanetary disks; a warm zone emitting at around 10 $\mu$m and a much colder region emitting longward to 20 $\mu$m. Olofsson et al. (2009) show in their Figure 14 a schematic view of the disk in one of these systems, which might imply a grand unification between the dust in protoplanetary disks and that found in AGN.

Note that, if a distance of 14 Mpc is adopted (commonly used in other studies, e.g., Mason et al. 2006) instead of the 10.6 Mpc used in this paper, the luminosity would be higher by a factor of $\sim 1.7$ and the physical lengths (such as the inner and outer torus radius) would be higher by a factor of $\sim 1.3$.

5.2. Dust Composition and Dust Grain Size

Besides the geometry, an important aspect explored in this work is that SED fitting allows studying the composition of the dust, which cannot be done with other techniques. Unfortunately, available SED libraries that explore grain size, size particle distribution or composition have not been produced to so far, although some works have made an effort to explore it (e.g., Höning & Kishimoto 2010). Thus, new radiative transfer simulations, such as those produced in this work, are mandatory to study if dust composition or dust grain size are important to accurately reproduce the shape of the AGN dust continuum.

In this work, we demonstrate that an important ingredient to explain the MIR $N$- and $Q$-band spectra of NGC 1068 is the size of the particles. Since significantly better spectral fits are found if both graphite and silicate grains have grain sizes in the range of 0.1–1 $\mu$m using the silicates used in Min et al. (2007). We also find an important improvement in the best-fit model from setting the maximum dust grain size to 1 $\mu$m, while varying the minimum particle size results in marginally changing the final SED. This particle size is much larger than that assumed for publicly available AGN dust models since they rely on the results for the ISM (usually 0.005–0.25 $\mu$m; Fritz et al. 2006; Nenkova et al. 2008b; Stalevski et al. 2016).

Some authors (e.g., Nikutta et al. 2009) have argued that the 10 $\mu$m silicate feature can be explained through a clumpy dust distribution with a standard ISM dust. In Section 3, we tested a clumpy torus model for NGC 1068, however the silicate absorption profile showed poor agreement. Feltre et al. (2012) performed a comparison between the smooth and clumpy models by Fritz et al. (2006) and Nenkova et al. (2008b), respectively. They found that the behavior of the silicate feature at 9.7 $\mu$m is quite distinct between the two models. However, they concluded that such difference arises from the dust chemical composition assumed by the models and not from the smooth or clumpy morphology, in agreement with our findings.

Some works have already explored the effect on the size of the particles in the context of AGN. Schartmann et al. (2005) explored models of dusty tori in AGNs. They tested effects of a broadening of the grain size distribution, spreading the grain size range with grains of 0.005–10 and 0.001–10 $\mu$m. They found that the differences are nearly negligible for a face-on view angle, but for inclination angles, close to edge-on, a reduced relative depth of the silicate feature toward smaller wavelengths is visible. NGC 1068 has an almost edge-on view of the torus ($\sim 71^\circ$) so the importance of the dust grain sizes is justified. Other authors have also found evidence supporting large dust sizes. Through the ratio of the optical extinction in the visual band to the optical depth of the 9.7 $\mu$m silicate absorption feature, $A_V/\Delta T_{9.7}$, Lyu et al. (2014) obtained a mean ratio of $A_V/\Delta T_{9.7} \approx 5.5$ from a sample of 110 type 2 AGNs, which is considerably lower than that of the local ISM of the Milky Way ($A_V/\Delta T_{9.7} \approx 18.5$), implying that AGN dust grain size could exceed $\sim 0.4$ $\mu$m (Shao et al. 2017).

Although the dependence of the dust sublimation radius on grain size might be complex (see Figure 1 in Absil et al. 2013), Kishimoto et al. (2007) suggested that the dust sublimation radius vary with the square root of the dust size. In the context of debris disks, Kobayashi et al. (2011) developed the equation that links the sublimation radius (we express it in units of parsecs), the grain size ($\mu$m), luminosity (erg s$^{-1}$), and sublimation temperature (K) as follows:

$$R_{\text{sub}} = 0.11 \left(1 + \frac{1}{x}\right)^{1/2} \left(\frac{L_{\text{bol}}}{10^{45}}\right)^{1/2} \left(\frac{T_{\text{sub}}}{1300}\right)^{-2},$$

