Inverse kinetic theory for incompressible thermofluids

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Abstract

An interesting issue in fluid dynamics is represented by the possible existence of inverse kinetic theories (IKT) which are able to deliver, in a suitable sense, the complete set of fluid equations which are associated to a prescribed fluid. From the mathematical viewpoint this involves the formal description of a fluid by means of a classical dynamical system which advances in time the relevant fluid fields. The possibility of defining an IKT for the 3D incompressible Navier-Stokes equations (INSE), recently investigated (Ellero \textit{et al}, 2004-2007) raises the interesting question whether the theory can be applied also to thermofluids, in such a way to satisfy also the second principle of thermodynamics. The goal of this paper is to prove that such a generalization is actually possible, by means of a suitable extended phase-space formulation. We consider, as a reference test, the case of non-isentropic incompressible thermofluids, whose dynamics is described by the Fourier and the incompressible Navier-Stokes equations, the latter subject to the conditions of validity of the Boussinesq approximation.

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I. INTRODUCTION

A remarkable aspect of fluid dynamics is related to the construction of inverse kinetic theories (IKT) for hydrodynamic equations in which the fluid fields are identified with suitable moments of an appropriate kinetic probability distribution. Recently the topic has been the subject of theoretical investigations on the incompressible Navier-Stokes (N-S) equations (INSE) [2, 3, 4, 5, 7]. The importance of the IKT-approach goes beyond the academic interest. In fact, fluid equations represent usually a mixture of hyperbolic and elliptic pde’s, which are extremely hard to study both analytically and numerically. As such, their investigation represents a challenge both for mathematical analysis and for computational fluid dynamics. For this reason in the past alternative approaches, based on asymptotic kinetic theories, have been devised which permit to advance in time the fluid fields, to be determined in terms of suitable moments of an appropriate kinetic distribution function. An example is provided by kinetic theories for incompressible fluids which adopt the so-called Lattice-Boltzmann approach [8] (see also related discussion in Refs. [10, 11]). These methods, which approximate the fluid equations only in an asymptotic sense, are based on the introduction of suitably modified (fluid) equations which permit to advance in time the fluid fields only in an approximate sense. In particular, typically, their modified fluid equations actually describe weakly-compressible fluids. The discovery of IKT [1] provides, however, a new starting point for the theoretical and numerical investigation of hydrodynamic equations, since it does not require any modification of the exact fluid equations, in particular it holds for strong solutions, and permits to advance in time exactly the fluid fields by means of a suitable kinetic distribution function \( f(x,t) \). Here \( x \) is the state vector \( x = (r_1, v_1) \), where respectively \( r_1 \) and \( v_1 \) denote the corresponding ”configuration” and ”velocity” vectors, and \( \Gamma \) is the phase-space spanned by \( x \). In the sequel we shall assume that \( \Gamma \) is an extended phase-space, i.e., it has a dimension \( 2n \) with \( n > 3 \). This is achieved introducing a phase-space classical dynamical system

\[
x_o \to x(t) = T_{t,t_o}x_o,
\]

(1)
which uniquely advances in time the fluid fields by means of an appropriate evolution operator $T_{t,t_o} \ [4, 5]$. This is assumed to be generated by a suitably smooth vector field $X(x,t)$,

$$\frac{d}{dt} x = X(x,t),$$

(2)

$$x(t_o) = x_o,$$

(3)

Therefore, introducing the corresponding microscopic distribution function $f(x,t)$, it fulfills necessarily in $\Gamma$ the differential Liouville equation

$$L f(x,t) = 0,$$

(4)

where $L$ denotes the Liouville streaming operator $L f \equiv \frac{\partial}{\partial t} f + \frac{\partial}{\partial x} \cdot \{X(x,t)f\}$. This equation, which may be interpreted as a Vlasov-type inverse kinetic equation (IKE), can in principle be defined in such a way to satisfy appropriate constraint equations. In particular, thanks to the arbitrariness of the dynamical systems $\Xi$ [i.e., the arbitrariness of $X(x,t)$], the velocity moments of $f(x,t)$ might be identified - in principle - so that suitable velocity moments (of $f$) coincide with the relevant fluid fields characterizing a prescribed classical fluid. For example, as in Refs. $[2, 3, 4, 5, 7]$ one can impose that the first velocity-moment coincides with the fluid mass density, i.e., there results $\rho = \int_{\mathbb{R}^n} dv_1 f(x,t)$.

