

Response to Referee 1

This manuscript aims at clarifying the long-debated definition of a passive variable along neutral/isopycnal layers, commonly referred as "spiciness". The paper clarifies and demonstrates that the use of thermohaline anomalies (in particular absolute salinity) along neutral surfaces is sufficient to provide orthogonality in physical space. The long sought orthogonality in thermohaline space is showed to be flawed and not necessary to construct an inert variable along neutral surfaces. Moreover, the author discusses and resolves several issues raised by the definition of a physical variable satisfying the properties of spiciness. The existence of neutral surfaces is revealed to be key to the construction of a spiciness-like variable. By using theoretical arguments and a quasi-linear transformation of T/S space, the author also compares published definitions based on different assumptions and unifies them under basic principles.

I found the manuscript very interesting and well written. It surely provides an important step forward to the study of water mass. I therefore only have a few minor comments and recommend this paper to be published.

Response and suggested changes I thank the referee for his/her supportive comments. I response to his/her specific comments, I have made the following main changes:

- Orthogonality in physical space has now been more clearly defined. In the revised version of the paper, it is now defined as the median of all angles between $\nabla\gamma$ and $\nabla\xi$ estimated for all available data points.
- The orthogonality between $\nabla\xi$ and $\nabla\gamma$ has now been quantified for all spiciness variables ξ , as well as for their anomaly $\xi = \xi - \xi_r(\gamma)$.

I have also made many additional changes in response to the other comments, the main ones being:

- I have replaced σ_1 by the more neutral thermodynamic neutral density γ^T , for which I have proposed a new and computationally simpler implementation that should facilitate the reproducibility of my results. Section 2 has been modified to include a description of the new variable.
- To work with γ^T , the potential spiciness/spicity variables need to be referenced to a variable reference pressure $p_r(S, \theta)$. How to do that is now the topic of Section 3.
- Section 4 provides an illustration of the results as before but has been completely rewritten to account for the remarks of the referees as well as to account for the use of γ^T instead of σ_1 .
- Many sections have been rewritten/rephrased in the light of the new insights achieved since the original submission.

Response to specific comments

- 160 and Fig 1 : What is the source of the data shown?
 Good point. I used the WOCE dataset, available at:
<http://icdc.cen.uni-hamburg.de/1/daten/index.php?id=woce&L=1> Reference has now been added to the text.
- Fig2 : In caption : $\sin(\nabla\sigma_1, \nabla\xi)$? Why is the yellow histogram closer to 0 (ie sine closer to 1, angle closer to $\pi/2$), but described as the less orthogonal? Have the blue and yellow histograms been swapped? How does Θ variable compare to S_A in terms of orthogonality?
 The caption is as suggested by the referee. I think salinity is correctly described as the variable the most orthogonal to σ_1 and can't quite reconcile what the referee says and what I say. This figure has been completely redone in the manuscript. Orthogonality is now defined in terms of the median of all the angles between $\nabla\gamma$ and $\nabla\xi$ (or $\nabla\xi'$). The results are depicted in the new Figure 2.
- 1149 : What would be the proportion of the world ocean covered in that range? To identify regions where a spiciness definition would be challenged could be an interesting add to the paper.
 I have not attempted to quantify the accuracy of the quasi-linear approximation of density for the ocean's water masses, as it does not really matter for the arguments developed in the paper. My main aim was to construct a variable that can be used as a proxy for the spiciness variables of Jackett and McDougall (1995) and McDougall and Krzysik (2015) extending such variables to a wider range of reference pressures, allowing among other things to use a reference pressure $p_r(S, \theta)$ or $p_r(S_A, \Theta)$.
- Along the manuscript, it is commonly referred to “orthogonality in physical space” and I think it would be nice to have a clear definition of what it means in introduction. I agree as I can see from the other comments that not doing so has created some confusion. This has now been fixed as described above.
- I have the feeling that in regions of the ocean with temperature-driven density, salinity anomalies will have be a better choice to construct an inert variable. Am I speculating too much? Would Θ' be any better than S'_A where density is salinity-driven (eg, coastal ocean, near sea-ice, Mediterranean, Red, Black Seas, . . .)?
 This is an interesting question, which I find difficult to answer. Indeed, as first showed by Jackett and McDougall (1995), all thermodynamic variables are approximately dynamically inert on a material approximately neutral $\gamma = \text{constant}$ density surface. Whether the approximation is better for S'_A than Θ' , and whether this can be proven, is an interesting suggestion that I am still not clear about.