where $x = 2\pi s_{\text{grain}}(T_{\text{sub}}/2898)$ K and $s_{\text{grain}}$ is the grain size. Therefore, the resulting larger grain sizes naturally imply dust located closer to the torus. Considering that the AGN dust models $s_{\text{grain}} = 0.25$ $\mu$m, while we have found $s_{\text{grain}} = 1$ $\mu$m, the largest grains might be located up to a factor of 2 closer to the accretion disk. However, we tested the inner radius without a significant improvement in the final fit. Conversely, also in the context of protoplanetary disks, the analysis of the shape and strength of both the amorphous 10 $\mu$m feature and the crystalline feature around 23 $\mu$m provides evidence for the prevalence of micron-sized (amorphous and crystalline) grains in the upper layers of disks (Olofsson et al. 2009). Observations of dust in disks from submillimeter to centimeter wavelengths have provided strong evidence for grain growth in disks (Testi et al. 2001; Calvet et al. 2002). Pérez et al. (2012) found that the maximum size of the particle-size distribution increases from submillimeter sizes in the outer disks to millimeter and centimeter sizes in the inner disks. Indeed, dust grains in the planet-forming regions around young stars are expected to be heavily processed due to coagulation, fragmentation, and crystallization (Olofsson et al. 2009), and similar mechanisms might also explain the large grains found in NGC 1068.

6. Summary

We have studied the dusty torus in NGC 1068 using $N$- and $Q$-band Michelle/Gemini spectra. For this purpose we perform the analysis into two steps: (1) we used the XSPEC spectral-fitting package to test already available models and (2) we used the 3D Monte Carlo radiative SED transfer code SKIRT to build grids of synthetic SEDs, based on the result obtained from the first step. The main results are as follows:

1. Available SED models: Among the available models, the resulting best fit was obtained using the clumpy disk + wind model by Höning & Kishimoto (2017). However, the best fit was statistically unsatisfactory. We then explored the possibility of adding complexity to the models by untying one and then two parameters when doing the fits of the $N$ and $Q$ spectra separately. We found that the fit significantly improves using the smooth torus model by Fritz et al. (2006) and four combinations of untied parameters. In this scenario, the emission in the two spectral ranges here considered is dominated by dust with different geometrical locations and distributions.
These components are characterized by different values of the equatorial optical depth, the opening angle, and the parameters regulating the dust density gradients. We interpret these results as a signal of the complexity of the dust in NGC 1068.

2. New SEDs with SKIRT: For the 3D Monte Carlo radiative simulations, we used two concentric tori that allow us to test more complex dusty geometries. The final best fit has the following common parameters for both tori: (1) a fractional contribution for graphite and silicate grains of 49% and 51%, respectively; (2) graphite from (Li & Draine 2001) and silicate from (Min et al. 2007); (3) size of graphite and silicate particles of 0.1–1 μm; (4) inner radius of both tori of 0.2 pc; (5) viewing angle i = 71°; and (6) foreground extinction $A_V = 2$ mag. The parameters changing from both tori are (1) the exponent of the power law describing the radial distribution $p_1 = 0.2$ and $p_2 = 1$, (2) the exponent of the polar distribution $q_1 = 3.2$, and $q_2 = 5.8$, (3) the half-opening angle $\sigma_1 = 42$ and $\sigma_2 = 58$, (4) the outer radius $R_{\text{max},1} = 1.8$ pc and $R_{\text{max},2} = 28$ pc, and (5) the equatorial optical depth to $\tau_{9.7 \mu m,1} = 12$ and $\tau_{9.7 \mu m,2} = 0.3$.

These findings can be interpreted as a compelling evidence for a complex dusty torus for NGC 1068. We speculate that this can be understood as inner compact disk/torus plus an outer extended torus/wind, conforming either a flared disk or a dynamical fountain model for the dust. Furthermore, some mechanism for grain growth needs to be claimed to explain the large grains to fit the MIR ground-based spectra of NGC 1068. Note that these results were obtained considering a smooth distribution of dust. Therefore, some parameters of the torus likely depend on the assumption of this distribution. In order to consider a similar geometry with other distributions, like clumpy, future efforts should test these scenarios. As a final remark, it has been largely discussed by the community that the complexity of the models, model parameter degeneration, and spatial resolution might be an issue when inferring the properties of the dust using SED fitting techniques (Ramos Almeida et al. 2014; González-Martín et al. 2019a). However, this detailed work demonstrates that useful information can be achieved from SED fitting when the full MIR spectral coverage is available and specific synthetic SEDs are produced to explain the observations.

