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Spiciness theory revisited, with new views on neutral density, orthogonality and passiveness

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Abstract. This paper clarifies the theoretical basis for constructing spiciness variables optimal for characterising ocean water masses. Three essential ingredients are identified: 1) a material density variable γ that is as neutral as feasible; 2) a material state function ξ independent of γ, but otherwise arbitrary; 3) an empirically determined function $\xi_r(\gamma)$ of γ quantifying the isopycnal mean behaviour of ξ. The key results are: It is the anomaly $\xi' = \xi - \xi_r(\gamma)$, rather than ξ, that is the variable optimally suited for characterising ocean water masses; Ingredient 1) is required, because contrary to what is usually assumed, it is not the property of ξ that determine its dynamical inertness, but the degree of neutrality of γ; Oceanic sections of ξ' are rather insensitive to the particular choice of ξ; Contrary to what has been usually assumed, it is orthogonality in physical space rather than in thermohaline space that is the relevant property for optimally characterising ocean water masses.

The results are important because: They unify the various ways in which spiciness has been defined and used in the literature; They provide for the first time a rigorous first-principles physical justification for the concept of neutral density.

1 Introduction

As is well known, three independent variables are needed to fully characterise the thermodynamic state of a fluid parcel in the standard approximation of seawater as a binary fluid. The standard description usually relies on the use of a temperature variable (such as potential temperature θ, in-situ temperature T or Conservative Temperature Θ), a salinity variable (such as reference composition salinity S or Absolute Salinity S_A), and pressure p. In contrast, theoretical descriptions of oceanic motions typically involve only two 'active' variables, namely in-situ density ρ and pressure. The implication is that S and θ can be regarded as being made of an 'active' part contributing to density, and a passive part associated with density-compensated variations in θ and S — usually termed 'spiciness' anomalies, which behaves as a passive tracer. Physically, such an idea is empirically supported by numerical simulation results showing that the turbulence spectra of density-compensated thermohaline variance is generally significantly different from that contributing to the density (Smith and Ferrari, 2009).

Although behaving predominantly as passive tracers, density-compensated anomalies may however occasionally 'activate' and couple with density and ocean dynamics. This may happen, for instance, when isopycnal mixing of θ and S leads to cabelling and densification, which may create available potential energy (Butler et al., 2013); when density-compensated temperature anomalies propagate over long distances to de-compensate upon reaching the ocean surface, thus modulating air-sea interactions (Lazar et al., 2001); when density-compensated salinity anomalies propagate from the equatorial regions to the regions of deep water formation, thus possibly modulating the strength of the thermohaline circulation (Laurian et al., 2006, 2009); when sopycnal stirring of density-compensated θ/S anomalies releases available potential energy associated with thermobaric instability (Tailleux, 2016a). For these reasons, the mechanisms responsible for the formation, propagation, and decay of spiciness anomalies have received much attention, with a key research aim being to understand their impacts on the climate system, e.g., Schneider (2000); Yeager and Large (2004); Luo et al. (2005); Tailleux et al. (2005).

Although in-situ density ρ is the most dynamically relevant variable, its strong dependence on pressure p makes it difficult to work with for unambiguously defining meaningful isopycnal surfaces and density-compensated θ/S anomalies. For this reason, it has become customary to define isopycnal surfaces in terms of some suitably defined material function $\gamma(S,\theta)$, generally defined in terms of some potential density appropriate to the range of pressures considered, in order for γ to most accurately capture the dependence of in-situ ρ on S and θ. Once a suitable γ has been selected, a second material function $\xi(S,\theta)$ is needed to fully characterise the (S,θ) properties of fluid parcels. The presumption so far has been that it might be advantageous to construct ξ so that it is 'orthogonal' to γ in thermohaline (S,θ) space. Indeed, this was originally thought to be required for ensuring that ξ be passive or dynamically inert, e.g., Veronis (1972). However, the notion was challenged by Jackett and McDougall (1985), who pointed out that it is the density-compensated part of any variable that is dynamically inert, not the variable itself, regardless of what the variable is. Jackett and McDougall (1985) also pointed out that orthogonality is a property that makes sense only if it is invariant upon any re-scaling of the axes, which is not the case for variables with different physical units such as S and θ. Nevertheless, rather than abandoning the idea, subsequent studies have sought to circumvent the above difficulty by defining orthogonality in a re-scaled system of coordinates $X(S)$ and $Y(\theta)$ expressing S and θ in a common system of density units. As showed in this paper, it is possible to classify existing constructions of ξ into two main categories:

1. those assuming $X(S)$ and $Y(\theta)$ to be linear functions of S and θ, as is the case of Veronis (1972); Huang (2011); Huang et al. (2018). In the following, we will generically refer to the corresponding state functions as spicity or potential spicity, denoted by π, following Huang et al. (2018);

2. those assuming $X(S)$ and $Y(\theta)$ to be nonlinear functions of S and θ, as it the case of Jackett and McDougall (1985); Flament (2002); McDougall and Krzysik (2015), although it is important to note that this is not how such variables were originally presented. In the following, we will generically refer to the corresponding state functions as spiciness or potential spiciness, generally denoted by τ_{jmd}. In this paper, illustrations will in general be based on the most recent paper by McDougall and Krzysik (2015).

Since orthogonality is at best ambiguously defined in (S,θ) space as well as unrelated to dynamical inertness, it is legitimate to ask whether it has any physical basis or any demonstrable benefits attached to it? So far, the presumption has been that orthogonality is somehow useful for optimally representing water masses and intrusions, e.g., Jackett and McDougall (1985);

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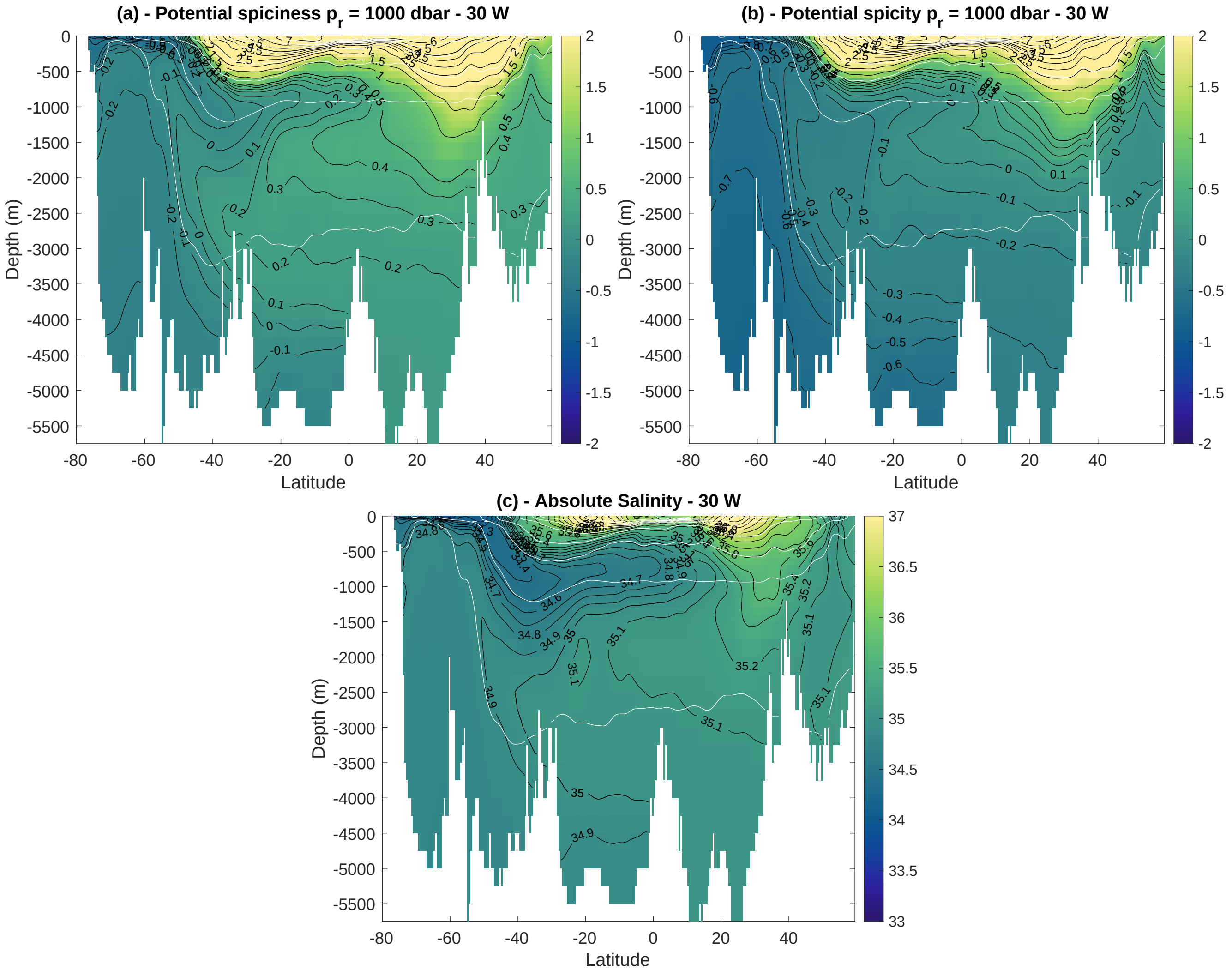

Figure 1. Atlantic section along $30°W$ of: (a) McDougall and Krzysik (2015) potential spiciness referenced to $1000\,\mathrm{dbar}$; (b) Huang et al. (2018) potential spicity referenced to $1000\,\mathrm{dbar}$; (c) Absolute Salinity. White contours indicate selected constant σ_1 isopycnal surfaces.