An interesting issue is whether the theory can be applied also to thermostats. Such a generalization, as shown in an accompanying paper $[10]$, is actually non-unique. In particular, the goal of this paper is to prove that an IKT can be achieved by means of a suitable extended phase-space formulation. We consider, as a reference problem, the case of incompressible thermostats subject, for greater generality, to the condition of non-isentropic flow.

For definiteness, we shall assume that the relevant fluids $\{\rho = \rho_o > 0, V, p \geq 0, T > 0, S_T\}$, i.e., respectively the (constant) mass density, fluid velocity, pressure, temperature and entropy describing the fluid, are defined in an appropriate existence domain. In particular if $\Omega$ is an open connected subset of $\mathbb{R}^3$ (denoted as configuration domain; with prescribed fixed boundary $\delta \Omega$ and closure $\Omega$ defined as the set where the mass density is a constant $\rho_o > 0$) and $I$ a finite time interval $I = [t_0, t_1]$ (with closure $\overline{I} = [t_0, t_1]$), we assume that the fluid fields $\{p, V, T\}$ are continuous in $\overline{\Omega} \times \overline{I}$, satisfy suitable initial and boundary conditions respectively at $t = t_o$ and on $\delta \Omega$, while in the open set $\Omega \times I$ they satisfy the so-called
non-isentropic and incompressible Navier-Stokes-Fourier equations (INSFE), i.e.,

\begin{align}
\nabla \cdot \mathbf{V} &= 0, \quad \text{(5)} \\
\frac{\partial}{\partial t} \mathbf{V} + \mathbf{V} \cdot \nabla \mathbf{V} + \frac{1}{\rho_0} \left[ \nabla p - \mathbf{f} \right] - \nu \nabla^2 \mathbf{V} &= 0, \quad \text{(6)} \\
\frac{\partial T}{\partial t} + \mathbf{V} \cdot \nabla T &= \chi \nabla^2 T + \frac{\nu}{2c_p} \left( \frac{\partial V_i}{\partial x_k} + \frac{\partial V_k}{\partial x_i} \right)^2 + \frac{1}{\rho_0 c_p} J, \quad \text{(7)} \\
\frac{\partial}{\partial t} S_T &\geq 0. \quad \text{(8)}
\end{align}

Here the notation is standard. Thus, Eq.(5) denotes the so-called isochoricity condition, while Eq.(6) is the Navier-Stokes equation in the Boussinesq approximation. Hence, in such a case the force density \( \mathbf{f} \) reads \( \mathbf{f} = \rho_0 g \left(1 - k_p T\right) + \mathbf{f}_1 \), where the first term represents the (temperature-dependent) gravitational force density, while the second one (\( \mathbf{f}_1 \)) the action of a possible non-gravitational externally-produced force. Moreover:

- Eq.(7) is the Fourier equation for the temperature \( T \), to be assumed strictly positive in \( \overline{\Omega} \times \overline{T} \), with \( J \) the quantity of heat generated by external sources per unit volume and unit time (for example, Joule heating). Thus for an isolated fluid there results by definition \( J \equiv 0 \) in \( \overline{\Omega} \times \overline{T} \).

- Eq.(8) defines the so-called 2nd principle for the thermodynamic entropy \( S_T \). For its validity in the sequel we shall assume that there results either everywhere in \( \overline{\Omega} \times \overline{T} \), \( J \equiv 0 \) (thermally-isolated thermofluid) or

\[ \int_\Omega d\mathbf{r} \left( \chi \nabla^2 T + \frac{1}{\rho_0 c_p} J \right) \geq 0 \quad \text{(9)} \]

(externally heated thermofluid).