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Software: XSPEC (Arnaud 1996), HEAsoft (NASA High Energy Astrophysics Science Archive Research Center (HEASARC), 2014), SKIRT (Baes et al. 2003, 2011), Python/C language (Oliphant 2007), NumPy (Harris et al. 2020), SciPy (Virtanen et al. 2020), and Matplotlib (Hunter 2007).

Appendix A

Dust Models

In order to show the geometry and dust distribution of the models tested in Section 2, a sketch of the models is shown in Figure 9. The smooth torus model by Fritz et al. (2006), the clumpy torus model by Nenkova et al. (2008b), and two-phase torus model by Stalevski et al. (2016) assume the dust distribution in a toroidal geometry. The clumpy disk and outflow model by Höning & Kishimoto (2017) consider the dust distributed in a disk-like geometry plus a polar hollow cone. The smooth torus model by Fritz et al. (2006) considers a continuous distribution of dust toward the torus. The clumpy torus model by Nenkova et al. (2008b) considers a toroidal distribution of dusty clumps. The two-phase torus model by Stalevski et al. (2016) considers a dust distribution of clumps embedded in a smooth component. The clumpy disk and outflow model by Höning & Kishimoto (2017) considers a dust distribution in a clumpy disk plus a polar hollow cone.
Appendix B
Models’ Parameters

In order to reproduce the SED of NGC 1068, we test the four dust models described in Section 2. Our best fit assuming that a single SED of the models is able to reproduce the N and Q bands at the same time is shown in Tables 5–8 (Column 2). In all cases, many of the parameters are not well restricted. We also show the goodness of the fit throughout the \( \chi^2 / \text{dof} \). Tables 5–8 (Column 3 onward) show the best fits obtained by unlinking one parameter in the Q band. The smooth torus model by Fritz et al. (2006) restricts all parameters by untying the optical depth at 9.7 \( \mu \text{m} \), \( \tau_{9.7 \mu \text{m}} \). The clumpy torus model by Nenkova et al. (2008b), the two-phase model by Stalevski et al. (2016), and the clumpy disk and outflow model by Höning & Kishimoto (2017) do not restrict all the parameters well in any case. Finally, Table 9, shows the best fits for the two-phase model by Stalevski et al. (2016) untying the half-opening angle with the other parameters. The table with the results for the smooth torus model by Fritz et al. (2006) untying two parameters is shown in Section 3.2.
The Astrophysical Journal, 926:192 (19pp), 2022 February 20

Victoria-Ceballos et al.

Table 5
Fitting Results of the N- and Q-band Spectra to the Smooth Torus Model by Fritz et al. (2006)

| Param | Linking Parameters | Band | \( i \) \( \sigma \) \( \gamma \) Unlinking |
|-------|-------------------|------|-------|---|---|---|---|
| \( i \) | >0.01 | \( N \) | 22.5 ± 0.2 | 60.16±0.17 | 49.15±0.1 | >0.01 | 34.76±0.5 | 1.13±0.48 |
| \( \sigma \) | >0.01 | \( Q \) | ... | ... | ... | ... | ... | ... |
| \( \gamma \) | >0.01 | \( N \) | >20 | >20 | >20 | 23.94±0.3 | 57.63±0.23 | 20.0±0.02 |
| \( \beta \) | >0.01 | \( Q \) | ... | 5.82±0.13 | ... | ... | ... | ... |
| \( Y \) | >0.01 | \( N \) | >10 | >10 | >10 | 9.7±0.13 | 3021.32 | 107.67 | 207.13 |

\( \chi^2/\text{dof} \) 1293.66/260

Note. Column 1: symbol of the parameter (see Table 1). Column 2: using a single SED by linking for the parameters in the \( N \) and \( Q \) bands. Columns 3–9: unlinking one of the parameters in the \( Q \) band with respect to those of the \( N \) band. The \( \chi^2/\text{dof} \) value for each fit is shown in the bottom row.