Flament (2002); Huang et al. (2018), but this may be wishful thinking. Indeed, the proposition seems to be easily refuted by plotting Absolute Salinity versus τ_{jmd} and π referenced to $1000\,\mathrm{dbar}$ for a selected Atlantic section, here chosen along $30°W$, as showed in Fig. 1. In the salinity plot, the Antarctic Intermediate Water (AAIW) is one of the most prominently visible signal and is seen to extend to about $20°N$. In the spiciness and spicity plots, however, the AAIW signal has a different shape and structure; it is much weaker and seen to only reach the equator, with the spiciness AAIW signal being somewhat stronger the spicity one. If orthogonality in (S,θ) space has any benefits or advantages, they are certainly not obvious, at least, as far as characterising ocean water masses is concerned. In their paper, Huang et al. (2018) suggested that without imposing orthogonality on ξ, it is otherwise hard to define a distance in (S,θ) space. As stated, however, this argument appears to be mathematically groundless, because it is not true that the concept of distance requires orthogonality. As can be checked in any good mathematics textbook, all is required is the introduction of positive definite metric $d(x,y)$ such that: 1) $d(x,y) \geq 0$ for all x and y; 2) $d(x,y) = 0$ is equivalent to $x = y$; 3) $d(x,y) = d(y,x)$; 4) $d(x,y) \leq d(x,z) + d(z,y)$, the so-called triangle inequality. As a result, $d(1,2) = \sqrt{\beta_0^2(S_1 - S_2)^2 + \alpha_0^2(\theta_1 - \theta_2)^2}$, where α_0 and β_0 are some constant reference values of α and β, define a valid distance in (θ,S) space. Obviously, there is an infinite number of ways to define distances in (θ,S) space. Any two material functions $\gamma(S,\theta)$ and $\xi(S,\theta)$ can also be used, i.e., $d(1,2) = \sqrt{(\gamma_1 - \gamma_2)^2 + K_0^2(\xi_1 - \xi_2)^2}$, where K_0 is a constant to express γ and ξ in the same system of units if needed, where $f_i = f(S_i,\theta_i)$, for $f = (\gamma,\xi)$.

Perhaps the most problematic aspect of regarding spiciness as a state function orthogonal to density, however, is that it appears to be fundamentally inconsistent with the way spiciness is defined in most of the literature seeking to understand the role of spiciness on climate. Indeed, as Jackett and McDougall (1985) originally remarked, it is the density-compensated part of any thermodynamic variable that is supposed to be dynamically inert, regardless of what the variable is. Mathematically, such an idea implies that it is the isopycnal anomaly $\xi' = \xi - \xi_r(\gamma)$ that is dynamically inert, regardless of how ξ is defined, where $\xi_r(\gamma)$ is a measure of the mean behaviour of ξ on the isopycnal surface $\gamma(S,\theta) = \mathrm{constant}$. In practice, the simplest and most natural choices of ξ are either S or θ, with the corresponding definitions of spiciness being $\theta' = \theta - \theta_r(\gamma)$ or $S' = S - S_r(\gamma)$. If the isopycnal mean $S_r(\gamma)$ and $\theta_r(\gamma)$ are defined so that $\gamma(S_r(\gamma_0),\theta_r(\gamma_0)) = \gamma_0$ for all γ_0, then at leading order $\gamma_S S' + \gamma_\theta \theta' \approx 0$, thus establishing that S' and θ' are density-compensated, as is expected physically. An immediate benefit of defining spiciness as an isopycnal anomaly is that it naturally ensures its vanishing in any spiceless ocean (one in which all iso-surfaces of S, θ and γ coincide), a property that is impossible to satisfy if spiciness is defined as a state function. Finally, it is important to remark that functions of state are usually reserved for describing intrinsic properties of a substance; spice, however, is fundamentally a relative property that can only be meaningfully defined after having determined the range of possible variations in θ/S values for samples of a given density. Physically, the concept of spice is therefore more naturally understood as an anomaly rather than as an absolute concept.

The main aim of this paper is to explore the above ideas further and to clarify their inter-linkages. Section 2 discusses what determines the dynamical inertness of spiciness, and shows that it is determined not by any of the properties of ξ, but by the properties of the quasi-linear material density variable γ that it is used in conjunction with. Section 3 examines the physical basis for using density units as the relevant joint system of units for making it possible to meaningfully define the concept of orthogonality in thermohaline space. Section 4 examines the link between orthogonality in thermohaline space and physical

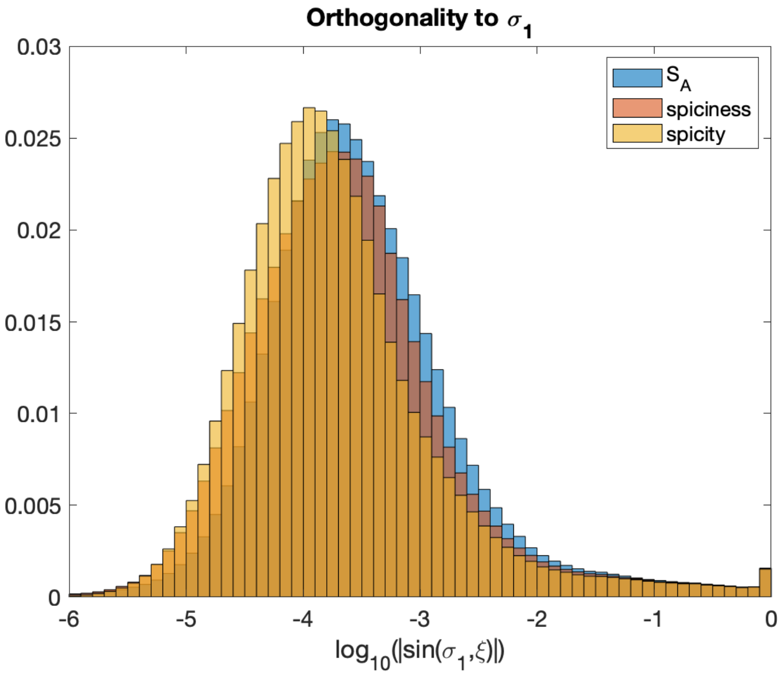

Figure 2. Histogram of the decimal logorithm of the (absolute value of the) sine of the angle between $\nabla\sigma_1$ and $\nabla\xi$ estimated for data restricted to the Atlantic section of Fig. 11 for: $\xi = S_A$ (Blue), $\xi = \tau_{jmd}$ (Potential spiciness referenced to $1000\,\mathrm{dbar}$, brown) and $\xi = \pi$ (potential spicity referenced to $1000\,\mathrm{dbar}$, orange). This shows that S_A (resp. π) is the variable the most (resp. less) orthogonal to σ_1 in physical space.

space. This idea is motivated by the results depicted in Fig. 2, which shows that the ability of a variable to characterise water masses is proportional to the degree of orthogonality between $\nabla\xi$ and $\nabla\gamma$, suggesting that the relevant concept is orthognality in physical space, rather than in thermohaline space. Section 5 summarises the results and discusses the implications and further work needed.

2 On what determines the dynamical inertness of spiciness

Near the freezing point, it is occasionally possible for the thermal expansion of seawater to vanish. In that case, Stipa (2002) pointed out that because potential temperature locally stops affecting density, it essentially becomes passive and therefore the most natural definition of spiciness. To extend the argument to the general case, one therefore needs to regard in-situ density as a function of the new (γ,ξ,p) coordinates, viz. $\rho = \rho(S,\theta,p) = \hat{\rho}(\gamma,\xi,p)$, and link the dynamical inertness of ξ to the smallness of the partial derivative $\partial\hat{\rho}/\partial\xi$. As showed by Tailleux (2016a), the partial derivatives of $\hat{\rho}$ with respect to γ and ξ are:

$$\frac{\partial\hat{\rho}}{\partial\gamma} = \frac{\partial(\hat{\rho},\xi)}{\partial(\gamma,\xi)} = \frac{1}{J}\frac{\partial(\xi,\rho)}{\partial(S,\theta)} = \frac{J_\gamma}{J}, \qquad \frac{\partial\hat{\rho}}{\partial\xi} = \frac{\partial(\gamma,\hat{\rho})}{\partial(\gamma,\xi)} = \frac{1}{J}\frac{\partial(\rho,\gamma)}{\partial(S,\theta)} = \frac{J_\xi}{J}, \tag{1}$$

where $J_\gamma = \partial(\xi,\rho)/\partial(S,\theta)$, $J_\xi = \partial(\rho,\gamma)/\partial(S,\theta)$ and $J = \partial(\xi,\gamma)/\partial(S,\theta)$. Of particular interest is the expression for the neutral vector $\mathbf{N}$ in the density/spiciness coordinates:

$$\mathbf{N} = -\frac{g}{\hat{\rho}}\left(\nabla\hat{\rho} - \hat{\rho}_p\nabla p\right) = -\frac{g}{\hat{\rho}}\left(\hat{\rho}_\gamma\nabla\gamma + \hat{\rho}_\xi\nabla\xi\right). \tag{2}$$