Response to Referee 2

General Comments This manuscript aims to clarify the theoretical foundation for a spiciness variable sought by many oceanographers. The main idea is that, before considering spiciness, one must first construct a good neutral density variable that is materially conserved, and then most any materially conserved function can be used to construct a spiciness variable, simply by constructing its anomaly along neutral surfaces. The author also clarifies that pursuing orthogonality of spiciness and neutral density in $S - \Theta$ space is misguided, and instead that the goal should be orthogonality of their gradients in physical space. Unfortunately, many of the advances of this paper are overstated, either lacking justification, detail, or novelty. There are several logical errors as well. These are discussed below. I believe this manuscript has the potential to nicely tie together the theory of spiciness variables, but Major Revisions are required to get there.

Response and proposed changes I thank the referee for his/her careful and comprehensive review, as well as for some thought provoking comments. In addition to addressing the numerous specific suggestions as detailed below, I have implemented the following main changes to address his/her most important comments.

1. To increase the novelty of the paper, I have redone all the calculations to be based on a new implementation of thermodynamic neutral density γ^T instead of σ_1 . Outside the southern ocean, this variable is significantly more neutral than σ_1 throughout the vertical column, and therefore a more satisfactory choice of quasi-neutral material density variable. I also showed how to construct potential spiciness and potential spiciness referenced to the non-constant reference pressure $p_r(S, \theta)$ underlying the construction of γ .
2. I have rephrased the abstract to link the present work to the previous work by Jackett and McDougall (1985) as well as to McDougall and Giles (1987). I have also tried to make it clear in the paper that these two studies represent important precursors of the present work.
3. I have completely rewritten the parts about orthogonality in physical space and significantly toned down its usefulness or importance
4. I have significantly rewritten various parts that appear to have been causes of confusion.
5. After thinking about it, I think that I agree with the referee that the arguments presented only offer support for the pursuit of a globally-defined material density variable maximising neutrality, but that they fell short of representing first-principles arguments.

6. Section 4 provides an illustration of the results as before but has been completely rewritten to account for the remarks of the referees as well as to account for the use of γ^T instead of σ_1 .
7. Many sections have been rewritten/rephrased in the light of the new insights achieved since the original submission.

Response to specific comments

- One of the major points of the paper, that what matters for spiciness is actually the neutral density variable, was made by Jacket and McDougall (1985). The author has acknowledged this in some places, but a reader could easily get the impression that this idea owes to this manuscript. A stand-out example is in the abstract (line 5): stating "contrary to what is usually assumed" is unfair. Anyone who has read Jackett and McDougall (1985) would not assume this. This phrase should be removed, and a citation to Jackett and McDougall (1985) given in the abstract.

Since the referee emphasises rigour and accuracy throughout his/her review, it seems important to point out that my point is actually that what determines the dynamical inertness of spiciness is the degree of neutrality of γ , which is quite different from what the referee says. Moreover, last time I checked, the term 'neutral density' is nowhere mentioned in Jackett and McDougall (1985) (JM85). Rather, JM85 use the term 'isopycnal surfaces', stating at the beginning of their paper: "In this paper we approximate the isopycnal surfaces by surfaces of constant potential density which we call ρ ." Moreover, JM85 also state: "the variations of any variable, when measured along isopycnal surfaces, are dynamically passive [...]". Since such a statement is technically true only on surfaces of constant in-situ density, there is no logical reason why readers would conclude that by 'isopycnal surfaces' JM85 actually mean 'neutral surfaces', especially as neither neutral surfaces nor patched potential density surfaces were yet in widespread use at the time. Even when such surfaces started to become popular, I am not aware that they have never associated with the dynamical inertness of spiciness before my paper.

I don't understand how my "contrary to what is usually assumed" is unfair to JM85, since what such a statement criticises is past studies contending that orthogonality and dynamical inertness are somehow connected, e.g., Veronis (1972). This is obviously not the case of JM85, which my paper praises for being the first to recognise that orthogonality is not connected with dynamical inertness. This being said, I agree that JM85 deserve a place in the abstract, not for promoting the use of neutral density, but for being the first to recognise the lack of connection between orthogonality and dynamical inertness, as well as for being the first to propose describing spiciness in terms of the isopycnal anomaly of some thermodynamic variable. As regards to the latter point, I don't think I give enough credit to JM85, which I hope has been

satisfactorily corrected in the revision of my paper.

As a final remark, I'd like to stress that I am not claiming credit for the idea that spiciness should be used in conjunction with neutral density, because there is no ambiguity that this is implied explicitly or implicitly in most if not all spicity/spiciness papers written post JM85, as is evident in Huang (2011) or McDougall and Krzysik (2015) for instance. I only claim credit for spelling a logical and rigorous argument establishing the link between dynamical inertness and neutrality, which had never been explicitly stated before, as far as I know.