- In these equations \( g, k_p, \nu, \chi \) and \( c_p \) are all real constants which denote respectively the local acceleration of gravity, the density thermal-dilatation coefficient, the kinematic viscosity, the thermometric conductivity and the specific heat at constant pressure. Thus, by taking the divergence of the N-S equation (5), there it follows the Poisson equation for the fluid pressure \( p \) which reads

\[ \nabla^2 p = -\rho_0 \nabla \cdot \left( \mathbf{V} \cdot \nabla \mathbf{V} \right) + \nabla \cdot \mathbf{f}, \quad \text{(10)} \]

with \( p \) to be assumed non negative and bounded in \( \overline{\Omega} \times \overline{T} \);
Finally, it is assumed that:

- Eqs. (5)-(7) satify a suitable initial-boundary value problem (INSFE problem) and that a smooth (strong) solution exists for the fluid fields \( \{ \rho = \rho_o > 0, \mathbf{V}, p \geq 0, T > 0 \} \);

- the entropy functional \( S_T \) can be defined so that it satisfies the 2nd principle.

II. EXTENDED PHASE-SPACE IKT FOR INCOMPRESSIBLE THERMOFLUIDS

Here we intend to show that an IKT for INSFE can be reached by introducing of a suitable extended phase-space formulation, based on a generalization of the IKT developed previously for the incompressible Navier-Stokes equations [2, 3, 4, 5, 7]. For definiteness, let us introduce the notations

\[
\begin{align*}
\mathbf{r}_1 &= (\mathbf{r}, \vartheta), \\
\mathbf{v}_1 &= (\mathbf{v}, w), \\
\mathbf{X} &= \{\mathbf{v}_1, \mathbf{F}_1(\mathbf{x}, t)\}, \\
\mathbf{F}_1(\mathbf{x}, t) &= \{\mathbf{F}(\mathbf{x}, t), H(\mathbf{x}, t)\}
\end{align*}
\]

where the vectors \( \mathbf{r} \) and \( \mathbf{v} \) span, respectively, the whole configuration domain of the fluid (\( \overline{\Omega} \)) and the 3-dimensional velocity space (\( \mathbb{R}^3 \)). Moreover, \( \vartheta, w \in \mathbb{R} \) are two additional real (hidden) variables, with \( \vartheta \) denoting in particular an ignorable configuration-space variable [both for the fluid fields and the kinetic distribution function \( f(\mathbf{x}, t) \)] defined in a bounded interval \( I_\vartheta = [\vartheta_0, \vartheta_1] \subset \mathbb{R} \). The streaming operator \( L \) in this case reads

\[ L \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + w \frac{\partial}{\partial \vartheta} + \frac{\partial}{\partial \vartheta} \cdot \{\mathbf{F}(\mathbf{x}, t)\} + \frac{\partial}{\partial \vartheta} \{H(\mathbf{x}, t)\}, \]

where \( \mathbf{F}_1(\mathbf{x}, t) = \{\mathbf{F}(\mathbf{x}, t), H(\mathbf{x}, t)\} \) can be interpreted as a mean field force acting on a particle with state \( \mathbf{x} = (\mathbf{r}, \vartheta, \mathbf{v}, w) \). In the sequel we intend to prove that, at least in a suitable finite time-interval \( I \), the fluid fields \( \mathbf{V}, p, T \) can be identified with the velocity moments \( \int_{\mathbb{R}^n} d\mathbf{v}_1 G(\mathbf{x}, t) f(\mathbf{x}, t) \), where respectively \( G(\mathbf{x}, t) = \frac{\mathbf{v}}{\rho_o}, (\mathbf{v} - \mathbf{V})^2/3, mw^2/3\rho_o \) and \( f(\mathbf{x}, t) \) is a properly defined kinetic distribution function. In addition, if the same distribution function \( f(\mathbf{x}, t) \) is strictly positive in the whole set \( \Gamma \times I \) and the statistical entropy functional \( S(f) = -\int_{\Gamma} d\mathbf{x} f(\mathbf{x}, t) \ln f(\mathbf{x}, t) \) exists for all
t ∈ I, we intend to show that the thermodynamic entropy can always be identified with $S(f)$, i.e., that
\[ S_T \equiv S(f). \] (12)

To reach the proof, let us first show that, by suitable definition of the "force" fields $F(x, t)$ and $Q(x, t)$, a particular solution of the the IKE (1) is delivered by the (extended-space) Maxwellian distribution:
\[ f_M(x, t) = \rho \frac{\pi^{3/2} v_{th,p} v_{th,T}}{v_{th}^3} \exp \left\{ -\frac{u^2}{2 v_{th,p}^2} - \frac{w^2}{2 v_{th,T}^2} \right\}. \] (13)