It is important to note that the Jacobian J is invariant upon transformation $\xi \to \xi - \xi_r(\gamma)$. In terms of $\xi' = \xi - \xi_r(\gamma)$, the expression for the neutral vector thus becomes:

$$\mathbf{N} = -\frac{g}{\rho}\left[\left(\hat{\rho}_\gamma + \hat{\rho}_\xi\frac{d\xi_r}{d\gamma}\right)\nabla\gamma + \hat{\rho}_\xi\nabla\xi'\right]. \tag{3}$$

According to (2) or (3), the condition for ξ or ξ' to be dynamically inert ($\hat{\rho}_\xi = 0$) is that γ be exactly neutral. As showed by Eq. (1), the condition for $\hat{\rho}_\xi$ to vanish is $\partial(\rho,\gamma)/\partial(S,\theta) = 0$, which is not possible because of thermobaricity, i.e., the pressure dependence of the thermal expansion coefficient (McDougall 1987; Tailleux (2016a)). As a result, the degree of dynamical inertness of ξ is related to the degree of non-neutrality of γ. This is an important result for two reasons. First, because it shows that it is not the properties (such as orthogonality) of ξ that determine its degree of dynamical inertness, but those of γ. Second, because it provides for the first time a rigorous and first-principles theoretical justification for seeking the construction of a globally-defined material density variable $\gamma(S,\theta)$ maximising neutrality (although this probably won't be a surprise to most oceanographers).

3 Spiciness and orthogonality to density

Physically, the pursuit of orthogonality as a constraint on ξ can only be justified if a physically-based way to re-scale S and θ in a join system of physical units can be identified. So far, studies that have pursued orthogonality in one form or the other have taken it for granted that such a joint system of units should be based on density units, but without really proving it. The use of density units can nevertheless be justified by remarking that the isopycnal variations of any arbitrary material function $\xi(S,\theta)$ on any given density surface $\gamma(S,\theta) = \text{constant}$ satisfy:

$$\mathrm{d}_i\xi = \frac{J}{\gamma_S\gamma_\theta}\gamma_S\mathrm{d}_iS = -\frac{J}{\gamma_S\gamma_\theta}\gamma_\theta\mathrm{d}_i\theta, \tag{4}$$

by using the result that $\gamma_\theta\mathrm{d}_iS + \gamma_S\mathrm{d}_iS = 0$, where $J = \partial(\xi,\gamma)/\partial(S,\theta)$ is the Jacobian of ξ and γ. Eq. (4) establishes that the isopycnal variations of any material ξ are all proportional to the quantity $\gamma_S\mathrm{d}_iS = -\gamma_\theta\mathrm{d}_i\theta$, the proportionality factor being $J/(\gamma_S\gamma_\theta)$. The two quantities $\gamma_S\mathrm{d}_iS$ and $\gamma_\theta d_i\theta$ have the same physical units: they can thus be regarded as the basic building blocks for the construction of any spiciness variable and motivate the introduction of re-scaled salinity and temperature scales $X(S)$ and $Y(\theta)$ such that $X'(S) \approx \gamma_S$ and $Y'(\theta) \approx -\gamma_\theta$. The following pursues such an idea by providing a concrete way to construct $X(S)$ and $Y(\theta)$ explicitly.

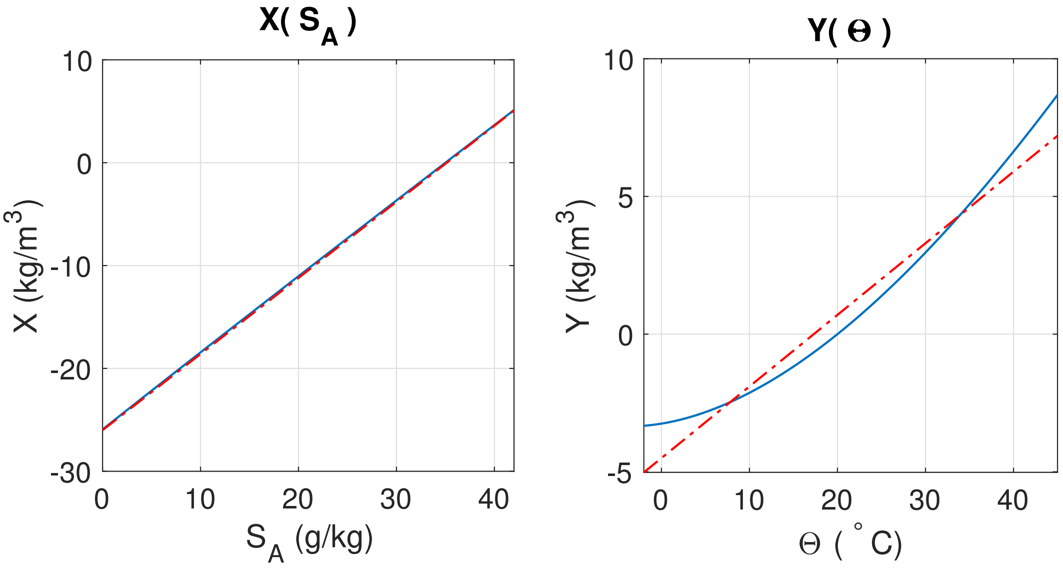

Figure 3. The functions $X(S_A)$ and $Y(\Theta)$ re-scaling S_A and Θ in a common system of density-like units. Red dashed line indicates linear regression. $X(S_A) = 0.74\,S_A - 26$ and $Y(\Theta) = 0.26\,\Theta - 4.5$

3.1 A quasi-linear approximation to density

For reasons made clear in the following, a useful and instructive explicit construction of $X(S)$ and $Y(\theta)$, parameterically dependent on pressure p, is as follows:

$$X = X(S,p) = \rho_{00} \ln \frac{\rho(S,\theta_0,p)}{\rho(S_0,\theta_0,p)}, \qquad Y = Y(\theta,p) = -\rho_{00} \ln \frac{\rho(S_0,\theta,p)}{\rho(S_0,\theta_0,p)}, \tag{5}$$

where S_0, θ_0 and ρ_{00} are constant reference values for S, θ, and ρ respectively. In principle, S_0 and θ_0 could also be made to depend on pressure p, but this complication is avoided here to keep the approach as simple as possible. Fig. 3 illustrates a particular construction based on the use of the most recent thermodynamic equation of state (IOC et al., 2010; Pawlowicz et al., 2012), in terms of absolute salinity S_A and Conservative Temperature Θ, using the values $S_0 = 35\,\mathrm{g/kg}$, $\Theta_0 = 20°C$, and $\rho_{00} = 1000\,\mathrm{kg.m^{-3}}$, for $p = 0\,\mathrm{dbar}$. This figure shows that $X(S_A)$ varies approximately linearly with S_A. However, $Y(\Theta)$ is clearly a nonlinear function of Θ, for which a linear approximation can nevertheless be constructed using linear regression (depicted as the red dashed line).

The re-scaled salinity/temperature coordinates given by Eq. (5) make it possible to construct a quasi-linear approximation $\rho_\ddagger = \rho_\ddagger(S,\theta,p;S_0,\theta_0)$ of in-situ density as follows:

$$\rho_\ddagger = \frac{\rho_0(p)}{\rho_{00}}(X - Y + 1) = \rho_0(p)\left[\ln\left\{\frac{\rho(S,\theta_0,p)\rho(S_0,\theta,p)}{\rho_0^2(p)}\right\} + 1\right] \tag{6}$$

where $\rho_0(p) = \rho(S_0,\theta_0,p)$, so that by construction, $\rho_\ddagger = \rho$ at the reference point (S_0,θ_0) for all pressures. In-situ density and its quasi-linear approximation are compared in Fig. 4 for $p = 0$, as a function of S_A and Θ (top panel) as well as of X and Y