- I find Fig 11 the most interesting aspect of this work. It is essentially a global test of the Jackett and McDougall (1985) idea, repeated here, that it is the anomaly ξ' is dynamically inert. The author's anomaly is defined as relative to a global isopycnal average. The results are evidently meaningful, but it is not entirely clear that more refined results could be obtained by refining the averaging procedure. McDougall and Giles (1987) argued in favor of studying property (salinity) anomalies relative to a local isopycnal average. To study a particular water mass intrusion, the state of the ocean far away should be irrelevant. It would therefore be prudent of the author to discuss the utility of using global isopycnal averages, and to locate the present work relative to the earlier work of McDougall and Giles (1987).

I fully agree with the referee and thank him/her for pointing out the highly relevant study by McDougall and Giles (1987), which I was not aware of. I have only touched upon global versus local definitions of $\xi_r(\gamma)$ as I haven't really explored the issue thoroughly enough yet.

- Moreover, it would be interesting to add another panel to Fig 11 that tests the anomaly of a state variable that is specifically designed to be quite poor as spiciness-as-a-state variable — but nonetheless may appear comparably good as spiciness-as-a-property (anomaly).

Conservative Temperature appears to be quite poor as a spiciness-as-a-state-function, and performs much better as an anomaly. It has now been added to the discussion.

- In addition to the question of which geographic data should enter the construction of the $\xi_r(\gamma)$ function, the question of how this data is used must also be asked. Early on in the paper, the author describes this as the isopycnal mean, which presumably implies an arithmetic mean (this should be clarified). However, Section 4 seems to make this more general, stating only that $\xi_r(\gamma)$ is a "suitably constructed function of density only". Should we use an arithmetic mean? If so, why? If we define ξ_r as the best such function, in some kind of a least-squares sense, would we discover that it is an arithmetic mean? Fig 8 provides a trivial example where γ and ξ are linear functions of space. Obviously, the real ocean presents a far more nonlinear problem, for there will not be a suitable function $\xi_r(\gamma)$ that renders $\nabla\xi'$ orthogonal to $\nabla\gamma$. Unless this general issue can be addressed, Section 4.1 is not of great theoretical or

practical interest.

After further testing and thinking about the issue, I am retracting my earlier response because I am now believe that trying to maximise the orthogonality of ξ' to γ in physical space is not the right way to approach the construction of $\xi_r(\gamma)$. In truth, I don't know what is the best way to construct $\xi_r(\gamma)$ and therefore decided to leave the issue open. In my paper, I chose a second order polynomial descriptor for $\xi_r(\gamma)$ in order to ensure the smoothness and differentiability of the function, which is not usually guaranteed if a standard isopycnal average is used. As far as I can see, my choice appears to result in ξ' that appear to succeed well as water masses' indicators. Moreover, two of the resulting variables, namely τ'_{ref} and S'_A , appear to have relatively small nonlinearities in S_A and Θ , which suggests that they might be sufficiently conservative in practice (which means that they can be expected to mix linearly to a good approximation). I can only hope at this stage that my paper will stimulate further research on the topic and that others may succeed in coming up with a better way of doing things.

- Section 3 provides one way (among many) to nonlinearly scale the $S - \Theta$ diagram so that both axes have common units [density], such that there is a well-defined spiciness variable $\tau_{\ddagger}$ that is orthogonal to density on this diagram. However, $\tau_{\ddagger}$ is subsequently dropped from the manuscript. It is claimed (line 168) that $\tau_{\ddagger}$ is similar to τ_{jmd} , but this is not proven or shown numerically. This manuscript would be considerably stronger if $\tau_{\ddagger}$ were tested in Section 4.2 and shown to have some advantage over other spiciness/ spicity variables (including τ_{jmd} , which it may well turn out to be very similar to). Otherwise, Section 3 seems to be of limited utility.

In the revised version of my paper, τ_{jmd} and $\tau_{\ddagger}$ are compared in Figs. 7 and 8, which appears to be sufficient to establish their similarity in (S_A, Θ) space. The main advantage of $\tau_{\ddagger}$ is its mathematically explicit character and continuous dependence on pressure, which makes it possible to construct the potential spiciness τ_{ref} referenced to the variable reference pressure $p_r(S, \theta)$ underlying the construction of thermodynamic neutral density. In the revised paper, Fig. 9 further establishes the similarity between the two variables.

Physically, I don't expect $\tau_{\ddagger}$ to have many advantages over τ_{jmd} for the study of spiciness anomalies. Its main advantages are practical ones, due to the Jacobian being non-zero everywhere in (S_A, Θ) space, and due to its dependence on adjustable parameters being more explicit.

- The theoretical argument, opening Section 3, reaches the conclusion that the $S - \Theta$ axes should be rescaled to have density as their common units, but this is commonly known. Huang et al (2018) pursues this, for example. The author does not make it clear why this rescaling of the $S - \Theta$ diagram is superior to other rescalings, even linear ones.

