

The authors would like to thank the reviewer for their comments and feedback. Our responses are presented in blue.

### # Reviewer 1

The paper applies the formulation developed by TK 21 (Torquato and Kim, Physical Review X 2021) to scattering by fresh snow. The merit of the non-local formulation is to extend the previous quasistatic model (Torquato 2002) to higher frequency so that the attenuation due to scattering is accounted for. The attenuation in scattering is included in the imaginary part of the effective permittivity. The TK21 method is supposedly valid up to  $ka = 6$  where  $k$  is the wavenumber and  $a$  is grain radius. The value  $ka=6$  means the grain radius is 1 wavelength

There are questions whether the TK21 model is applicable to snow

a. A microscopic picture of snow shows that the ice grains have irregular shapes and that they also have “stickiness” that the grains adhere together. A limitation of classical mixture formula as given in the book by Sihvola (1999) is that the mixture formula depends on the shape of the scatterers. The mixture formula is developed for simple shapes such as spheres, ellipsoids, disks etc. The problem with irregular shape is that the solutions of Maxwell equations are “discontinuous” across the boundaries between the scatterers and the background. Boundary conditions indicate that although the tangential component of electric field is continuous, but the normal component electric field is discontinuous with the normal component in air that is 3.2 times that of in ice. For well-defined shapes such as ellipsoids, such boundary value problems are solved by ellipsoid coordinates. But such problems cannot be solved analytically for irregular shapes. The TK21 model is strongly dependent on the choice of exclusion volume which is analogous to particle shape. The examples in the paper TK21 are limited to regular shapes such as spheres, disks etc. In TK21, the beta  $p_q$  in equation (33) with  $d=3$  indicates the shape of a sphere.

This comment raises 2 main points, the boundary problem and the question of the equivalence between the exclusion volume and the particle shape.

It concerns our section 4 which aims to highlight that TK21 theory does not need the notion of individual particles (with some shapes and sizes) even though it solves (exactly up to some point) the Maxwell equations and hence, takes the boundary conditions into account, overcoming the problem highlighted by the reviewer.

More precisely, regarding **the boundary problem**: We agree that classical formulations explicitly solve the boundary problem for given particles, which is relatively straightforward for simple geometrical shapes, but is not for irregular shapes. TK21 does not solve this problem explicitly but implicitly because the medium is not represented by particles but by local information on whether phase 1 or 2 (air and ice in our case) is present at any point  $r$  in space. Actually, this information is

given in a statistical way by the n-point correlation functions. For a medium made of particles, the n-point correlation functions hold all the information about both the shape and the relative arrangement of the particles. However TK21 approach is more general because it also applies to non-granular media. In this sense, the TK21 formalism is “non-classical”, it has a much wider range of applicability than previous classical formulas. TK21 is not unique in this category, IBA and the Strong Fluctuation Theory (SFT) share similarities about the medium description.

Regarding the exclusion volume: While it is correct to state that TK21 formalism results in different formulas depending on the shape of the exclusion region associated with the Green's function singularity, this volume is not analogous to the particle shape. The notion of particle is not used anywhere in the derivation of the equations. This exclusion region is infinitesimally small and is not a physical entity. It is a mathematical entity. For example, choosing a spherically-shaped exclusion region does not at all mean one can only apply such formulas to spherical particles. One can still apply them to non-spherical shapes, including cubes, ellipsoids, etc. Importantly, as alluded above, the n-point correlation functions incorporate the information of particle shapes, in an indirect manner. Despite this fundamental difference, the fact that the equation (33) corresponds to that of spherical particles is certainly not a coincidence, it is because the polarizability of a spherical particle (smaller than the wavelength) is the same as the polarizability of a spherical exclusion volume, since it does not depend on the size (as long as the spheres are small).

TK21 goes a step further by indicating that rather than being related to the particle shape, the shape of the exclusion region is actually related to the symmetry of the effective dielectric constant tensor. For example, a spherical exclusion volume gives an isotropic effective dielectric constant and thus is optimal when the effective dielectric constant tensor is expected to be isotropic. This point is novel and important, this is where TK21 advances from IBA and SFT which relied on some assumptions about the particle shape. Some similar element was already in Improved Born Approximation via the K field factor proposed in Mätzler, 2002, but TK21 makes it more explicitly.

Our text is faithful to this response, and only minor editing is proposed:

“The SCE derivation does not rely on the scatterer concept, the medium is **exhaustively** described by the **n-point** correlation functions and the electromagnetic derivation uses the Green function formalism [\citep{tsang\\_2001\\_vol3}](#).”

“Further noting that the spherical exclusion volume provides a faster convergence (TK21 sec III B) as a function of the dielectric contrast **in case of isotropic media**, the conclusion is that **a spherical exclusion volume is recommended for any isotropic microstructure, i.e. independently of the existence (and shape) of individual scatterers.**”

b. In computational electromagnetics, such boundary value problems of irregular shape/boundary have been handled by more accurate numerical techniques such as edge elements in vectorial finite element method, RWG basis function in the method of moment, and Nystrom method for volume integral equations. The popular FDTD method which is used in TK21 is not accurate This is because FDTD uses rectangular grids in the discretization. It is unclear that the formulation of TK21 can handle the irregular shape of ice grains to correctly obey the boundary conditions on the surface of a scatterer.