Here $u = v - V(r, t)$ is the relative velocity, while $v_{th,p} = \sqrt{2p_1(r, t)/\rho}$ and $v_{th,T} = \sqrt{2T(r, t)/m}$ denote respectively the pressure and temperature thermal velocities. Furthermore $p_1(r, t) = p_0 + p(r, t)$ is the kinetic pressure. In these definitions, $p_0(t)$ (to be denoted as pseudo-pressure) is an arbitrary strictly positive and suitably smooth function defined in $I$, while the mass $m > 0$ is an arbitrary real constant. The following theorem can immediately be proven:

**Theorem 1 - Local Maxwellian solution for INSFE-IKT** Let us identify respectively the vector and scalar fields $F(x, t)$ and $H(x, t)$ with
\[
F(x, t; f_M) = F_0 + F_1 \tag{14}
\]
\[
H(x, t; f_M) = \frac{w}{2T} K + \frac{w}{2} u \cdot \frac{\partial}{\partial r} \ln T, \tag{15}
\]
where $F_0, F_1$ and $K$ read respectively
\[
F_0(x,t;f_M) = \frac{1}{\rho_o} \mathbf{f} + \frac{1}{2} \mathbf{u} \cdot \nabla \mathbf{V} + \frac{1}{2} \nabla \mathbf{V} \cdot \mathbf{u} + \nu \nabla^2 \mathbf{V}, \tag{16}
\]
\[
F_1(x,t;f_M) = \frac{u}{2p_1} A + \frac{v_{th}^2}{2} \nabla \ln p_1 \left\{ \frac{u^2}{v_{th}^2} - \frac{3}{2} \right\}, \tag{17}
\]
\[
K = \chi \nabla^2 T + \frac{\nu}{2c_p} \left( \frac{\partial V_k}{\partial x_k} + \frac{\partial V_i}{\partial x_i} \right)^2 + \frac{J}{\rho c_p}, \tag{18}
\]
while, denoting $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla$, $A$ reads:
\[
A \equiv \frac{D}{Dt} p_1 = \frac{\partial}{\partial t} p_1 - \mathbf{V} \cdot \left[ \frac{\partial}{\partial t} \mathbf{V} + \mathbf{V} \cdot \nabla \mathbf{V} - \frac{1}{\rho_o} \mathbf{f} - \nu \nabla^2 \mathbf{V} \right]. \tag{19}
\]

It follows that:
1) The local Maxwellian distribution (13) is a solution of the IKE (4) if and only if the fluid fields \( \{\rho = \rho_o > 0, V, p, T\} \) satisfy the fluid equations (5)-(7);

2) The velocity-moment equations obtained by taking the weighted velocity integrals of Eq.(4) with the weights \( G(x, t) = 1, v/\rho_o, (v - V)^2/3, w^2/3 \) deliver identically the same fluid equations (5)-(7).

**PROOF** - First we notice that if the fluid equations (5)-(7) are satisfied identically in \( \Omega \times I \), the proof that (13) is a particular solution of the IKE [Eq.(4)] follows by direct differentiation. The converse implication, i.e., the proof that if (13) is a solution of Eq.(4) then the fluid equations (5)-(7) are satisfied identically in \( \Omega \times I \), follows by evaluating the velocity moments of Eq.(26) for the weights \( G = 1, v, (v - V)^2/3, w^2/3 \). In analogy to the case of isothermal fluids the present theorem can be generalized to suitably smooth non-Maxwellian initial distribution function [3]. In such a case the fields \( F_0, F_1 \) and \( H \) read respectively

\[
F_0(x; t; f) = \frac{1}{\rho_o} \left[ \nabla \cdot \Pi - \nabla p_1 + f \right] + u \cdot \nabla V + v \nabla^2 V, \tag{20}
\]

\[
F_1(x; t; f) = \frac{1}{2} u \left\{ \frac{1}{p_1} A + \frac{1}{p_1} \nabla \cdot Q - \frac{1}{p_f} \left[ \nabla \cdot \Pi \right] Q \right\} + \frac{v_{th}^2}{2p_1} \nabla \cdot \left\{ \frac{u^2}{v_{th}^2} - \frac{3}{2} \right\}, \tag{21}
\]

while the scalar field \( H(x, t; f) \) now reads

\[
H(x, t; f) = \frac{w}{2T} K_1 + \frac{w}{2} u \frac{\partial}{\partial r} \ln T. \tag{22}
\]