I have decided to remove this part of the paper as I think that it was confusing and

not really necessary.

- In terms of structure, Section 4.2 "Illustrations" is more of a "Results" section, and does not fit well with the theoretical Section 4.1. I recommend splitting Section 4 into two sections, and expanding both, as described above.

I have completely rewritten Section 4, which is now entirely a 'results' section.

- The author claims that the anomaly ξ' "is the variable optimally suited for characterising ocean water masses" (line 4-5). However, this is not proven, nor is there any discussion about how such optimality would be measured. Claims of optimality appear in several other places in the manuscript. I recommend this loose language be qualified and proved, or else changed.

The term optimal now only appears in the abstract as part of the stated goal of the paper and has been removed from the rest of the paper. Optimal is only used in the sense of 'best', not in the sense of satisfying any particular metric. I think that this is common usage. It is proven in the sense that ξ' is demonstrably better than ξ for the purpose.

- Another one of the major results claimed is that this paper presents a "rigorous and first-principles theoretical justification for... a globally-defined material density variable $\gamma(S, \theta)$ maximising neutrality" (e.g. lines 10, 115-116, 251-252). However, this justification is predicated upon the desire of oceanographers to have a spiciness variable. Though such a variable may be useful to possess, it does not itself have a rigorous and first-principles theoretical foundation, and so cannot be leveraged to justify such a γ .

It is not true that the theoretical justification for γ is "predicated upon the desire of oceanographers to have a spiciness variable". Indeed, the justification is predicated on the recognition that because in-situ density surfaces are inconvenient to use due to their strong dependence on pressure, there is a need for a material variable that for all practical purposes capture most of the dynamical features of in-situ density. This need is independent of the construction of a spiciness variable. Maximising neutrality is what maximise the ability of a material variable to behave like in-situ density for practical purposes. One such application is defining density-compensated (S, θ) anomalies that are as passive as possible, but others exist: predicting thermal wind, static stability and so on...

Specific Comments

- 29: Another citation for thermobaric instability would be apt, here, such as Ingersoll (2005; JPO).

I have now cited this reference. Thanks for reminding me about it.

- 71: Some additional conditions are necessary to make this example true. As counterexample, take $\gamma(S, \theta)$ and $\xi(S, \theta)$ as constants: both are material, but the given

d does not satisfy property 2, since two distinct points (S_1, θ_1) and (S_2, θ_2) would nonetheless have $d = 0$.

I think the counterexample is not in the spirit of the paper. I have rephrased using the term 'nontrivial' ξ and γ .

- 80: Please provide further detail on the derivation of $\gamma_S S' + \gamma_\theta \theta' \approx 0$. Is one supposed to take the gradient of $\gamma(S - S', \theta - \theta') = \gamma_0$ in the neutral tangent plane, and assume that γ is an approximately neutral density variable? This would lead to $\gamma_S \nabla_n S' + \gamma_\theta \nabla_n \theta' \approx 0$, but this differs from the stated equation by the presence of gradients. It is not clear whether the condition $\gamma(S_r(\gamma_0), \theta_r(\gamma_0)) = \gamma_0$ is necessary “for all γ_0 ”, or just the γ_0 under consideration.

The equation is simply obtained from a Taylor series expansion around the reference $S_r(\gamma_0)$ and $\theta_r(\gamma_0)$ values, i.e., $\gamma(S_r(\gamma_0) + S', \theta_r(\gamma_0) + \theta') \approx \gamma(S_r(\gamma_0), \theta_r(\gamma_0)) + \gamma_S S' + \gamma_\theta \theta' + \dots = 0$, which implies $\gamma_S S' + \gamma_\theta \theta' \approx 0$ at leading order.

- 93-94: Fig 2 does not show, as stated, that “the ability of a variable to characterise water masses is proportional to the degree of orthogonality between $\nabla \xi$ and $\nabla \gamma$...” It simply shows that the spatial gradient of different candidate spiciness variables make different angles with $\nabla \gamma$. Fig 2 can only be interpreted as the author desires by referencing the interpretation of Fig. 1, that SA is a better spiciness variable than the other two. Even still, this is merely an interpretation or a “suggestion” at this stage.

I completely rewrote this part in the revision, hopefully in a more satisfactory way.

- Eq. (1): Please provide some details on the derivation of this equation. Tailleux (2016a) also lacks such details.

This equation is obtained by the Jacobi method. It is explained in much details in Appendix A of Feistel (2018): Thermodynamic properties of seawater, ice and humid air: TEOS-10, before and beyond. Ocean Sciences, 14, 471–502.

