Principle of Maximum Entropy Applied to Rayleigh-Bénard Convection

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A statistical-mechanical investigation is performed on Rayleigh-Bénard convection of a dilute classical gas starting from the Boltzmann equation. We first present a microscopic derivation of basic hydrodynamic equations and an expression of entropy appropriate for the convection. This includes an alternative justification for the Oberbeck-Boussinesq approximation. We then calculate entropy change through the convective transition choosing mechanical quantities as independent variables. Above the critical Rayleigh number, the system is found to evolve from the heat-conducting uniform state towards the convective roll state with monotonic increase of entropy on the average. Thus, the principle of maximum entropy proposed for nonequilibrium steady states in a preceding paper [T. Kita: J. Phys. Soc. Jpn. 75 (2006) 114005] is indeed obeyed in this prototype example. The principle also provides a natural explanation for the enhancement of the Nusselt number in convection.

I. INTRODUCTION

In a preceding paper, we have proposed a principle of maximum entropy for nonequilibrium steady states: The state which is realized most probably among possible steady states without time evolution is the one that makes entropy maximum as a function of mechanical variables. We here apply it to Rayleigh-Bénard convection of a dilute classical gas to confirm its validity.

Rayleigh-Bénard convection is a prototype of nonequilibrium steady states with pattern formation, and extensive studies have been carried out to clarify it. However, no calculation seems to have been performed on entropy change through the nonequilibrium “phase transition,” despite the fact that entropy is the key concept in equilibrium thermodynamics and statistical mechanics. There may be at least four reasons for it. First, there seems to have been no established expression of nonequilibrium entropy. Second, the standard starting point to describe Rayleigh-Bénard convection is a set of deterministic equations for the particle, momentum and energy flows, with all the thermodynamic effects pushed into phenomenological parameters of the equations. Third, one additionally adopts the Oberbeck-Boussinesq approximation to the equations in the conventional treatment. Despite many theoretical efforts over a long period, a well-accepted systematic justification for it seems still absent, thereby preventing a quantitative estimation of entropy change. Fourth, there is ambiguity on what to choose as independent variables of entropy for open systems.

In a preceding paper, we have derived an expression of nonequilibrium entropy together with the evolution equations for interacting bosons/fermions. We here apply them to a classical gas of the dilute high-temperature limit where the evolution equations reduce to the Boltzmann equation. We carry out a microscopic derivation of the hydrodynamic equations for the particle, momentum and energy densities (i.e., the basic conservation laws) from the Boltzmann equation. We then provide a systematic justification for the Oberbeck-Boussinesq approximation to describe the convection. With these preliminaries, we perform a statistical-mechanical calculation of entropy change through the convective transition by choosing mechanical quantities as independent variables. It is worth pointing out that classical gases have been used extensively for detailed experiments on Rayleigh-Bénard convection over the last two decades. Thus, quantitative comparisons between theory and experiment are possible here.

This paper is organized as follows. Section II derives (i) equations of motion for the particle, momentum and energy densities and (ii) an explicit expression for the distribution function $f$, both starting from the Boltzmann equation. Section III reduces the equations of II in a way appropriate to treat Rayleigh-Bénard convection of a dilute classical gas. This includes a systematic justification of the Oberbeck-Boussinesq approximation and a derivation of the expression of entropy for convection. Section IV transforms the equations of III into those suitable for periodic structures with the stress-free boundaries. Section V presents numerical results obtained by solving the equations of IV. It is shown explicitly that the principle of maximum entropy is indeed obeyed by the convection. Concluding remarks are given in VI.

II. DISTRIBUTION FUNCTION, CONSERVATION LAWS AND ENTROPY

A. The Boltzmann equation and entropy

We shall consider a monatomic dilute classical gas under gravity. This system may be described by the Boltzmann equation:

$$ \frac{\partial f}{\partial t} + \frac{p}{m} \cdot \frac{\partial f}{\partial r} - mg \frac{\partial f}{\partial z} = C. $$

(1)

Here $f = f(p, r, t)$ is the distribution function, $t$ the time, $p$ the momentum, $m$ the mass, $r$ the space coordinate, and $g$ the acceleration of gravity. With a unified description of classical and quantum statistical mechanics in mind, we choose the normalization of $f$ such that it is

$$ \int f(p, r, t) dp \, dr \, dz = 1. $$

(2)