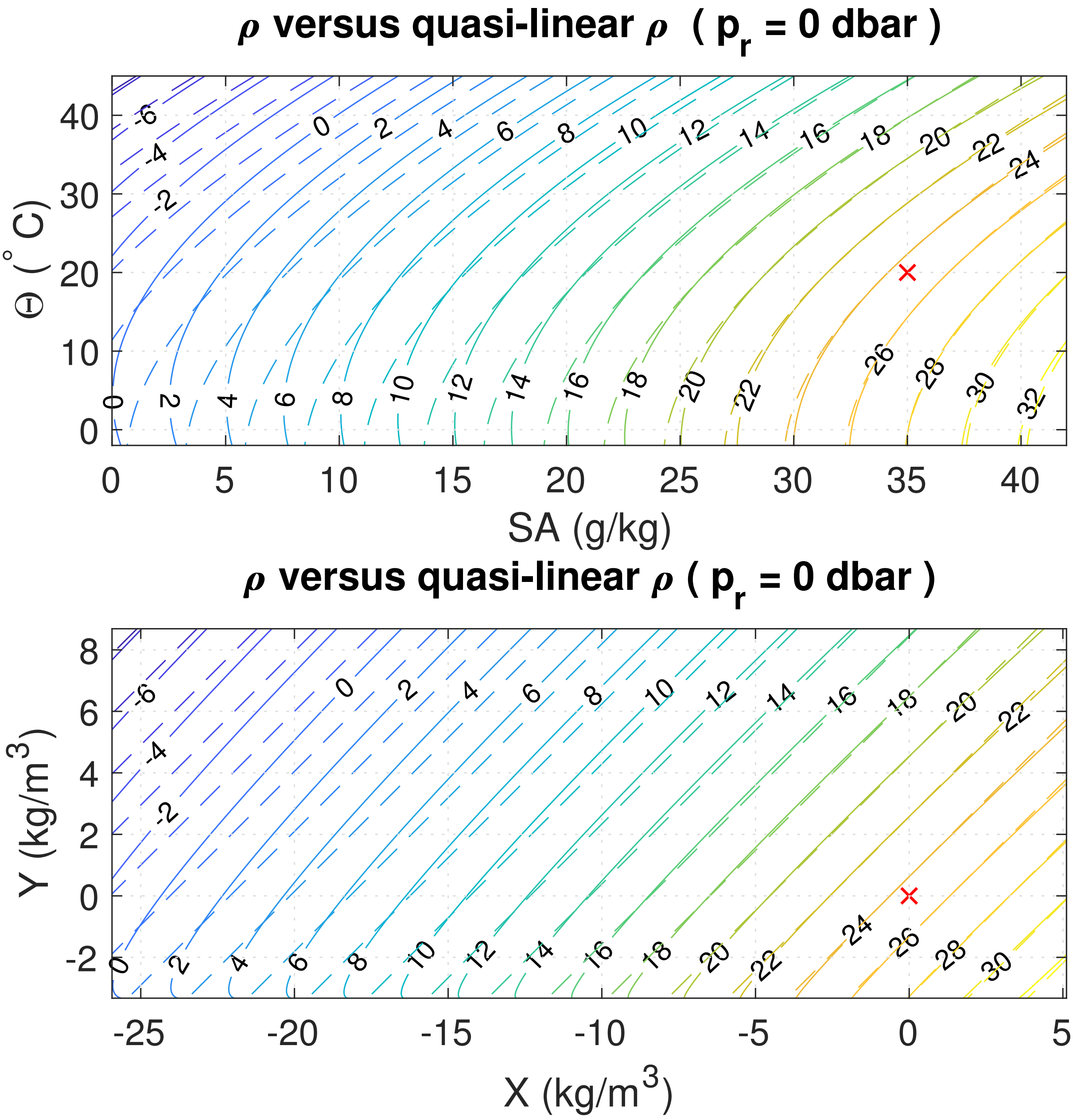

Figure 4. Comparison between potential density (referenced at $p = 0\mathrm{dbar}$) (solid line) and its quasi-linear approximation (dashed line), seen as function of S_A and Θ (top panel) and re-scaled coordinates X and Y (bottom panel). The red cross denotes the point $(S_A, \Theta) = (35., 20.)$ at which the two functions are imposed to be equal.

(bottom panel), with the red cross indicating the reference value ($S_A = 35\,\mathrm{g/kg}, \Theta = 20°C$) used in the definition of $\rho_\ddagger$. As expected, the accuracy of $\rho_\ddagger$ decreases away from the reference point, but appears to be reasonable in the restricted salinity range $[30\,\mathrm{g/kg}, 40\mathrm{g/kg}]$ that pertains to the bulk of ocean water masses. Interestingly, the bottom panel of Fig. 4 reveals that a significant fraction of the nonlinear character of the equation of state is captured by X and Y, so that ρ appears to be approximately linear in such coordinates.

The accuracy of the quasi-linear approximation $\rho_\ddagger$ can also be evaluated by examining how its thermal expansion, haline contraction and compressibility compare with that of in-situ density. These are given by:

$$\alpha_\ddagger = -\frac{1}{\rho_\ddagger}\frac{\partial \rho_\ddagger}{\partial \theta} = \frac{\rho_0(p)\alpha(S_0,\theta,p)}{\rho_\ddagger}, \tag{7}$$

$$\beta_\ddagger = \frac{1}{\rho_\ddagger}\frac{\partial \rho_\ddagger}{\partial S} = \frac{\rho_0(p)\beta(S,\theta_0,p)}{\rho_\ddagger}, \tag{8}$$

$$\kappa_\ddagger = \frac{1}{\rho_\ddagger}\frac{\partial \rho_\ddagger}{\partial p} = \kappa(S_0,\theta_0,p) + \frac{\rho_0(p)}{\rho_\ddagger}\left[\kappa(S,\theta_0,p) + \kappa(S_0,\theta,p) - 2\kappa(S_0,\theta_0,p)\right]. \tag{9}$$

These relations show that the first partial derivatives of $\rho_\ddagger$ with respect to its three variables also coincide with their exact values at the reference point (S_0,θ_0), with the accuracy of the approximations decaying away from it, as expected.

3.2 A mathematically explicit quasi-linear spiciness variable

Because $\rho_\ddagger$ is a simple linear function of X and Y, it is trivial to construct a variable $\tau_\ddagger$ orthogonal to it in (X,Y) space, and hence approximately orthogonal to in-situ density. In this paper, we consider the following construction:

$$\tau_\ddagger = X + Y + \tau_0 = \rho_{00}\ln\left\{\frac{\rho(S,\theta_0,p)}{\rho(S_0,\theta,p)}\right\} + \tau_0, \tag{10}$$

where $\rho_{00} = 1000\,\mathrm{kg.m^{-3}}$ for simplicity, while $\tau_0 = \tau(S_0,\theta_0,p)$ specifies the reference value of $\tau_\ddagger$ at the reference point (S_0,θ_0). At fixed pressure, the total differential of $\tau_\ddagger$ is

$$\mathrm{d}\tau_\ddagger = \rho_{00}(\beta(S,\theta_0,p)\,\mathrm{d}S + \alpha(S_0,\theta,p)\,\mathrm{d}\theta), \tag{11}$$

and is clearly an approximate solution to the differential problem $\mathrm{d}\tau \approx \rho(\alpha\mathrm{d}\theta + \beta\mathrm{d}S)$ set out by Jackett and McDougall (1985) to define their own spiciness variable (see McDougall and Krzysik (2015)), which is also the problem considered by Flament (2002). Defining τ_0 as

$$\tau_0(p) = -\rho_{00}\ln\left\{\frac{\rho(S_{ref},\theta_0,p)}{\rho(S_0,\theta_{ref},p)}\right\}, \tag{12}$$

allows one to choose (S_{ref},θ_{ref}) as the point in (S,θ) space at which $\tau_\ddagger$ vanishes. In terms of the TEOS10 variables (S_A,Θ), we use $S_{ref} = 35.16504\,\mathrm{g/kg}$ and $\Theta_{ref} = 0°C$ to fix the zero of $\tau_\ddagger$ as in McDougall and Krzysik (2015). As a result, the pressure dependence of $\tau_\ddagger$ becomes:

$$\frac{\partial \tau_\ddagger}{\partial p} = \rho_{00}\left(\kappa(S,\theta_0,p) - \kappa(S_0,\theta,p) - \kappa(S_{ref},\theta_0,p) + \kappa(S_0,\theta_{ref},p)\right). \tag{13}$$

Eq. (13) shows that $\partial_p \tau_\ddagger$ vanishes at the two reference points (S_0,θ_0) and (S_{ref},θ_{ref}); it follows that by design, $\tau_\ddagger$ is only weakly dependent on pressure, and hence naturally quasi-material.

Our new quasi-linear spiciness variable $\tau_\ddagger$ is compared with that of McDougall and Krzysik (2015) in Figs. 5 and 6, as a function of (S_A,Θ) and (X,Y) respectively. These figures show that the two spiciness variables behave in essentially the same way, except for cold temperature and low salinity values where the contours of McDougall and Krzysik (2015) spiciness variable become parallel to that of density, resulting in the Jacobian of the transformation to vanish, a problem not affecting our variable.

Jackett and McDougall (1985) sought to construct a spiciness variable satisfying the constraint $\nabla_i \tau \approx 2\rho_0 \beta \nabla_i S$. From the viewpoint of Eq. (4), this is mathematically equivalent to impose the condition $J/(\gamma_S \gamma_\theta) \approx 1$ on the proportionality factor, which can also be viewed as the constraint $J \approx \gamma_S \gamma_\theta$ on the Jacobian of the transformation. Because γ_θ may change sign at a point of maximum density, the implication is that Jackett and McDougall (1985)'s approach yields a density/spiciness coordinate system that is not invertible everywhere. In contrast, the Jacobian associated to $\tau_\ddagger$ does not vanish anywhere in (S,θ) space. As a result, the isopycnal variations of $\tau_\ddagger$, which are given by:

$$\nabla_i \tau = \rho_{00}\left(\beta(S,\theta_0,p)\nabla_i S + \alpha(S_0,\theta,p)\nabla_i \theta\right) = \rho_0 \left\{ \frac{\beta(S,\theta_0,p)}{\beta(S,\theta,p)} + \frac{\alpha(S_0,\theta,p)}{\alpha(S,\theta,p)} \right\} \beta \nabla_i S \tag{14}$$

are similar but not identical to that of Jackett and McDougall (1985)'s spiciness variable. Near the reference point (S_0,θ_0), $\nabla_i \tau \approx 2\rho_0 \beta \nabla_i S = 2\rho_0 \alpha \nabla_i \theta$ as for Jackett and McDougall (1985) spiciness variable. As showed by Fig. 7, the factor within brackets is close to the factor 2 for most (S,θ) values, but becomes very large near the point of maximum density, the necessary trade-off for allowing the transformation to remain invertible.