<https://os.copernicus.org/articles/14/471/2018/os-14-471-2018.pdf>

- Eq. (4): d_i needs to be defined. Also, it needs to be stated that this assumes is a perfectly neutral density variable, rather than “on any given density surface...”

The expression is correct as stated. d_i is defined as the restriction of the total differential operator to an isopycnal surface $\gamma = \text{constant}$. The restriction depends on how γ is constructed. This has been clarified in the text.

- Eq. (6): Units error in the middle expression. X and Y have units of density, so cannot be added to the unitless value 1, which should be ρ_{00} .

I agree. Thank for spotting this. Corrected.

- Eq. (11): This isn’t really the total differential of $\tau_{\mp}$ if it’s at fixed pressure. But we can say that this is the total differential of potential spiciness. This has now been clarified

- 165: τ has not been defined. All that can be said is that τ_0 is an arbitrary constant with units of density, and that $\tau_{\ddagger}(S_0, \theta_0, p) = \tau_0$.
I did not really understand this so did not act on it.
- 168: $\tau_{\ddagger}$ is the exact solution to an approximate differential equation, but this does not mean $\tau_{\ddagger}$ is an approximate solution of the exact differential equation. Here, Eq. (11) is the "approximate differential equation", which approximately matches (exactly in form, approximately in coefficients) with the "exact differential equation" set out by Jackett and McDougall (1985). If this logic were true, chaos (theory) would not exist.
The referee has lost me. I have tried to rephrase the whole section, but am not sure that I have addressed this comment.
- Eq. (14): How did ρ_{00} become ρ_0 ? I assume the neutral relation $\nabla_i \theta = \alpha(S, \theta, p) \beta(S, \theta, p)^{-1} \nabla_i S$ was used, but this provides the second equality in (14) only if $\rho_0 = \rho_{00}$.
 ρ_0 should be ρ_{00} , thanks for spotting it. Corrected.
- 196-7: Here, the author states that Section 3 showed spiciness can be theoretically justified to be orthogonal to density in thermohaline space, but elsewhere (e.g. line 208) stated that orthogonality in thermohaline space is "fundamentally ill-defined". This is confusing, to say the least. I remain unconvinced that Section 3 delivered what has been advertised here (line 196-7). Rather, Section 3 just showed that we can define an alternative, but only approximate, equation of state under which orthogonality in thermodynamic space is well-defined. This does not answer the theoretical questions surrounding spiciness in the real ocean.
After further thinking about the issue, I am withdrawing my previous response to this comment. Indeed, I have come to realising that orthogonality in physical space is not as useful as I initially thought. I have therefore completely rewritten all the relevant parts. Hopefully, the revision makes more sense and is less controversial.
- 204 and Eq. (15): This is introduced a bit sloppily. No definition is given for $\hat{f}$ so the reader is left to figure that out by understanding Eq. (15) and/or by comparison with $\hat{\rho}$ earlier. Also, $\partial \hat{f} / \partial p = \partial f / \partial p$ is used but not stated in Eq. (15), which would probably benefit by using the latter in the middle expression. Actually, since the same thing appears in Eq. (16), it may be better to simply provide an equation that does nothing more than define $\hat{\nabla}$, thereby eliminating these multi-part equations (15) and (16).
This bit has been removed in the revision.
- 206: "efficient" does not seem like the right word here. Maybe "compact"?
I have removed this part altogether.
- 230: What is meant by "the values of σ_1 contours retained in the nonlinear regression"? Is only some of the data shown in Fig 9 actually used in the nonlinear

regression that produces its red lines? And the data that is used has σ_1 values between the largest and smallest of the thick black contours in Fig 10? The caption of Fig 10 helps support this interpretation, but even there it is confusing: the restricted range of σ_1 used to compute the nonlinear regression should be defined by two σ_1 values (a lower and upper bound) rather than four values (the thick contours).
The relevant plot has been completely redrawn in the revision. Hopefully, it is now much clearer.