This provides a well-accepted principle for the normalization of the distribution function $f$.
The collision integral $\mathcal{C}$ is given explicitly by

$$
\mathcal{C}(\mathbf{p}, \mathbf{r}, t) = \frac{\hbar^2}{(2\pi)^3} \int \frac{d^3p_1}{(2\pi)^3} \int \frac{d^3p_1'}{(2\pi)^3} \int \frac{d^3p_1''}{(2\pi)^3} V_{\mathbf{q}}^* \delta(p - p_1 - p_1' + p_1'') f(p, p_1) f(p, p_1') f(p, p_1'') f(p, p_1'') \delta(p_1' + p_1' - p_1) \delta(p_1'' + p_1' - p_1),
$$

where $V_{\mathbf{q}}$ is Fourier transform of the interaction potential and $E_p = p^2/2m$.

Equation (2) also results from eq. (63) of ref. [1] as follows: (i) approximate the spectral function as $A(p_1, r) = 2\pi\delta(\varepsilon_E - E_p - mgz)$; (ii) substitute the second-order self-energy of eq. (66) into the collision integral of eq. (64); (iii) take the high-temperature limit; and (iv) integrate eq. (63) over $\varepsilon$ to obtain an equation for

$$
f(\mathbf{p}, \mathbf{r}, t) = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} A(p_1, rt) \phi(p_1, rt).
$$

This whole procedure amounts to treating the interaction potential only as the source of dissipation in the dilute high-temperature limit; and naturally results from the Boltzmann equation.

With a change of variables $p_1 = p + q$, $p_1' = p - q/2$ and $p_1'' = p + q/2$ in eq. (2), the collision integral is transformed into

$$
\mathcal{C} = \int \frac{d^3q}{(2\pi)^3} \frac{q}{m} \int d\sigma \left[ f(p + (q - q)/2) f(p + (q + q)/2) - f(p) f(p + q) \right],
$$

where $d\sigma = d\Omega_q' \int dq' \delta(q' - q) [m|V(q' - q)/2|/4\pi\hbar^2]^2$ is the differential cross section in the center-of-mass coordinate of the scattering with $d\Omega_q'$ denoting the infinitesimal solid angle. We shall use the contact interaction with no $\mathbf{q}$ dependence in $V_{\mathbf{q}}$, where $d\sigma$ reduces to

$$
d\sigma = a^2 d\Omega_q' \int dq' \delta(q' - q),
$$

with $a = m|V|/4\pi\hbar^2$ denoting the scattering length. Now, the differential cross section acquires the form of the two-particle collision between hard-sphere particles with radius $a$.\footnote{Entropy per unit volume is given in terms of $f$ by

$$
S = -\frac{k_B}{V} \int \frac{d^3r d^3p}{(2\pi)^3} f((\log f) - 1),
$$

with $V$ denoting the volume. This expression also results from eq. (69) of ref. [1] for entropy density by: (i) adopting the quasiparticle approximation $A(p_1, rt) = 2\pi\delta(\varepsilon_E - E_p - mgz)$; (ii) defining $f$ by eq. (3) above; (iii) taking the high-temperature limit; and (iv) performing integration over $r$. The term $-1$ in the integrand of eq. (3) is absent in the Boltzmann $H$-function\footnote{The collision integral is also related to the differential cross section in the center-of-mass coordinate of the scattering with $d\Omega_q'$ denoting the infinitesimal solid angle.} but naturally results from the procedure (iii) above. Indeed, eq. (3) reproduces the correct expression of entropy in equilibrium.\footnote{This whole procedure amounts to treating the interaction potential only as the source of dissipation in the dilute high-temperature limit; and naturally results from the Boltzmann equation.}}