Here \( K_1 \) denotes the scalar function \( K_1 = K - [\Phi_T \cdot \nabla \ln T + \nabla \cdot (V_T T) - V \cdot \nabla T] \), where \( K \) is defined by Eq.(18) and furthermore the moments \( Q, \Pi, \Phi_T \) and \( V_T \) are defined respectively as \( Q = \int d^3v d\omega w^2 f, \Pi = \int d^3v d\omega u f, \Phi_T = \int d^3v d\omega w^2 u f \) and \( V_T = \frac{1}{\rho_o} \int d^3v d\omega w^2 v f \).

### III. H -THEOREM AND THE 2ND PRINCIPLE OF THERMODYNAMICS

In this section we want to prove that, provided the pseudo-pressure \( p_0(t) \) is suitably defined (i.e., is a uniquely-prescribed function of time), an H Theorem can be established for the statistical entropy \( S(f) = -\int_\Gamma dxf \ln f \), which warrants the strict positivity of the kinetic distribution function in the whole set \( \Gamma \times I \). As a further consequence, the position (12) holds too. For this purpose we distinguish between isothermal and non-isothermal fluids, i.e., fluids in which the fluid temperature is respectively a constant in the whole set \( \Omega \times I \), or not. In particular, we intend to prove that, in the first case (isothermal...
fluid), a constant H-theorem holds for the statistical entropy under suitable conditions, i.e., by suitably prescribing the pseudo-pressure. Instead, to reach an H-theorem for a non-isothermal fluid, it is necessary to include also a suitable prescription on the r.h.s. of the Fourier equation [and in particular on the scalar field \( J \); see Eq. (11)], which defines the quantity of heat generated by external sources. In both cases, the result can be proven to hold at least in a finite time interval \( I \) and for an arbitrary strictly positive (and suitably summable) distribution function \( f \).

**Theorem 2 - H-theorem** Let us assume that: 1) \( \Omega \) is a bounded subset of \( \mathbb{R}^3 \); 2) the kinetic distribution function \( f \) coincides identically in \( \Omega \times I \) with the local Maxwellian distribution \( f_M \) defined by Eq. (13). Furthermore, let us distinguish respectively the cases in which the fluid is isothermal in \( \Omega \times I \) or not. In the first case we demand that the following assumption is fulfilled: 3) the pseudo-pressure \( p_0(t) \) is \( p_0(t) > 0 \) determined in such a way to satisfy identically \( \forall t \in I \) the constraint

\[
\int_{\Omega} \frac{d\mathbf{r}}{p_1} \left[ \frac{\partial}{\partial t} p_1 + \nabla \cdot \mathbf{Q} - \frac{1}{p_1} \nabla p \cdot \mathbf{Q} \right] = 0. \tag{23}
\]

Instead, for non-isothermal fluids, we require that the following two assumptions are satisfied (3B and 4): 3B) the pseudo-pressure \( p_0(t) \) is \( p_0(t) > 0 \) and satisfies identically \( \forall t \in I \) the constraint

\[
\frac{3}{2} \rho_o \int_{\Omega} \frac{d\mathbf{r}}{p_1} \left[ \frac{\partial}{\partial t} p_1 + \nabla \cdot \mathbf{Q} - \frac{1}{p_1} \nabla p \cdot \mathbf{Q} \right] - \frac{1}{2} \rho_o \int_{\Omega} \frac{d\mathbf{r}}{T} \left[ \Phi_T \cdot \nabla \ln T + \nabla \cdot (\mathbf{V}_T T) \right] = 0; \tag{24}
\]

4) the quantity of heat generated by external sources \( J \), either vanishes identically in \( \Omega \times T \) (isolated fluid) or \( \forall t \in I \) is externally heated in the sense of the inequality (9).