- 250: Jackett and McDougall (1985) should be cited here.
Agreed
- 266-7: What would happen if you used a non-constant reference pressure for $\tau_{\ddagger}$, as suggested here? Actually, it's not clear what this even means: where does a reference pressure fit into $\tau_{\ddagger}$?
The paper has been completely rewritten to now rely on the use of a non-constant reference pressure $p_r(S, \theta)$. This has led to the introduction of the potential spiciness variable $\tau_{ref} = \tau_{\ddagger}(S, \theta, p_r(S, \theta))$ referenced to $p_r(S, \theta)$.
- 270: This claim, that Tailleux (2016b)'s density variable "maximizes neutrality while also being the only one that accounting for thermobaricity", is unfounded. Tailleux (2016b) only compared the neutrality of his density variable against a select few competitor density variables, namely two potential density variables, γ^n of Jackett and McDougall (1997), and a rational approximation of γ^n defined by McDougall and Jackett (2005; JMR). Conspicuously missing is the orthobaric density of de Szoeke et al (2000), not to mention the neutral density of Eden and Willebrand (1999). Moreover, since Tailleux (2016b)'s density variable was custom-built to mimic γ^n of Jackett and McDougall (1997), and the latter exhibits better neutrality (Fig 6 of Tailleux (2016b)), it is unclear how the author can make this claim even if orthobaric density had been tested
Orthobaric density is not a purely material variable so does not fit in the present framework. However, McDougall and Jackett (2005) γ_a and Eden and Willebrand (1999)'s variable are presumably affected by thermobaricity on account to the way that they are constructed, so I agree with the referee that I was imprecise. The whole claim has been dropped in the revision.
- 275-6: The author has not shown that ξ' appears to be insensitive to the particular choice of $\xi_r(\gamma)$, since only one method for empirically constructing $\xi_r(\gamma)$ was tested, namely the (arithmetic?) mean.
The use of the verb 'appears' makes my statement a subjective one. Nevertheless, I can try to be somewhat more precise in the revision.
- 278: Isn't ξ' conservative by definition? Since ξ and γ are assumed to be conservative throughout this manuscript, then ξ' should be too.

γ and ξ are assumed to be material and therefore Lagrangian invariants in the absence of diffusive sources/sinks of temperature and salinity, not conservative. The term conservative is used in the same sense as in McDougall (2003) paper on Conservative Temperature, i.e., as a variable satisfying an equation of the form

$$\frac{DH}{Dt} + \nabla \cdot \mathbf{F}_h = 0. \quad (1)$$

A priori, γ is not conservative since there are nonlinear production terms due to cabelling and thermobaricity. ξ will be similarly conservative depending on the magnitude of its linearities in S and θ .

- Fig 2: The source data should be restricted to be between, say, 500 and 1500 dbar, to remain near the reference pressure of σ_1 .
I have redone all the calculations using a new implementation of thermodynamic neutral density to avoid the issue altogether. The new Figure 4(b) shows that this variable is satisfactorily neutral throughout the water column outside the southern ocean.
- Fig 2: The colors are a bit confusing. In the caption, spiciness and spicity are described as brown and orange, respectively – quite similar colors! This seems (to me) to describe more how they appear in the histogram when blended with other colors, not how they are in the legend.
This figure has been redone and redrawn completely and should be much clearer now
- Fig 9: It is nearly impossible to get much information from these panels. It is likely that most of what we see is due to outliers, and the vast majority of the data is lying on top of itself. Instead of a simple scatter plot, I suggest using a 2D histogram.
I don't understand what would be the purpose of what the referee suggests. In any case, this figure has been modified to include data points from the global ocean as well. I suppose that this probably does not address the referee's comments, but I am not sure exactly what he/she has in mind.
- Fig 11: The colorbars all range between -2 and 2, but the units vary across panels. It would be better to let each colorbar cover the entire range of its variable, or perhaps to cover the variable's range up to two standard deviations, say.
Dr. Zika suggested to normalise each variable by its standard deviation, which I did. The relative ranges of each variable is now much more comparable I think.
- Fig 11: Caption: Which contours of σ_1 are shown in white?
As said previously, all the calculations have been redone using a new implementation of thermodynamic neutral density. The contour labels for $\gamma_{analytic}^T$ are now given in the new Figure 1 (panel d).

Technical Corrections [Thank you for these. All these have been taken into account in the revision.](#)

- 4-8: "The key results are:" should be "The key results are as follows." and each key result that follows should be a separate sentence. (What comes before a colon must be a complete sentence.)
- 9-10: Same issue as above.
- 19: behaves -> behave
- 28: sopycnal -> isopycnal
- 48 and 53: At this stage, it's unclear why or when "potential" should appear before "spicity" and "spiciness".
- 50: remove "in general"
- 56, 277, 278: question mark should be a period, or rephrase so that a question is actually asked, rather than stating what the question is.
- 61: signal -> signals
- 67: The statement "checked in any good mathematics textbook" is rather cavalier, and would be better omitted. Simply naming the mathematical object d as a metric is enough.
- 69: Using "1" and "2" to identify data leads to the unfortunate notation of $d(1; 2)$. I'd suggest using A and B instead of numbers.
- 72: The definition of f_i is quite confusingly written, since (γ, ξ) is really meant to say γ or ξ
- 105: This is usually called the "dianeutral vector" not the "neutral vector".
- 120: join $\rightarrow$ joint
- 125: typo in the inline equation: the first S should be θ
- 125: J has already been defined and does not need to be stated again.
- Eq (14) and line 191: τ should be $\tau_{\dagger}$.
- 192: brackets -> braces in Eq. (14).
- 207: tilde is placed incorrectly, should be over ∇
- 259: all -> are all