4 Orthogonality in thermohaline space versus in physical space

4.1 Theoretical considerations

Although we saw in the previous section that the construction of a spiciness variable orthogonal to density in thermohaline space can be justified theoretically, at least to some extent, we also saw in the introduction that the resulting variable does not appear to do a particularly good job at identifying the standard ocean water masses, which is at odds with widespread claims in the spiciness literature about its supposed optimality for characterising water masses and intrusions. In this section, we make the case that the main reason for the failure of published definitions of spiciness is because the property that is actually the most useful for characterising ocean water masses is not orthogonality in thermohaline space, as erroneously assumed, but orthogonality in *physical space*.

To see this, let us first note that for any density/spiciness (γ,ξ) set of variables, the gradient of any thermodynamic function $f(S,\theta,p) = \hat{f}$ corrected for pressure is:

$$\tilde{\nabla} f = \nabla f - \frac{\partial \hat{f}}{\partial p}\nabla p = \frac{\partial \hat{f}}{\partial \gamma}\nabla \gamma + \frac{\partial \hat{f}}{\partial \xi}\nabla \xi. \tag{15}$$

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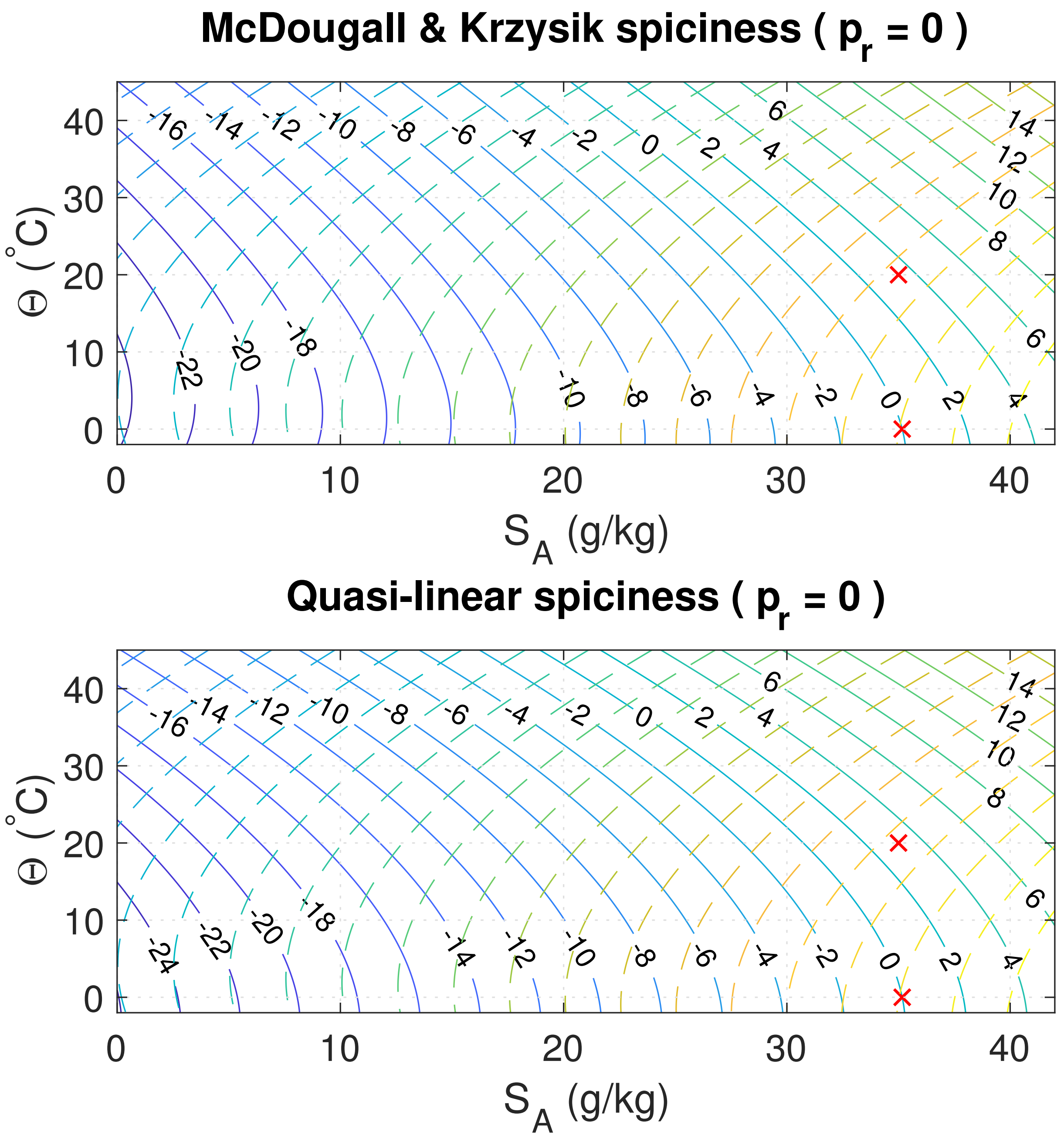

Figure 5. Comparison between McDougall and Krzysik (2015) spiciness variable versus the mathematically explicit quasi-linear spiciness variable discussed in this paper (solid lines). The crosses indicate the reference point $(S_A,\Theta) = (35, 20)$ at which $X = Y = 0$ and the reference point $(S_A,\Theta) = (35.16504, 0.)$ at which both spiciness variable are imposed to vanish. The dashed contours represent the isolines of the potential density referenced to $p = 0\,\mathrm{dbar}$.

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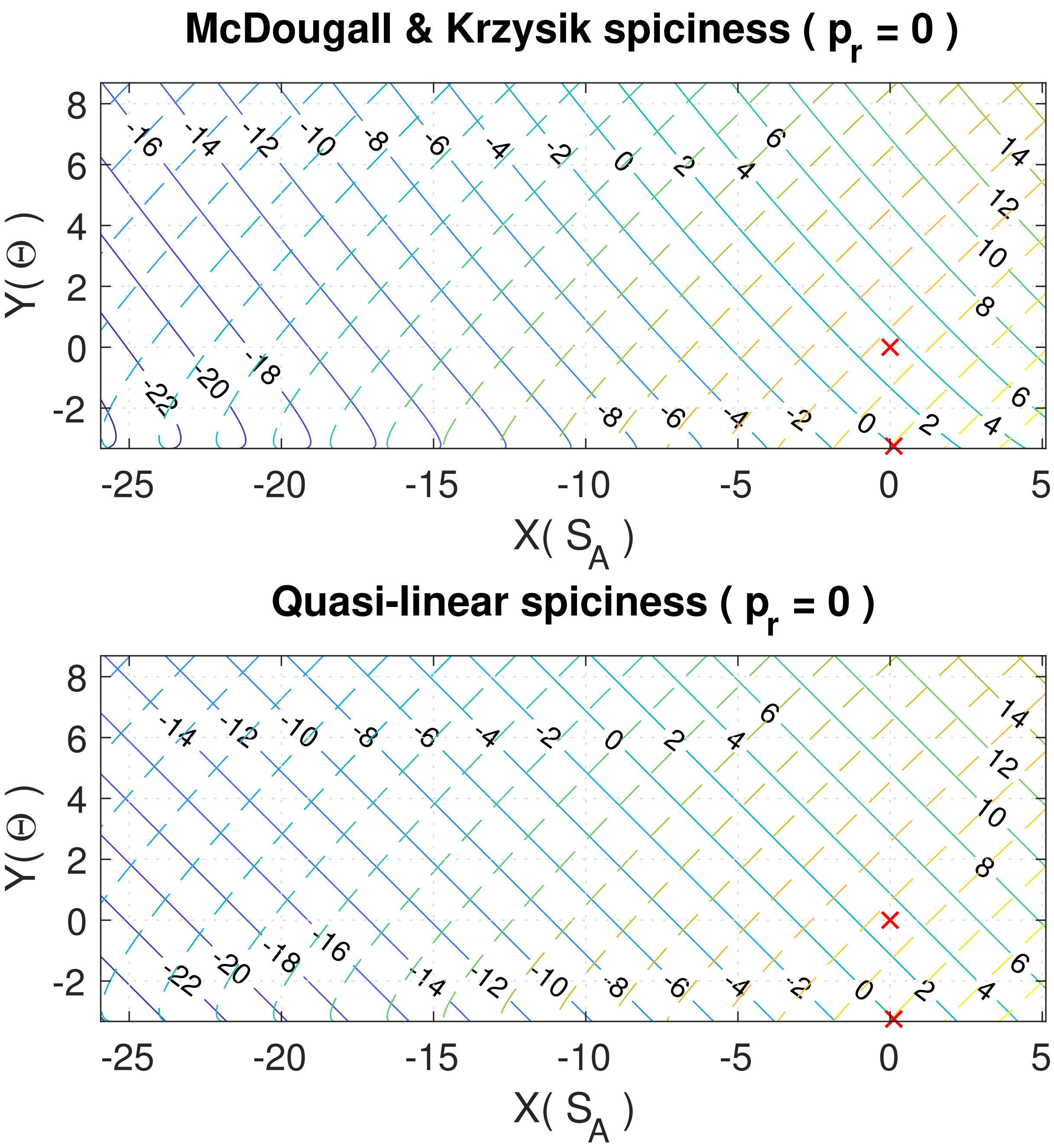

Figure 6. Same as in Fig. 5 but as a function of the re-scaled salinity and temperature X and Y.