It is not possible to explicitly check that the boundary conditions on the surface of a particle is verified, at least because the description of the medium is statistical in TK21. However the starting point of TK21 theory is the wave equation in two-phase media (which is an exact consequence of the Maxwell equations) and the development is very similar to that of other authors (e.g. Strong Fluctuation Theory, Chap 4, Section 3, Tsang and Kong 2021). The key breakpoint is from Eq 38 in TK21 and the benefit of this new treatment is explained in Remark viii. In TK21.

Regarding FDTD, we propose to remove the term “precise” in our paper, which was to be understood relative to the analytical formulations, not to other numerical methods. However, we admit this is misleading.

“Moreover TK21 conducted **numerical** electromagnetic simulations (FDTD technique) that compare favorably with SCE for a dielectric contrast comparable to that of ice and air, and up to  $k a \approx 1$  (fig. 9 in TK21)”

c. For TK21, the methodology is based on point geometries and correlation functions associated with point geometries. In principle, the point geometry has correlation functions of infinite order which makes the solution “exact”. But in practice to infinite order is not possible. Only the second order correlation function is used which means that the solutions have inaccuracies.

We fully agree with this and this point is explicitly addressed (last two paragraphs in Section 2) in the initial version of the paper, where we state our use of the truncation for  $n=2$ . This is not ideal as discussed in Section 2 but it is equivalent to the approximations found in the other formulations that we consider in our Section 3 (namely DMRT QCA and IBA). In this respect, TK21 with the truncation  $n=2$ , is the state of the art for snow, not beyond. However the TK21 methodology is not restricted to “point geometries” (in the sense of decorated point processes) a similar hierarchy emerges for continuous, non-particulate phases.

A benefit of TK21, for the future, is that the expressions for higher order truncation ( $n \geq 3$ ) are given explicitly which paves the way for further work. However, this is challenging for two reasons: 1) the  $n$ -point correlation function is required, and although a statistical estimator of these functions can be obtained from micro-computed tomography images, the inaccuracy is certainly very high based on our experience. Our intuition at this stage is that the inaccuracy will cancel the benefit of using such advanced truncation, but this is very open.

2) the numerical implementation of the terms  $n \geq 3$  is not trivial, and it is likely that the expressions in the form given by TK21 would be subject to numerical instability. A bit more mathematical work is needed even though TK21 already provides a significant advance.

At last, we question the interest of exploring this route, as of 2022, given that practical field snow measurement techniques (excluding micro-computed tomography,) are actually insufficient to even characterize the 2-point correlation function with full accuracy.

d. For  $ka$  extended beyond 0.5, there is incoherent field that contributes to radiative transfer equation. In addition to the attenuation due to scattering, there also is the phase matrix. This part of phase matrix

has not been treated in TK21. Recently, the cross-polarization of the phase matrix at C band, X band and Ku band have drawn significant interests in microwave remote sensing of snow.

This is correct, the phase matrix is not explicated in TK21. It could be derived from their equation 39 with probably very significant work. In our paper, most of the results concern the scattering coefficient only. However to produce Fig 2, we had to assume a phase matrix. We did so by taking the same form as predicted by IBA. This information was missing in our first version, it is now stated in the manuscript:

“Note that for this calculation, the phase matrix of the radiative transfer equation is needed. It is not available for the SCE theory and we assumed that its angular variations are the same as predicted by IBA.”

We are confident that this hypothesis is valid because of the proximity between IBA and TK21 at  $n=2$ . However, more mathematical work is needed to demonstrate this result.

e. In Mie scattering, there are two series with two sets of coefficients: one is “electric” and the other is “magnetic”. For  $ka \ll 1$ , the electric series dominate. However, when  $ka$  gets larger such as in TK21, the magnetic series contribute. It is unclear that TK21 include the magnetic series if the model is applied to dense Mie scattering

It is unclear which approximation in TK21 motivates this concern. As explained above, the medium description and the derivation of the electromagnetic equations are very different between TK21 and particle-based theories (such as Mie), which makes it difficult to compare the equations.

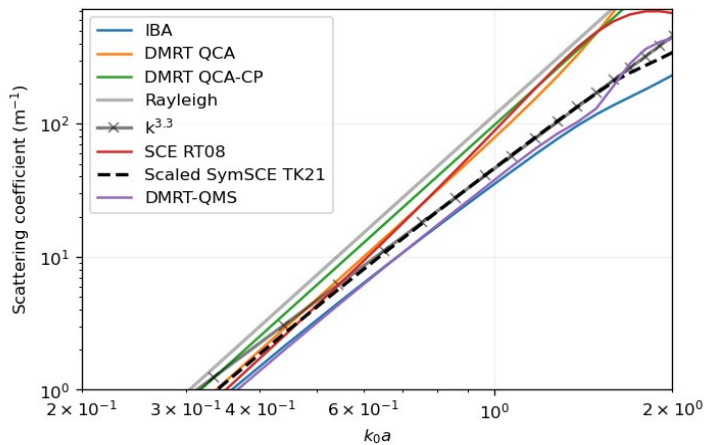
Although I have the above reservations about the applicability of TK21 to snow, I do think it is worthwhile for this paper to compute the results of attenuation of TK21 in snow and compare with other models.