- 260: "the one used in this study": it's unclear what "one" is referring to, since four candidates were tested, and the author's own variable was also presented.
- 263: "as the ... variable" -> "as ... variables"
- 264: mimic -> mimics
- Fig 2: The x axis label is missing two gradient symbols, in front of σ_1 and ξ . Also, "11" -> "1". Also, "less" -> "least".
- Fig 9: "Fig. 11" -> "Fig. 1". Also, shouldn't "spiciness" and "spicity" be changed to "potential spiciness" and "potential spicity" throughout this caption? Also, the subscript for $\tau_{\ddagger}$ is sideways on the y-axis label of panel (a).
- various: showed -> shown

Response to Referee 3

Tailleux presents new ideas around spiciness in the ocean. I think this is a worthwhile paper with some interesting points being made. A number of the key conclusions don't seem well supported though. Some points are presented as self-evident, yet their justification seems far from obvious. Furthermore, some analysis lacks rigour. I feel these are largely matters of presentation and I expect I will be able to recommend publication after major revision.

Response and proposed changes I thank Dr. Zika for his careful review and useful suggestions. After thinking more about his comments and doing some more calculations and analysis, I have come to realise that part of my analysis was indeed not sufficiently rigorous, especially the part related to orthogonality in physical space, which I now regard as not as useful as originally thought, although still relevant. The main changes implemented in response to his suggestions are:

1. I have completely rewritten the discussion of orthogonality in physical space and considerably toned down its significance and usefulness;
2. I have improved Fig. 11 by rescaling the variables by their standard deviation as suggested

In addition to such changes, I have also implemented several other changes in response to all the other comments received, the main ones being:

- I have replaced σ_1 by the more neutral thermodynamic neutral density γ^T , for which I have proposed a new and computationally simpler implementation that should facilitate the reproducibility of my results. Section 2 has been modified to include a description of the new variable.
- To work with γ^T , the potential spiciness/spicity variables need to be referenced to a variable reference pressure $p_r(S, \theta)$. How to do that is now the topic of Section 3.
- Section 4 provides an illustration of the results as before but has been completely rewritten to account for the remarks of the referees as well as to account for the use of γ^T instead of σ_1 .
- Many sections have been rewritten/rephrased in the light of the new insights achieved since the original submission.

Specific issues:

1. **Orthogonality** Tailleux argues that the most appropriate spice variable should be orthogonal in geographical coordinates. I actually think this is a very important point

but words like orthogonal and optimal are used frequently without their implementation actually being globally orthogonal, nor evidently ‘optimal’ in any way. Firstly, the importance of orthogonality is introduced with “As is well known, the most efficient way to represent a vector is achieved by decomposing it in an orthogonal basis” This statement (and similar statements about orthogonality) should be made more precisely. For example, does the word ‘efficient’ have a precise meaning here? If we are to apply rigour to the idea of developing an orthogonal basis, surely there is a fundamental issue that the gradient of any spice variable can vanish on an isopycnal (and clearly the along-section isopycnal gradient of all the spice variables shown in figure 11 vanish at various locations). The problem Tailleux is dealing with is in three-dimensional space yet neutral density and spice offer only two basis vectors. This should be clarified with regard to the motivation to have an orthogonal basis since the basis developed is clearly incomplete. I suggest a severe tone down of the language of ‘orthogonal coordinates’ unless these issues are to be discussed carefully. Perhaps more crucially, it is unclear where and to what degree the modified spice variable η' is actually orthogonal. How do we know if the reference profile $\xi_r(\sigma_1)$ is ‘suitably constructed’? Fig.11 uses a polynomial fit of $\xi_r(\sigma_1)$ for a specific section for ξ_r . Doesn’t this imply there is no perfect orthogonality anywhere? Why not choose η_r to be η at a specific latitude and longitude so at least local orthogonality is ensured? Or one could use the global isopycnal average of η Why not these other choices? More generally, there is no attempt to quantify how ‘optimal’ different methods for making η' orthogonal are despite the word optimal being used frequently throughout the paper.

After further thinking about Dr. Zika’s remarks, I would like to withdraw my previous response to this comment because I now think that the importance of orthogonality in physical space was overstated in my originally submitted paper and that its usefulness for constraining the choice of ξ or $\xi_r(\gamma)$ is not as clear as I thought. As a result, I have significantly toned down the importance of orthogonality in the revision of my paper. As it turns out, ξ' is not always more orthogonal to γ in physical space than ξ , and upon further consideration, there is no strong reason that it should necessarily be. I hope that the referee will find the revised version of the paper more satisfactory in this respect. I am grateful to the referee for challenging me on that point, as I now realise that I had not fully taken into account all aspects of the problem. Because I completely rewritten the relevant parts of the manuscript, I believe that most of the other problems have been eliminated as a result.