### B. Conservation laws

We next consider conservation laws which originate from the Boltzmann equation. The basic physical quantities relevant to them are the density $n(r, t)$, the velocity $v(r, t)$, the temperature $T(r, t)$, the momentum flux density tensor $\Pi(r, t)$ in the reference frame moving with the local velocity $v$, and the heat flux density $j_Q(r, t)$. They are defined by

$$
n(r, t) = \int \frac{d^3p}{(2\pi)^3} f(\mathbf{p}, \mathbf{r}, t),
$$

$$
v(r, t) = \frac{1}{n(r, t)} \int \frac{d^3p}{(2\pi)^3} \frac{p}{m} f(\mathbf{p}, \mathbf{r}, t),
$$

$$
T(r, t) = \frac{2}{3k_B n(r, t)} \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{2m} f(\mathbf{p}, \mathbf{r}, t),
$$

$$
\Pi(r, t) = \int \frac{d^3p}{(2\pi)^3} \frac{pp}{2m} f(\mathbf{p}, \mathbf{r}, t),
$$

$$
j_Q(r, t) = \int \frac{d^3p}{(2\pi)^3} \frac{\rho^2}{2m} \frac{\rho}{m} f(\mathbf{p}, \mathbf{r}, t),
$$

with $\rho = p - mv$. The expressions (4a-4c) also result from eqs. (C.1a), (C.1b), (C.20a), (C.14) and (C.20b) of ref. [1], respectively, by noting eq. (3), neglecting the interaction terms, and identifying the local internal-energy density $\hat{E}$ as $\hat{E} = \frac{3}{2} n k_B T$. To obtain the number, momentum and energy conservation laws, let us multiply eq. (4) by $p$ and $p^2/2m$, respectively, and perform integration over $p$. The contribution from the collision integral (2) vanishes in all the three cases due to the particle, momentum and energy conservations through the collision.\footnote{The collision integral is also related to the differential cross section in the center-of-mass coordinate of the scattering with $d\Omega_q'$ denoting the infinitesimal solid angle.} The resulting hydrodynamic equations can be written in terms of the quantities of eq. (7) as

$$
\frac{\partial n}{\partial t} + \nabla (nv) = 0,
$$

$$
\frac{\partial v}{\partial t} + v \cdot \nabla v + \frac{1}{mn} \nabla \Pi + ge_z = 0,
$$

$$
\frac{3}{2} n k_B \left( \frac{\partial T}{\partial t} + v \cdot \nabla T \right) + \nabla \cdot j_Q + \Pi : \nabla v = 0,
$$

where $e_z$ is the unit vector along the $z$ axis and $A \cdot \vec{B}$ denotes the tensor product: $A \cdot \vec{B} \equiv \sum_i A_i B_{ji}$. These equations are identical in form with eqs. (C.2), (C.9) and (C.21) of ref. [1], respectively, with $\hat{U} = mgz$ and $\hat{E} = \frac{3}{2} n k_B T$.\footnote{Entropy per unit volume is given in terms of $f$ by

$$
S = -\frac{k_B}{V} \int \frac{d^3r d^3p}{(2\pi)^3} f((\log f) - 1),
$$

with $V$ denoting the volume. This expression also results from eq. (69) of ref. [1] for entropy density by: (i) adopting the quasiparticle approximation $A(p_1, rt) = 2\pi\delta(\varepsilon_E - E_p - mgz)$; (ii) defining $f$ by eq. (3) above; (iii) taking the high-temperature limit; and (iv) performing integration over $r$. The term $-1$ in the integrand of eq. (3) is absent in the Boltzmann $H$-function but naturally results from the procedure (iii) above. Indeed, eq. (3) reproduces the correct expression of entropy in equilibrium.}
The Enskog series

We now reduce the whole procedures of solving eq. [11] for \((p, r, t)\) to those of solving eq. [8] for \(r, t\). We adopt the well-known Enskog method\(^{16,17}\) for this purpose, i.e., the expansion from the local equilibrium. We here describe the transformation to the extent necessary for a later application to Rayleigh-Bénard convection.

Let us expand the distribution function formally as

\[
    f(p, r, t) = f^{(eq)}(p, r, t) \left[1 + \varphi^{(1)}(p, r, t) + \cdots\right],
\]

where \(f^{(eq)}\) is the local-equilibrium distribution given explicitly by

\[
    f^{(eq)} = \frac{(2\pi\hbar)^4}{(2\pi m k_B T)^{3/2}} \exp\left(-\frac{\bar{p}^2}{2mk_BT}\right),
\]

with \(\bar{p} \equiv p - mv\). This \(f^{(eq)}\) has been chosen so as to satisfy the two conditions\(^{16,17}\): (i) the local equilibrium condition that the collision integral vanishes; (ii) eqs. [10]-[12] by itself. It hence follows that the higher-order corrections \(\varphi^{(j)} (j=1, 2, \ldots)\) in eq. [9] should obey the constraints:

\[
    \int \frac{d^3 p}{(2\pi\hbar)^3} p^n f^{(eq)} \varphi^{(j)} = 0 \quad (n=0, 1, 2). \tag{11}
\]

Note that we have incorporated five space-time dependent parameters in \(f^{(eq)}\), i.e., \(n, v\) and \(T\), which can be determined completely with eqs. [8]-[10] of conservation laws.