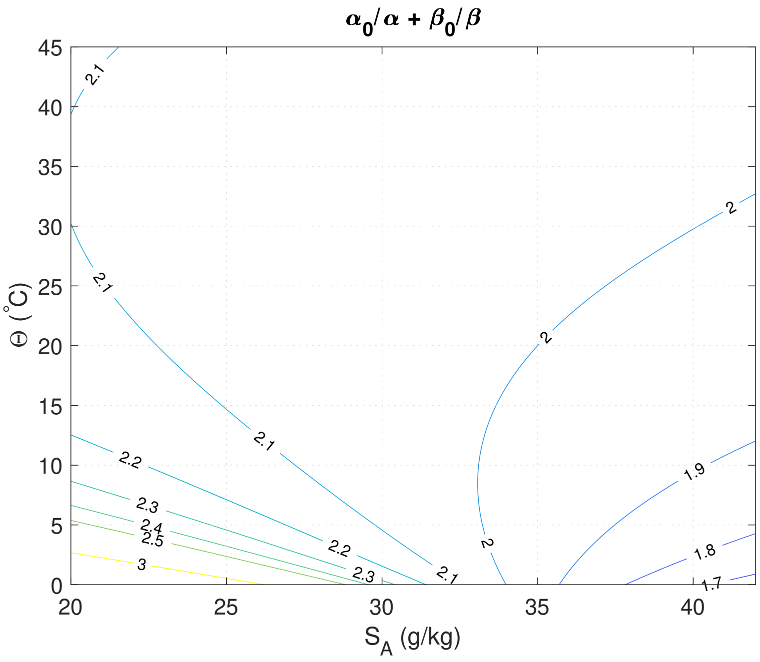

Figure 7. The factor $\frac{\beta(S_A,\Theta_0,p)}{\beta(S_A,\Theta,p)} + \frac{\alpha(S_0,\Theta,p)}{\alpha(S_A,\Theta,p)}$ controlling the isopycnal variations of spiciness. Reference pressure $p_r = 0\,\mathrm{dbar}$. Only a restricted range of (S_A, Θ) is showed. The factor becomes very large when α becomes very small near the region of maximum density.

As is well known, the most efficient way to represent a vector is achieved by decomposing it in an orthogonal basis. It follows therefore the most efficient representation of the pseudo gradient $\tilde{\nabla f}$ would be one in which $\nabla\gamma$ and $\nabla\xi$ are orthogonal to each other. Now, it is important that whereas the orthogonality of ξ and γ in thermohaline space is fundamentally ill-defined, the orthogonality of $\nabla\gamma$ and $\nabla\xi$ is always mathematically well defined. Importantly, orthogonality in thermohaline space does not imply orthogonality in physical space. As a result, even if ξ is constructed to be orthgonal to density in thermohaline space, this will not in general be the case in physical space. As an illustration of this, the isolines of ξ and γ in an oceanic section may look like that schematically depicted in the left panel of Fig. 8. In that case, $\nabla\xi$ and $\nabla\gamma$ are non-orthogonal, and each vector has a significant projection onto the other.

The right panel of Fig. 8 illustrates how to make spiciness locally orthogonal to density in physical space by introducing the spiciness anomaly $\xi' = \xi - \xi_r(\gamma)$, where $\xi_r(\gamma)$ is a suitably constructed function of density only. In terms of ξ', the representation of $\tilde{\nabla} f$ becomes:

$$\tilde{\nabla} f = \nabla f - \frac{\partial \hat{f}}{\partial p}\nabla p = \left(\frac{\partial \hat{f}}{\partial \gamma} + \frac{\partial \hat{f}}{\partial \xi}\frac{d\xi_r}{d\gamma}\right)\nabla\gamma + \frac{\partial \hat{f}}{\partial \xi}\nabla\xi'. \tag{16}$$

Two important remarks need to be made. First, adding or subtracting a function of γ from ξ does not affect the Jacobian of the transformation, so that $\partial(\xi,\gamma)/\partial(S,\theta) = \partial(\xi',\gamma)/\partial(S,\theta)$. Moreover, this also does not affect the isopycnal variations of ξ so that $\nabla_i\xi = \nabla_i\xi'$, both in physical space and thermohaline space. As a result, the factor $J/(\gamma_S\gamma_\theta)$ is identical for ξ and

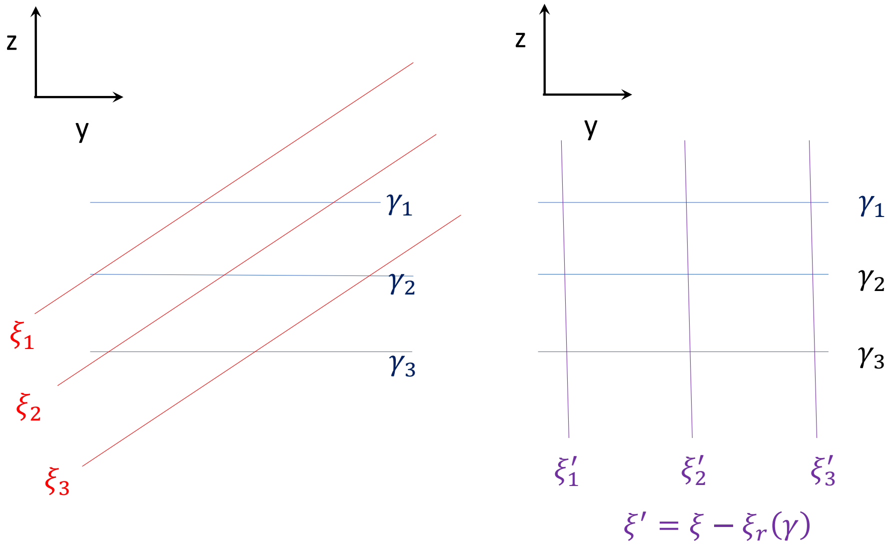

Figure 8. Schematics of the effect of subtracting a suitably defined function of density from an initial definition of spiciness state function. Left panel shows the isolines of idealised γ and ξ given by $\gamma = az+b$ and $\xi = cz+dy$. The right panel shows isolines of $\xi' = \xi - \xi_r(\gamma) = dy$, with $\xi_r(\gamma) = c[\gamma - b]/a$, which removes the z-dependent part of ξ, resulting in ξ' and γ to be orthogonal in physical space.

ξ'. Second, if ξ is originally constructed to be orthogonal to γ in thermohaline space, removing a function $\xi_r(\gamma)$ from it will destroy such orthogonality.

4.2 Illustrations

To illustrate the above ideas, we consider 4 possible spiciness state functions: McDougall and Krzysik (2015)'s potential spiciness τ_{jmd} referenced to $1000\,\mathrm{dbar}$, Huang et al. (2018)'s potential spicity π referenced to $1000\,\mathrm{dbar}$, Conservative Temperature Θ and Absolute Salinity S_A. Fig. 9 shows a scatter plot of each variable against σ_1, restricted to the values pertaining to the Atlantic section along $30^\circ W$ depicted in the introduction. As can be seen on the figure, each variable exhibit a different degree of scatter. The red line in each panel represents a best fit second order polynomial in σ_1 obtained by nonlinear regression of each variable against σ_1. Each of these variables is showed in (S_A, Θ) space in Fig. 10, where the black thick lines emphasise the values of σ_1 contours retained in the nonlinear regression.

Fig. 11 shows oceanic sections of the isopycnal anomaly $\xi' = \xi - \xi_r(\sigma_1)$ for each variable. Interestingly, although τ_{jmd}, π and S_A look quite different from each other in (S_A, Θ) space, their isopycnal anomalies exhibit strong similarities on an oceanic section, although Θ' looks somewhat different, so that visually, all variables appear to perform similarly in characterising ocean water masses. In particular, in all plots, the AAIW is seen to have the same shape and extent; in particular, it extends to about $20^\circ N$, similarly as in the salinity plot of Fig. 1.