2. **Fig 11.** I think the variables shown in Fig. 11 are even closer than they appear. Both potential spiciness and spicity are in units of kg/m^3 while Θ is in $^\circ\text{C}$ and S is in g/kg . As a consequence $\Theta - \Theta_r$ is saturated and $S - S_r$ is poorly resolved by the colour scale. There seems to not be a fundamental reason to care about the units of any of these coordinates since their utility is primarily in tracing water masses. So,

I strongly encourage the author to rescale the colour axes (e.g. by dividing each by 1 standard deviation) so the variations in each variable are highlighted rather than their absolute values. This will likely show that all four variables look very similar in terms of their relative variations.

This is a very good idea that I have implemented and that indeed appears to be sufficient to considerably reduce the inter-differences between the different ξ' .

3. I am not sure if I saw it mentioned but it would be nice to see it pointed out that if the equation of state is indeed linear then all four of the diagnostics shown in Fig.11 should be proportional (at least I am sure this is the case for Θ and S).

This is not mentioned in the text. I am not convinced that this is really necessary as the true equation of state is not linear.

4. General references to previous work There are a lot of instances where what is written in previous work is generalised. These need to be either removed or replaced with concrete examples. For example on line 120 it says “So far, studies that have pursued orthogonality: : have taken for granted: : :”. Unless complete knowledge of all such studies can be claimed, it would be more appropriate to just point out that this has happened in some studies and provide references.

I have kept this in mind in revising the paper. I have tried to make more specific statements and to avoid excessive generalisations.

Other comments and suggestions:

Thank for these. I have done my best to address these.

1. There were a large number of typos and a few terms left un-defined. I have had the paper proof-read and converted to Word to try to minimise these problems. I hope the revision is better in this respect.
2. Generally, it makes more sense to me that ‘I’ is used instead of ‘we’ since this is a sole author paper. This goes against my nature, but I gave it a try.
3. A lot of the mathematics was difficult to follow often because basic variables and notation were not defined.

I hope the revision is better

4. Line 14: What is a ‘binary fluid’

I think that most oceanographers know what a binary fluid is.

5. Line 25: What is “de-compensate”

At the surface, a density-compensated temperature anomaly will be modified by air-sea interactions, without necessarily modifying the associated density-compensated salinity anomaly. As a result, the modified temperature anomaly can no longer be density compensated, hence the term ‘de-compensate’.

6. Line 28: “isopycnal”
corrected. thanks.
7. Line 45: “As *shown* in this paper”
Part removed from the paper so no longer relevant
8. Line 72: I think I understand that f can be either gamma or eta. But as written it looks like f maps from Theta and S into gamma and eta space (e.g. the author writes $f = (\gamma, \eta)$). This whole paragraph could be expanded for clarity as it is important.
I have tried to clarify notations
9. Line 80: What is γ_S ? The partial derivative of gamma with respect to S ?
Yes. I think it is clear enough from context
10. Line 102: “As shown by” or “As Tailleux (2016a) showed”
Corrected. Thanks
11. Eq 2: Define ρ_p and ρ_η Done. Thanks.
12. Line 120: “in a join*t* system”. Also – its not clear what a ‘joint system of physical units’ is.
This part has been removed so no longer relevant
13. Eq (5): Why no brackets around what is being logged here?
This does not seem necessary here, as there is no ambiguity as to what is being logged.
14. Line 139: Why ρ_{00} and not just ρ_0 ?
I tend to use ρ_0 as a function of p or z , hence the choice of ρ_{00} to refer to a constant reference density.
15. Line 177: Define ‘quasi-material’
I have replaced quasi-material by material
16. Personal note: In our recent paper, Zika, J. D., J-B. Sallée, A. C. Naveira-Garabato, A. J. Watson, A. Meijers, M-J. Messias, B. King, 2020: Tracking the spread of a passive tracer through Southern Ocean water masses. Ocean Science.,16, 323–336, 2020, we attempted to construct a coordinate which was locally orthogonal to the along isopycnal direction and also materially conserved. The coordinate was essentially $S - S_r$. We chose $S - S_r$ because it was simpler to define than spice. Fig. 11 of this paper suggests this was a reasonable choice. Our salinity anomaly variable was used to help understand the isopycnal spreading of a passive tracer. There are likely other examples of work that benefited from, or would have benefitted from, such ‘spicy’ coordinates. I feel this paper would be better motivated if more references

were made to such studies.

I now remember that Dr. Zika mentioned this study to me at Ocean Sciences, and I am sorry that I forgot to cite it. This has been cited in the revision.