The remaining task here is to express the extra quantities \(\Pi\) and \(j_Q\) in eq. [8] as functionals of \(n, v\) and \(T\).

Let us substitute eq. [9] into eq. [11], regard the space-time differential operators on the left-hand side as first-order quantities, and make use of the fact that the collision integral \(\Pi\) vanishes for \(f^{(eq)}\). We thereby arrive at the first-order equation:

\[
    \frac{\partial f^{(eq)}}{\partial t} + \frac{p}{m} \cdot \frac{\partial f^{(eq)}}{\partial r} + \frac{p^2}{k_BT} f^{(eq)} = C^{(1)}, \tag{12}
\]

where \(C^{(1)}\) is obtained from eq. [11] as

\[
    C^{(1)} = \int \frac{d^3 q}{(2\pi\hbar)^3} q \int d\sigma f_{p+q}^{(eq)} f_{p+q}^{(eq)}
    \times \left[\varphi^{(1)}_{p+q} + \varphi^{(1)}_{p+q}/2 - \varphi^{(1)}_p - \varphi^{(1)}_{p+q}\right]. \tag{13}
\]

With eq. [10], the derivatives of \(f^{(eq)}\) in eq. [12] are transformed into those of \(n, v\) and \(T\). We then remove the time derivatives by using eq. [8] in the local-equilibrium approximation, where

\[
    \Pi^{(eq)} = P_1, \quad j_{Q}^{(eq)} = 0, \tag{14}
\]

with \(P = nk_BT\) the pressure and \(I\) the unit tensor. The left-hand side of eq. [12] is thereby transformed into

\[
    \frac{\partial f^{(eq)}}{\partial t} + \frac{p}{m} \cdot \frac{\partial f^{(eq)}}{\partial r} + \frac{p^2}{k_BT} f^{(eq)}
    = f^{(eq)} \left[2 \left(\kappa k - \frac{k^2}{3}\right) \cdot \nabla v + \left(\kappa^2 - \frac{5}{2}\right) \bar{p} \cdot \nabla \ln T\right], \tag{15}
\]

with \(\kappa\) a dimensionless quantity defined by

\[
    \kappa \equiv \bar{p}/\sqrt{2mk_BT}. \tag{16a}
\]

It is convenient to introduce the additional dimensionless quantities:

\[
    \hat{v} \equiv \sqrt{\frac{m}{2k_BT}} v, \quad \hat{r} \equiv n^{1/3} r, \tag{16b}
\]

and the mean-free path:

\[
    l \equiv \frac{1}{4\sqrt{2\pi n^2}}. \tag{17}
\]

Using eqs. [16] and [17] and noting eqs. [8], [10], [18] and [19], we can transform eq. [12] into the dimensionless form:

\[
    \frac{2\sqrt{2}}{\sqrt{\pi n^{1/3}}} \int \frac{d^3 q}{4\pi} \int \frac{d^3 q'}{4\pi} \frac{q}{q'} e^{-\kappa^2-(k+q)^2}
    \times \left[\varphi^{(1)}_{k+(q'-q)/2} + \varphi^{(1)}_{k+(q+q')/2} - \varphi^{(1)}_k - \varphi^{(1)}_{k+q}\right]
    = e^{-\kappa^2} \left[2 \left(\kappa k - \frac{k^2}{3}\right) \cdot \nabla \hat{v} + \left(\kappa^2 - \frac{5}{2}\right) \bar{p} \cdot \nabla \ln T\right], \tag{18}
\]

where \(\nabla \equiv \partial/\partial \hat{r}\), and we have redefined \(\varphi^{(1)}\) as a function of \(k \equiv \bar{p}/\sqrt{2mk_BT}\). Similarly, eq. [11] now reads

\[
    \int d^3 k e^{-\kappa^2} \Pi_k^{(eq)} \varphi_k^{(1)} = 0 \quad (n=0, 1, 2). \tag{19}
\]

Equation [18] with subsidiary condition [19] forms a linear integral equation for \(\varphi_k^{(1)}\).