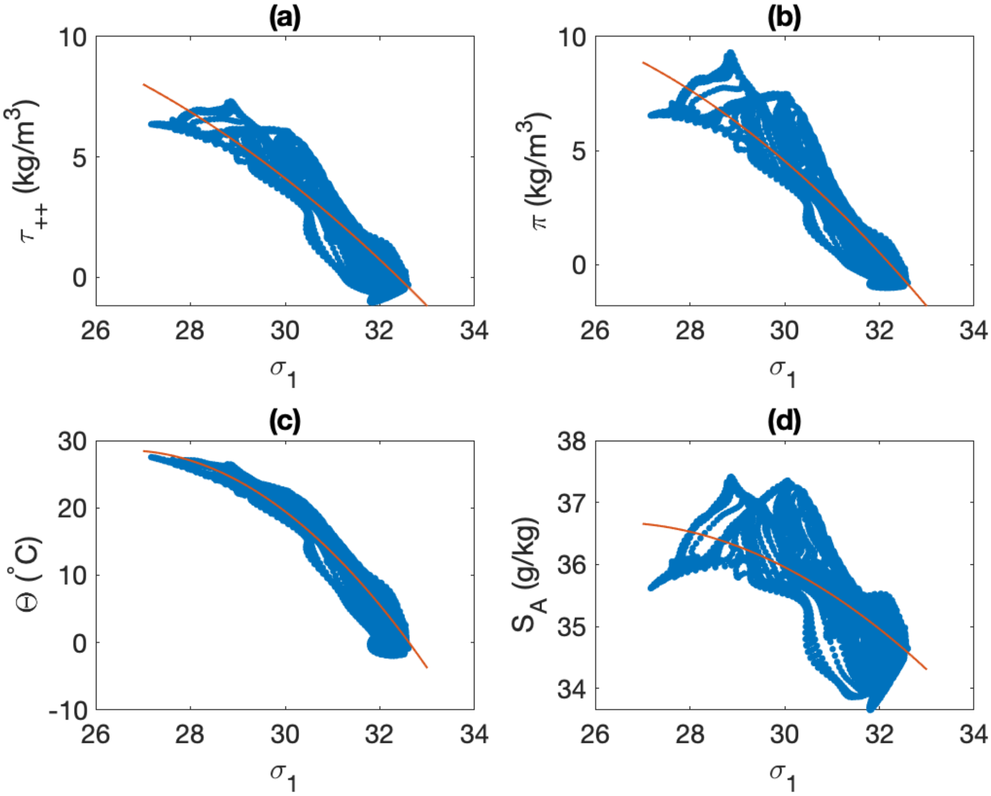

Figure 9. Nonlinear regression between σ_1 and various forms of spiciness state functions estimated for data restricted to the Atlantic section along $30°W$ depicted in Fig. 11: (a) $\tau_{\ddagger}$ defined in this paper, which is similar to McDougall and Krzysik (2015) spiciness variable; (b) Huang et al. (2018) spicity; (c) Conservative Temperature; (d) Absolute Salinity. Both spiciness and spicity potential are referenced to $1000\,\mathrm{dbar}$. The nonlinear regression curve is indicated in red.

Fig. 12 illustrates the consequences of subtracting the polynomial function of σ_1 in (S_A, Θ) space. In the restricted range of σ_1, all isopycnal anomalies are seen to behave similarly. Unlike McDougall and Krzysik (2015) and Huang et al. (2018) variables, which increase with both Θ and S_A, all the spiciness anomalies increase with salinity but decrease with temperature, but very weakly. Removing the function $\xi_r(\gamma)$ from ξ therefore erases many of the differences that may exist between different choices of ξ, an important result that suggests that the particular choice of ξ is not necessarily as important as previously envisioned.

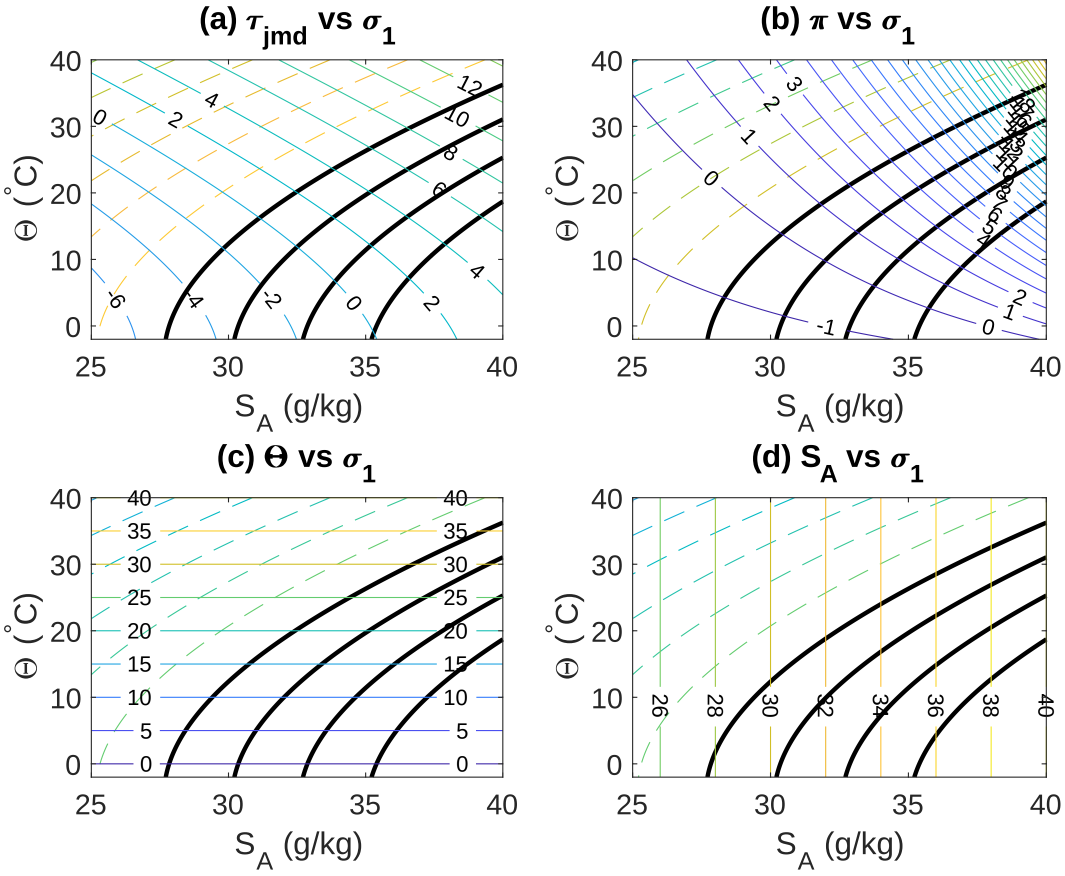

Figure 10. Isocontours of γ and ξ in (S_A, Θ) space for various ξ state functions: (a) McDougall and Krzysik (2015) potential spiciness referenced to 1000 dbar; (b) Huang et al. (2018) potential spicity referenced to 1000 dbar; (c) Conservative Temperature; (d) Absolute Salinity. The black solid lines represent the σ_1 isocontours for 27., 29., 31. and 33 $\mathrm{kg.m^{-3}}$ respectively, corresponding to the restricted range of σ_1 values over which the nonlinear regressions depicted in Fig. 9 were performed. Dashed contour lines correspond to σ_1 isocontours not involved in the nonlinear regression. Thin solid lines represent contours of ξ.