Table 6
Same as in Table 5 for the Clumpy Torus Model by Nenkova et al. (2008b)

| Param | Linking Parameters | Band | \( i \) \( N_0 \) \( \sigma \) \( Y \) \( q \) \( \tau \) |
|-------|-------------------|------|-------|---|---|---|---|
| \( i \) | >0.01 | \( N \) | >0.01 | >0.01 | >0.01 | >0.01 | >0.01 |
| \( N_0 \) | <15 | \( N \) | <15 | <15 | <15 | <15 | <15 |
| \( \sigma \) | <70 | \( N \) | 56.44±0.78 | 65.07±0.34 | 64.86±0.23 | <70 | <70 | 64.92±0.22 |
| \( Y \) | <100 | \( N \) | <100 | <100 | <100 | <100 | <100 |
| \( q \) | 1.84±0.04 | \( N \) | 0.52±0.03 | 0.57±0.01 | 0.58±0.06 | 1.83±0.04 | 0.5±0.03 | 1.32±0.04 |
| \( \tau_V \) | >10 | \( N \) | 20.0±0.02 | 20.0±0.01 | 19.99±0.03 | >10 | 13.48±0.19 | 20.0±0.02 |

\( \chi^2/\text{dof} \) 2682.42/260

Table 7
Same as in Table 5 for the Two-phase Torus Model by Stalevski et al. (2016)

| Param | Linking Parameters | Band | \( i \) \( \sigma \) \( p \) \( q \) \( Y \) \( \tau \) |
|-------|-------------------|------|-------|---|---|---|---|
| \( i \) | >0.01 | \( N \) | 40.0±0.05 | 88.66±0.23 | >0.01 | >0.01 | 88.84±0.02 | 89.15±0.02 |
| \( \sigma \) | 69.9±0.04 | \( N \) | 69.99±0.05 | 11.99±0.04 | 69.99±0.04 | 53.59±0.44 | <80 | <80 |
| \( p \) | <1.5 | \( N \) | <1.5 | <1.5 | <1.5 | <1.5 | 1.5 | <1.5 |
| \( q \) | <1.5 | \( N \) | <1.5 | 0.54±0.28 | 0.5±0.27 | <1.5 | <1.5 | <1.5 |
| \( Y \) | <30 | \( N \) | <30 | <30 | <30 | <30 | <30 | <30 |
| \( \tau_{9.7 \mu m} \) | 5.0 | \( N \) | <11 | <11 | <11 | <11 | <11 | <11 |

\( \chi^2/\text{dof} \) 3201.44/260

15
Table 8
Same as in Table 5 for the Clumpy Disk Plus Outflow Model by Hönig & Kishimoto (2017)

| Param | Linking Parameters | Band | Unlinking |
|-------|--------------------|------|-----------|
| $i$   | $>0.01$ | $N$ | $>0.01$ | $>0.01$ | $>0.01$ | $>0.01$ | $>0.01$ | $>0.01$ |
| $\sigma$ | $Q$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ |
| $\theta$ | $N$ | $<0.10$ | $>0.01$ | $>0.01$ | $>0.01$ | $>0.01$ | $>0.01$ | $>0.01$ |
| $\sigma$ | $Q$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ | $<0.01$ |
| $h$ | $<0.05$ | $Q$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ |
| $f_{\text{un}}$ | $a_w$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ |
| $a_w$ | $<0.05$ | $N$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ | $<0.05$ |

$\chi^2$/dof: 1138.56/258, 1138.51/257, 651.11/257, 618.99/257, 736.4/257, 540.26/257, 1057.5/257, 769.98/257, 538.73/257

Table 9
Same as in Table 2 for the Two Phase Torus Model by Stalevski et al. (2016) When We Unlink Two Parameters between the $N$ and $Q$ bands

| Param | Band | Unlinking |
|-------|------|-----------|
| $\sigma/p$ | $N$ | $80.0^{+2.1}_{-0.03}$ | $80.0^{+0.13}_{-0.08}$ | $89.17^{+0.05}_{-0.07}$ | $80.0^{+0.11}_{-0.08}$ |
| $\sigma/q$ | $Q$ | $...$ | $...$ | $...$ | $...$ |
| $\sigma/Y$ | $N$ | $19.0^{+1.35}_{-0.38}$ | $19.25^{+0.28}_{-0.16}$ | $10.67^{+0.18}_{-0.12}$ | $18.53^{+0.45}_{-0.13}$ |
| $\sigma/\tau$ | $Q$ | $11.8$ | $11.99^{+0.16}_{-0.09}$ | $10.0$ | $11.59^{+0.1}$ |
| $\rho$ | $N$ | $<1.5$ | $<1.5$ | $<1.5$ | $<1.5$ |
| $q$ | $Q$ | $<1.5$ | $<1.5$ | $<1.5$ | $<1.5$ |
| $Y$ | $N$ | $<30$ | $<30$ | $<30$ | $<30$ |
| $\tau$ | $Q$ | $3.93^{+0.11}_{-0.04}$ | $3.9^{+0.13}_{-0.04}$ | $<11$ | $4.04^{+0.14}_{-0.04}$ |