The right-hand side of eq. [18] suggests that we may seek the solution in the form\(^{16,17}\)

\[
    \varphi_k^{(1)} = -ln^{1/3} \left[A^{5/2}(\kappa) \left(\kappa k - \frac{k^2}{3}\right) \cdot \nabla \hat{v}
    + A^{3/2}(\kappa) \kappa \cdot \nabla \ln T\right], \tag{20}
\]

where \(A^{5/2}\) and \(A^{3/2}\) are two unknown functions; the use of fractions \(n=5/2\) and \(3/2\) to distinguish them will be rationalized shortly. Substituting eq. [20] into it, we can transform eq. [18] into separate equations for \(A^n\) as

\[
    \frac{2\sqrt{2}}{\sqrt{\pi}} \int \frac{d^3 q}{4\pi} \int \frac{d^3 q'}{4\pi} \frac{q}{q'} e^{-\kappa^2-(k+q)^2}
    \times \left[T_k^{(1)} + T_{k+q}^{(1)} - T_{k+(q'-q)/2}^{(1)} - T_{k+(q+q')/2}^{(1)}\right]
    = e^{-\kappa^2} R_k^n, \tag{21}
\]

where \(A^{5/2}\) and \(A^{3/2}\) are two unknown functions; the use of fractions \(n=5/2\) and \(3/2\) to distinguish them will be rationalized shortly. Substituting eq. [20] into it, we can transform eq. [18] into separate equations for \(A^n\) as

\[
    \frac{2\sqrt{2}}{\sqrt{\pi}} \int \frac{d^3 q}{4\pi} \int \frac{d^3 q'}{4\pi} \frac{q}{q'} e^{-\kappa^2-(k+q)^2}
    \times \left[T_k^{(1)} + T_{k+q}^{(1)} - T_{k+(q'-q)/2}^{(1)} - T_{k+(q+q')/2}^{(1)}\right]
    = e^{-\kappa^2} R_k^n, \tag{21}
\]
where tensor $R^\alpha_\ell$ and $T^\alpha_\ell$ are defined in Table I together with another tensor $W^\alpha_\ell$. Since the factor $e^{-k^2}$ is present on the right-hand side of eq. (21), we expand $A^\alpha(\varepsilon)$ further in the Sonine polynomials $S^\alpha(\varepsilon)$ as:

$$A^\alpha(\varepsilon) = \sum_{\ell=0}^{\infty} c^\alpha_\ell S^\alpha_\ell(\varepsilon).$$  \hspace{1cm} (22)

Use of two different complete sets $\{S^\alpha_\ell\}_\ell$ ($\alpha = 5/2, 3/2$) is only for convenience to transform the right-hand side of eq. (21) into a vector with a single nonzero element. With eq. (20) and (22) and the orthogonality of $S^\alpha_\ell(\varepsilon)$, we find that the constraint (19) reduces to the single condition:

$$c^\alpha_0 = 0.$$  \hspace{1cm} (23)

We hence remove the $\ell=0$ term of $\alpha = 3/2$ from eq. (22) in the subsequent discussion. We now take the tensor $\alpha = 5/2$ or the vector $\alpha = 3/2$ product of eq. (21) with $S^\alpha_\ell(k^2)W^\alpha_\ell/k^4\pi$ and perform integration over $k$. Equation (21) is thereby transformed into an algebraic equation for the expansion coefficients $\{c^\alpha_\ell\}_\ell$ as

$$\sum_{\ell'} T^\alpha_{\ell\ell'} c^\alpha_{\ell'} = R^\alpha_\ell.$$  \hspace{1cm} (24)