I recommend the following revisions of this paper.

- 1, The authors should discuss the 5-bullet points a, b, c, d, and e that are raised above.
2. In figure 1, the frequency dependence power law should be extracted and tabulated. For Rayleigh scattering, it is frequency to the 4th power. The power law dependence makes the model comparisons easier to digest and remember.

We include here a loglog plot equivalent to Fig 1 with a power law fit. We found (dark gray curve) that SymSCE behaves as a power law of 3.3 around  $ka=1$  and for the specific conditions (density, stickiness) of Fig 1. However this power law is quite different for other  $ka$  which makes this information context-specific. While this figure provides interesting information, the main message in our text is the divergence between the short vs long range theories first, and then between the long range theories, and for this the actual Fig 1 is clear. Since in addition tabulating exponent values or

adding a new figure are not suitable for the short format of this paper, we have briefly integrated this question of the power law in the main text in the paragraph on the interpretation of Fig 1, as follows:



“The results for a density of  $300 \text{ kg m}^{-3}$  show a sharp increase as a function of  $k_0 a$  for all models. This increase indeed follows a power law in  $k_0^4$  at low frequencies which tend to slow down in the case of the long range theories (TK21, IBA, and the Mie-DMRT version implemented in the DMRT-QMS model (Tsang et al. 2007) when  $k_0 a$  is increasing (e.g. an apparent  $k_0^{3.3}$  for SymSCE if fitted around  $k_0 a = 1$ ). These results also indicate that the short range theories (RT08 and the two DMRT flavors available in SMRT) diverge for  $k_0 a > \sim 0.6$  from the long range theories.”

3. The Mie-DMRT in figure 1 may not be correct. This is because when  $ka$  exceeds 1, more terms in both the electric series and the magnetic series should be included. It is unlikely that Mie-DMRT go off like that as in figure 1. The Mie-DMRT has weaker frequency dependence than the power law of 4. I suggest that the author delete the Mie-DMRT unless their results are correct.

The Mie DMRT was obtained with the DMRT-QMS model that may involve numerical approximations responsible for this unexpected behavior. We propose to keep the curve (which is the correct results of the numerical calculation) and relabel the legend with DMRT-QMS instead of Mie DMRT to make clear that the curve is specific to one implementation (this was already explicit in the text).

We prefer not to remove the “strange” part of the curve because the purpose of this figure is specifically to identify when the different theories diverge from each other. Our belief is that even though IBA and SCE (with  $n=2$ ) seems to show a more continuous behavior for  $ka > 1.5$ , it is not sufficient to trust their results. All these three theories are not supposed to work in this high range, and we interpret the divergence noted by the reviewer between these theories as an illustration of this global limitation, not a specific limitation to one or another theory.

4. The results in figure 2 should be done for larger grain size. At least, a new figure with  $a=0.4 \text{ mm}$  should be added at 19GHz. The use  $a=0.2 \text{ mm}$  is too small. The scattering coefficient is only a fraction

per meter which is too small for real life problem. The measured volume radar backscattering at 19 Ghz is much larger for a snow depth of 1 meter.

Actually the graph was produced with  $a=0.3\text{mm}$  as stated in the text, but the value in our legend was erroneous. We have increased the radius  $a=0.4\text{mm}$  to follow the Reviewer's comment and have updated the figure.

We have also propagated this change in the text, specifically on the value of the difference between the theories which is now a bit larger: "Despite this secondary role, the differences between the theories reach  $15\text{K}$  in a wide range of densities, a significant uncertainty."

5. In equation (1), the summation over index  $n$  is up to infinity. However, in practice only second order,  $n=2$ , is used. The results in this paper are based on  $A_2$ . The expression for  $A_2$  should be explicitly given so that readers can write a computer code for  $A_2$  readily.

To keep the paper in the brief communication format, we prefer not to include the  $A_2$  equation which is quite complex and requires the definition of many terms, needing space. But we agree that direct access to the equation is helpful so we have added in our text the precise equation number for  $A_2$  in TK21.

Regarding the implementation of such an equation, TK21 makes it clear that the numerical computation is tricky and provides useful hints in supplementary materials (eq S111). We will provide a computer code (in the SMRT model) as open source on github and in the Zenodo permanent repository, as stated in the code availability section. Our code is fully documented with all the equation numbers referring to TK21. Verification and improvement of our implementation by other research groups are facilitated as much as possible.

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