$\chi^2$/dof: 207.14/258, 184.63/258, 145.01/258, 174.9/258

Appendix C
The Bayes Factor

In order to evaluate to what extent a model is better than another one we calculate the Bayes factor through the Akaike information criterion, $AIC_c$. To this end, we use Equation (5) in Emmanoulopoulos et al. (2016) to calculate the $AIC_c$

$$AIC_c = 2k - 2C_L + \chi^2 + \frac{2k(k + 1)}{N - k - 1}$$

where $C_L$ is the constant likelihood of the true hypothetical model, $k$ is the number of free model parameters, and $N$ is the number of data points.

We then calculate the difference between two different models, $\Delta[AIC_c]$

$$\Delta[AIC_c] = AIC_{c,2} - AIC_{c,1}.$$  (3)

Finally, we estimate the evidence ratio, $\epsilon$

$$\epsilon = e^{-\frac{\Delta[AIC_c]}{2}}.$$  (4)

The evidence ratio or Bayes factor, is a measure of the relative likelihood of one versus other model. When the Bayes factor is $<0.01$, the first model is more likely to be the correct model. When the Bayes factor is $\geq 100$ the second model is more likely to be the correct model.

Appendix D
Graphite/Silicate Fraction

Several of the AGN dust models (e.g., Hönig & Kishimoto 2010) rely on composition constants derived by Mathis et al. (1977) for the ISM. In particular, the normalization with respect to hydrogen abundance is $log(A) = -15.24$ and $-15.21$ for graphite and silicate grains, respectively (i.e., 51.7% of silicate). However, Draine & Lee (1984) updated these numbers to $log(A) = 25.11$ and $25.16$ for silicate and graphite, respectively (i.e., 52.9% of silicate). This is the composition assumed by the smooth torus model by Fritz et al. (2006). Weingartner & Draine (2001) also gave the same abundance for the silicate but a different number for graphite with $log(A) = -25.13$ (i.e., 52.4% of silicate). This is the assumed normalization factors in the two-phase torus model presented by Stalevski et al. (2016). This fraction might have an impact on the results. In Section 3 we used ratios of 49% and 51% for graphite and silicate grains, respectively. However, this is further explored in this section. We create a grid covering a range percentages of silicates, $f_{\text{sil}} = [30, 40,$
45%–55%, 60%, and 70%). Note that in this grid, we do not include the previously used ratios of particles (49% and 51% for graphite and silicate grains, respectively). We obtained the best fit with $c = 0.51r^2$ for 51% of graphite and 49% of silicates. This fit has a Bayes factor of $4 \times 10^{-7}$ compared to the best fit obtained in Section 4.3. Figure 10 shows the best fit obtained with 51% graphite and 49% silicate.

Appendix E

Inner Radius of the Torus

We explored the scenario when the inner radius of the largest torus is different from that of the smallest torus. We initially kept the inner radius of the smallest torus fixed to 0.2 pc and we tested a range of values of the largest torus: $R_{in,2} = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6] \text{ pc}$. The other parameters are fixed to the best values obtained in Section 4.3. The grid has 2376 SEDs and the best fit was obtained with $\chi^2 = 1.06$ for $R_{in,2} = 0.1 \text{ pc}$, with an inclination angle of $i = 61^\circ$ and $A_v = 5 \text{ magnitudes}$. This fit has a Bayes factor of $3.9 \times 10^{-39}$ compared to the best fit in Section 4.3. Figure 11 (top-left panel) shows this result.

Graphite grains can sustain higher temperatures than silicate grains, with the former being able to heat up to $\sim$1900–2000 K and the latter sublimating at $\sim$800–1200 K, depending on density (García-González et al. 2017, and references therein). This implies a different sublimation radius for the graphite compared to silicate grains. In order to explore this, we create a complex system of tori, composed by two tori for graphite and two tori for silicate grains. All the parameters are the same, changing the sublimation radius for each kind of particle. For this, we made two grids of SEDs: first, we assume sublimation temperatures of 1500 and 1000 K for graphite and silicate, respectively (i.e., the sublimation radii for graphite and silicate grains at 0.4 and 1.2 pc, respectively). However, this fit is not

Figure 10. Best model exploring for different graphite/silicate ratios (see Appendix D). The description in this figure is the same as that reported in Figure 4.