Then it follows respectively: A) for isothermal fluids: the statistical entropy \( S(f) \) is constant, i.e., there holds identically the constant H-theorem:

\[
\frac{\partial}{\partial t} S(f) = 0; \tag{25}
\]

B) for non-isothermal fluids: the statistical entropy \( S(f) \) is a monotonic function of time, i.e., it holds, instead, the H-theorem \( \forall t \in I \)

\[
\frac{\partial}{\partial t} S(f) \geq 0. \tag{26}
\]
PROOF - For definiteness let us first consider an isothermal fluid, i.e., requiring $T = \text{const.}$ in $\Omega \times T$. In this case the proof of Eq.(25) is immediate. In fact for an arbitrary, suitably smooth and non-vanishing, non-Maxwellian distribution the entropy production rate $\frac{\partial}{\partial t} S(f)$ results

$$\frac{\partial}{\partial t} S(f) = -\frac{\partial}{\partial t} \int dxf \ln f =$$

$$= \frac{3}{2} \rho_o \int_{\Omega} d\mathbf{r} \frac{1}{p_1} \left[ \frac{\partial}{\partial t} p_1 + \nabla \cdot \mathbf{Q} - \frac{1}{p} \nabla p \cdot \mathbf{Q} \right],$$

which thanks to the constraint equation Eq.(23) for $p_0(t)$ vanishes identically. In particular, in the case in which the kinetic distribution function $f$ coincides with the local Maxwellian distribution (4) the same equation delivers

$$\frac{\partial}{\partial t} S(f) = \frac{3}{2} \rho_o \int_{\Omega} d\mathbf{r} \frac{1}{p_1} \left[ \frac{\partial}{\partial t} p_0(t) + \nabla \cdot \mathbf{Q} - \frac{1}{p} \nabla p \cdot \mathbf{Q} \right],$$

Let us now consider the case of a non-isothermal fluid obeying the fluid equations (5)-(7). In this case, imposing on $p_0(t)$ the constraint (24) the entropy production rate reads

$$\frac{\partial}{\partial t} S(f) = \frac{3}{2} \rho_o \int_{\Omega} d\mathbf{r} \frac{1}{p_1} \left[ \frac{\partial}{\partial t} p_0(t) + p_r(t) \right] = 0. \quad (28)$$

Hence, for a fluid which is either isolated or subject to external heating, in the sense of the inequality (9), the H-theorem (26) manifestly holds.

This result is consistent with the second principle if thermodynamics [i.e., the inequality (8)]. As a consequence, this enables us to specify also the thermodynamic entropy in terms of a suitable phase-space moment of the kinetic distribution function $f$.

IV. CONCLUDING REMARKS

A basic implication of the IKT here developed for INSFE is that it has been constructed in such a way to satisfy the following requirements:

1. **completeness**: all fluid fields are expressed as moments of the kinetic distribution function and all hydrodynamic equations can be identified with suitable moment equations of IKE;

2. **closure condition of moment equations**: there must exist a subset of moments of IKE which form a complete system of equations, to be identified with the prescribed set of hydrodynamic equations;
3. **smoothness for the fluid fields**: the fluid fields are assumed suitably smooth so that the solution of the kinetic distribution function exists everywhere in a suitable phase-space;

4. **arbitrary initial and boundary conditions for the fluid fields**: the initial conditions for the fluid equations are set arbitrarily while Dirichlet boundary conditions are considered on the boundary;

5. **self-consistency**: the kinetic theory holds for arbitrary (and suitably smooth) initial conditions for the kinetic distribution function.

6. **non-asymptotic IKE**: i.e., the correct hydrodynamic equations must be recovered by the inverse kinetic theory independently of any dimensionless parameter.

The present approach has the following main features:

1. a suitable classical dynamical system has been constructed which uniquely determines the evolution of the fluid fields;

2. the IKT is based on an extended phase-space formulation which relies of the microscopic statistical description of the dynamical system;

3. the theory satisfies the second principle of thermodynamics.

An interesting result of the theory, relevant for the mathematical investigation of the fluid equations, concerns the discovery of the underlying dynamical system, i.e., the phase-space classical dynamical system (10). We have found that this can be identified with a - generally non-conservative - dynamical system advancing in time the microscopic distribution function and generated by the kinetic equation itself. The evolution of the fluid fields is thus determined uniquely by this dynamical system, a result that in principle may be achieved without solving explicitly the fluid equations themselves.

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**Notice**

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