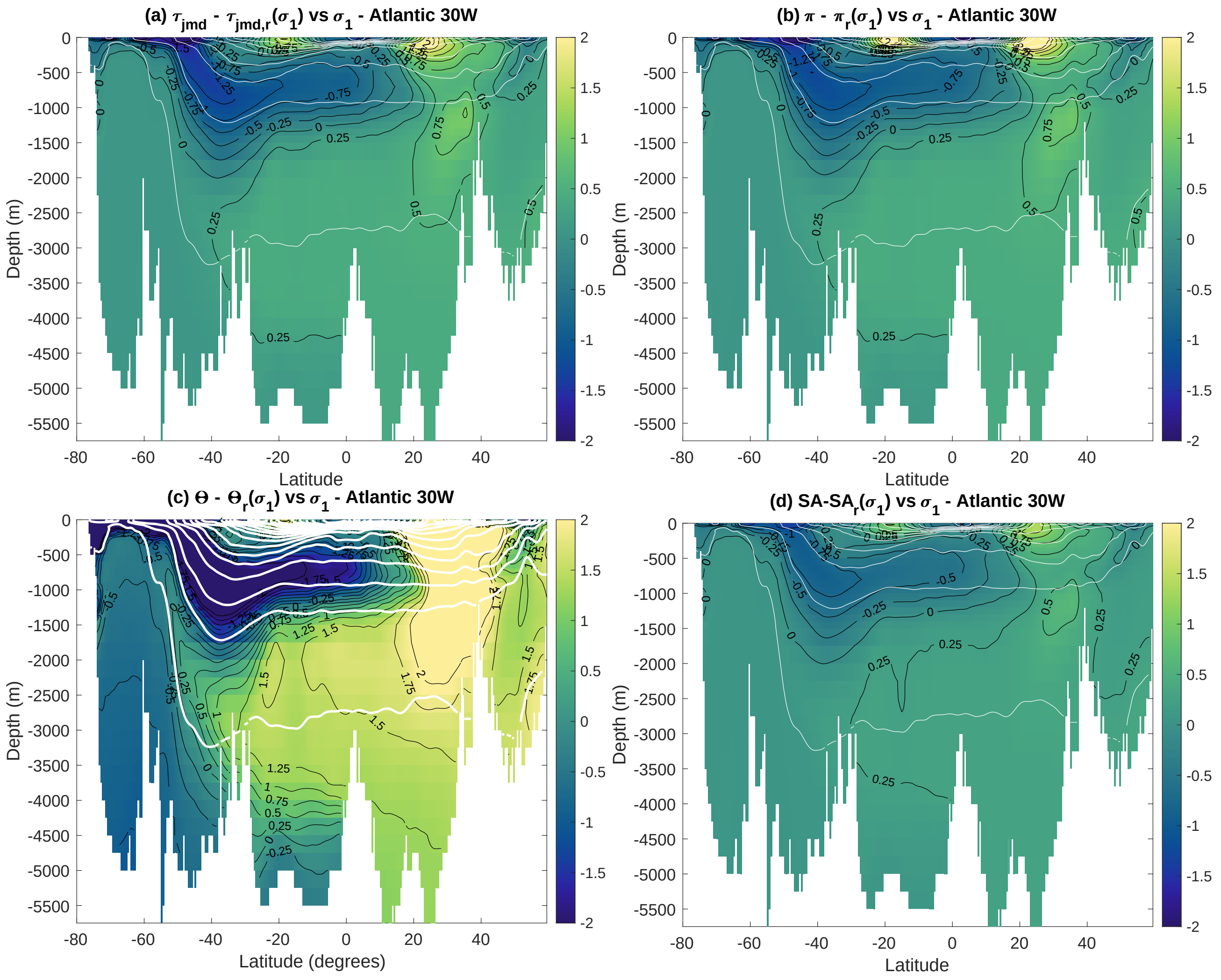

Figure 11. Oceanic sections along $30°W$ of the spiciness anomaly function $\xi' = \xi - \xi_r(\sigma_1)$, with $\xi_r(\sigma_1)$ corresponding to the nonlinear regression function depicted in Fig. 9, for different choices of ξ: (a) McDougall and Krzysik (2015) potential spiciness referenced to 1000 dbar; (b) Huang et al. (2018) potential spicity referenced to 1000 dbar; (c) Conservative Temperature; (d) Absolute Salinity. White solid lines represent selected isopycnal contours for σ_1.

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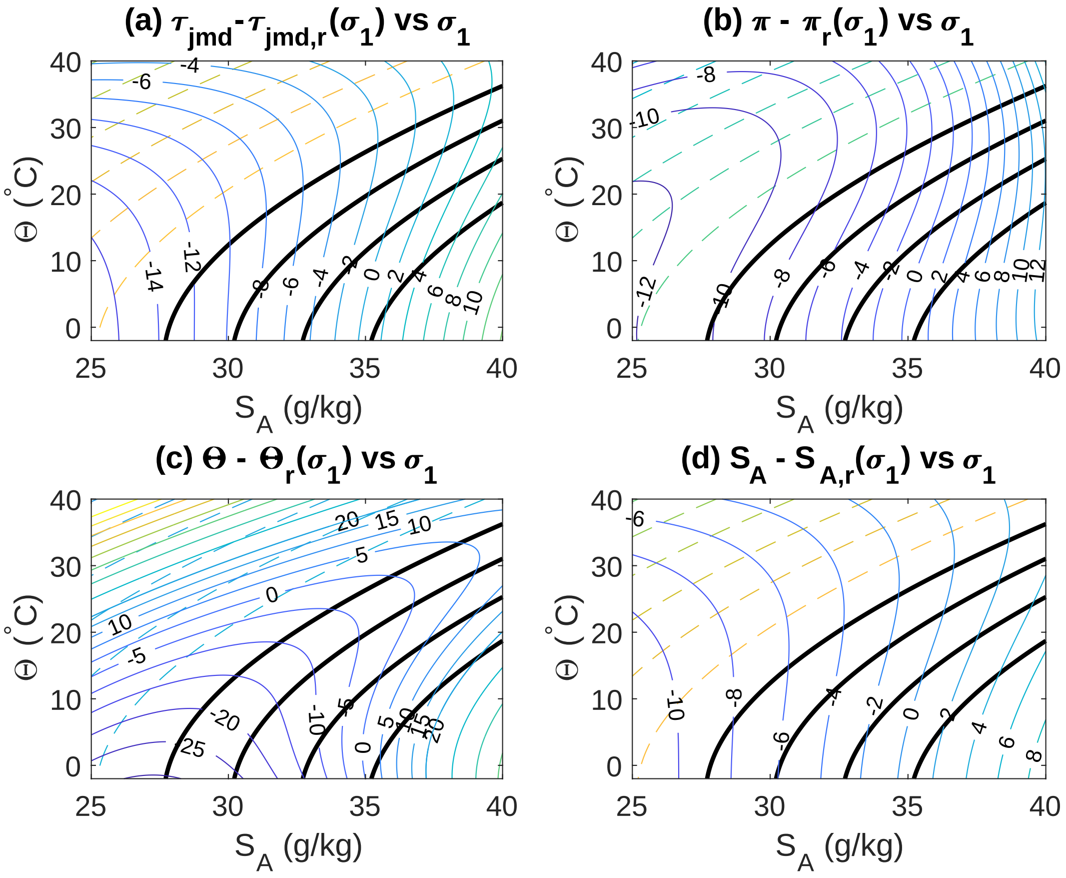

Figure 12. Same as Fig. 10 but showing isocontours of $\xi' = \xi - \xi_r(\sigma_1)$ instead of ξ.

5 Conclusions

In this paper, we have revisited the theory of spiciness and clarified the inter-linkages between different approaches. Our main conclusion is that the theory of spiciness must contain the following ingredients: 1) a quasi-material density like variable $\gamma(S,\theta)$ constructed to be as neutral as feasible; 2) a quasi-material spiciness-as-a-state-function $\xi(S,\theta)$ independent of γ, so that (ξ,γ) can be inverted to recover the (S,θ) properties of any fluid parcel; 3) an empirically defined function $\xi_r(\gamma)$ of γ constructed so that the quasi-material spiciness-as-a-property $\xi' = \xi - \xi_r(\gamma)$, would vanish in an hypothetical spiceless ocean in which all surfaces of constant S, θ and γ would coincide.

Ingredient 1) is required because contrary to what is often assumed, it is not the properties of ξ that determines its degree of dynamical inertness, but the degree of neutrality of γ, regardless of what ξ is. This result is important because it establishes that the theory of spiciness is not independent of the theory of isopycnal analysis; it also establishes for the first time a rigorous physical basis for pursuing the construction of a quasi-material density variable maximising neutrality, as originally pursued by Jackett and McDougall (1997) and subsequently revisited by Eden and Willebrand (1999), and more recently by Tailleux

(2016a, b). Because spiciness is not a substance but a property measuring the various possible variations in thermohaline properties of a fluid parcel of given density, it is important to realise that spiciness-as-a-property is really measured by $\xi' = \xi - \xi_r(\gamma)$ rather than by ξ itself. As is easily realised, one of the key problem with any state function ξ is that there is a priori no reason for it to vanish in a spiceless ocean. One of the most remarkable results of this paper is the fact that visually, plots of ξ' on oceanic sections appear to be rather insensitive to the particular choice of ξ. In particular, we showed that even though τ_{jmd}, π and S_A all look very different from each other in (S_A,Θ) space, τ'_{jmd}, π', and S'_A all very similar to each other both in thermohaline and physical spaces, at least over the restricted range of densities for which they are defined. Since it is ξ', rather than ξ, which provides the most useful quantify for characterising water masses, the need for a dedicated variable such as the one used in this study is unclear, especially since removing $\xi_r(\gamma)$ from ξ completely destroys orthogonality in (S,θ) space. Nevertheless, as the spiciness as-a-state-function variable orthogonal to density in the nonlinear $X(S),Y(\theta)$ coordinates have been extensively used, we provided an analytical expression that mimic the behaviour of McDougall and Krzysik (2015)'s spiciness variable that fully depends on pressure, making it possible to construct a potential spiciness variable referenced to a reference pressure $p_r(S,\theta)$ that is not necessarily constant, as in Tailleux (2016b)'s construction of thermodynamic neutral density.

To make further progress towards a complete theory of water masses, several outstanding issues remain to be resolved. First, how to construct a globally defined material density variable maximising neutrality, which is key to maximise the dynamical inertness of ξ, is still not fully understood. As showed by Tailleux (2016b), the density variable that currently maximises neutrality while also being the only one accounting for thermobaricity is one that is based on Lorenz reference density entering the theory of available potential energy (Tailleux, 2013; Saenz et al., 2015; Tailleux, 2018). This is far from being the last word on the issue, however. Indeed, Tailleux (2016a) recently outlined some new theoretical ideas suggesting that it should be possible, at least in principle, to construct material density-like variables with even better neutrality, as we hope to demonstrate in future work. Second, since ξ' appears to be provide a characterisation of water masses that does not appear to be very sensitive to the particular choice of ξ and $\xi_r(\gamma)$, the question is whether a physical basis or physical arguments can nevertheless be identified in favour of any particular choice? For instance, one could ask the question of whether it is possible to construct ξ and $\xi_r(\gamma)$ so that ξ' is as conservative as possible? Another important question is whether constraining ξ to be orthogonal to γ in thermohaline space, as pursued by McDougall and Krzysik (2015) or Huang et al. (2018), yields any special benefit for ξ'? Hopefully, the present work will help stimulate further research on these issues.

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Competing interests. The author declares no competing interests.

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