Figure 11. (Top left) Best model obtained when we test for different inner radius for the largest torus. (Top right) Best fit obtained from the model with a reshaped inner wall of the torus. (Bottom) Best fit when we consider different sublimation temperature for graphite and silicate using $T(\text{graphite}) = 1500 \text{ K}$ and $T(\text{silicate}) = 1000 \text{ K}$ (left) and $T(\text{graphite}) = 2000 \text{ K}$ and $T(\text{silicate}) = 1500 \text{ K}$ (right). The description in this figure is the same as that reported in Figure 4.
satisfactory ($\chi^2 = 2.38$), with $i = 64^\circ$ and $A_V = 0$ mag. Then, we assume sublimation temperatures of 2000 and 1500 K for graphite and silicate, respectively (i.e., the sublimation radius for graphite and silicate was set to 0.17 and 0.4 pc, respectively). However, this fit is not statistically acceptable with $\chi^2 = 2.48$, with $i = 62^\circ$ and $A_V = 0$ mag. These SEDs have Bayes factors of $5.9 \times 10^{-116}$ and $9 \times 10^{-122}$ compared to the best fit in Section 4.3, respectively. Figure 11 (bottom panels) shows these two fits. While they are quite good at reproducing the slope between the $N$ and $Q$ bands, they fail to reproduce the 10 $\mu$m silicate feature.

Finally, the inner region of the torus might be reshaped to account for this anisotropic irradiation by the accretion disk, with the strongest emission perpendicular to the disk and none in the equatorial plane (Stalevski et al. 2016). In this case, the incident flux is a function of the distance and the polar angle. In order to explore this, we used the anisotropic disk emission by Netzer (1987), where the flux as a function of the polar angle $\Theta$ is (see also Netzer 2013):

$$F_{AGN} = (1/3) \cos \theta (1 + 2 \cos \theta). \quad (5)$$

In this case, the sublimation radius is

$$R_d(\theta) = (0.4)L_{45}(\theta)^{1/2}T_{sub}^{2.5} \rho_{pc}, \quad (6)$$

where $L_{45}(\theta) = [s + (1 - s)(1/3)\cos \theta (1 + 2 \cos \theta)]L_{bol,AGN}$, where $L_{bol,AGN}$ is the AGN luminosity in units of $10^{45}$ erg/s and $s$ is the softening factor introduced to prevent the inner dust radius from reaching zero at the equatorial plane ($s = 1$ recovers the isotropic scenario).

We created a new grid including 48 SEDs with a range of inner radii of $R_{in} = [0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 1.0]$ pc; and a cutoff radius at half of the $R_{in}$ (i.e., $R_{cutoff} = [0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.5]$ pc). We have obtained that the best fit shows $\chi^2_r = 1.14$ for $R_{in} = 0.5$ pc and $R_{cutoff} = 0.25$ pc, with an inclination angle of 68° and extinction of 0 magnitudes (see Figure 11, top-right panel). The reshaping of the inner radius of the torus is not an improvement compared to those SEDs obtained without taking this effect into account. Indeed, the model shown in Section 4.3 without reshaping has a Bayes factor of $1.1 \times 10^{45}$ compared to this fit.

**Appendix F Nonconcentric Tori**

In order to test the scenario in which the two components found through our analysis are associated with two different AGN (according to recent literature, see the Discussion section), we produced new synthetic SEDs for two nonconcentric tori, with the same parameters obtained in our final best model but considering each torus hosts an AGN. For simplicity, we assume that the luminosity of each AGN is half of the total luminosity of NGC 1068. We explored several distances between the two AGN, from 0.1–25 pc (11 steps), where the radiation from both AGNs reaches both tori, and from 30–40 pc (six steps), where each AGN affects only one of the tori. We also explore the resulting SED when the separation occurs along the height or along the width of the torus. Our best model shows a statistic of $\chi^2_r = 0.63$ with an offset of 10 pc between each AGN, a viewing angle of 90° and a foreground extinction of $A_V = 3$ mag. This fit has a Bayes factor of $4.1 \times 10^{-14}$ compared to the best fit in Section 4.3. Figure 12 shows the resulting SED with these two nonconcentric tori. Although the fit is quite good, in particular around the silicate absorption feature at 10 $\mu$m, it is not better than that provided by the two concentric torus, discussed in the main body of this paper.

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![Figure 12](image-url)