Here $R^\alpha_\ell$ is defined by

$$\begin{align*}
R^\alpha_\ell &\equiv \int \frac{d^3k}{4\pi} e^{-k^2} S^\alpha_\ell(k^2) (W^\alpha_\ell(k), R^\alpha_\ell(k)) \\
&= \begin{cases} \\
\frac{5}{4\sqrt{\pi}} \delta_{00} : \alpha = 5/2 \\
-\frac{15}{16\sqrt{\pi}} \delta_{11} : \alpha = 3/2,
\end{cases} \hspace{1cm} (25)
\end{align*}$$

with $(W, R) \equiv W : R$ and $W \cdot R$ for $\alpha = 5/2$ and $3/2$, respectively. Also, $T^\alpha_{\ell\ell'}$ is obtained with a change of variable $k \to k - q/2$ in the $k$ integral as

$$T^\alpha_{\ell\ell'} = \frac{2\sqrt{3}}{\sqrt{\pi}} \int_0^\infty dk e^{-2k^2} \int_0^\infty dq e^{-q^2/2} q^3 \int_0^\infty dq' \delta(q'-q)$$

$$\times [I^\alpha_{\ell\ell'}(k, q, q) + I^\alpha_{\ell\ell'}(k, q, -q) - 2I^\alpha_{\ell\ell'}(k, q, q')] ,$$  \hspace{1cm} (26)

with $I^\alpha_{\ell\ell'}(k, q, q')$ defined by

$$I^\alpha_{\ell\ell'}(k, q, q') \equiv \int \frac{d\Omega_k}{4\pi} \int \frac{d\Omega_{k'}}{4\pi} S^\alpha_\ell((k-q/2)^2) S^\alpha_\ell((k-q'/2)^2)$$

$$\times (W^\alpha_{k-q/2}, W^\alpha_{k-q'/2}).$$  \hspace{1cm} (27)

The quantities $I^\alpha_{\ell\ell'}(k, q, q)$ and $I^\alpha_{\ell\ell'}(k, q, -q)$ are obtained from eq. (27) by removing the integral over $d\Omega_{q'}/4\pi$ and setting $q' \to q$ and $q' \to -q$ in the integrand, respectively.

The first few series of eq. (26) are easily calculated analytically as $T^\alpha_{00} = T^\alpha_{3/2} = 1$, $T^\alpha_{5/2} = T^\alpha_{5/2} = -1/4$, $T^\alpha_{11} = 205/48$ and $T^\alpha_{22} = 45/16$, in agreement with the values given below eq. (10.21,3) of Chapman and Cowling. The matrix element for a general $\ell'\ell$ can be evaluated numerically. With $T^\alpha_\ell$ and $R^\alpha_\ell$ thus obtained, eq. (21) is solved by cutting the infinite series at a finite value $\ell_c$ and $\ell_e$ is increased subsequently to check the convergence. Table I lists the values of $c^\alpha_\ell$ thereby obtained.

Those of $c^\alpha_0/\ell$ and $c^\alpha_2/\ell$ are about 2% larger in magnitude than the analytic ones $5\sqrt{\pi}/4$ and $-15\sqrt{\pi}/16$ with $\ell_c = 0$ and 1 for $\alpha = 5/2$ and $3/2$, respectively. This rapid convergence as a function of $\ell_e$ was already pointed out by Chapman and Cowling.

Substituting eqs. (9), (10) and (20) into eqs. (7a) and (7b), we arrive at the first-order contributions to the momentum flux density tensor and the thermal flux density as

$$\Pi^{(1)}_{ij} = -\mu v_i \frac{\partial v_j}{\partial r} + \frac{\partial v_i}{\partial r_j} - \frac{\kappa}{2} \frac{\partial T}{\partial r} ,$$  \hspace{1cm} (28a)

$$j^{(1)}_q = \frac{3}{2} \kappa k_B T \frac{\partial T}{\partial r} ,$$  \hspace{1cm} (28b)

respectively, where $\nu$ and $\kappa$ are the kinematic viscosity and the thermal diffusivity, respectively, defined by

$$\nu = \frac{1}{4} \sqrt{\frac{2k_B T}{m}},$$  \hspace{1cm} (29a)

$$\kappa = \frac{5}{6} \sqrt{\frac{2k_B T}{m}} c^{3/2}.$$  \hspace{1cm} (29b)

These quantities clearly have the same dimension. Using them as well as the specific heat at constant pressure $C_P$ and constant volume $C_V$, we can introduce an important dimensionless quantity $Pr = (\nu/\kappa)(C_P/C_V)$ called the Prandtl number. Adopting $C_P/C_V = 5/3$ of the ideal monatomic gas, we find $Pr = 0.66$ from eq. (29) and Table II which is in excellent agreement with the value 0.67 for Ar at $T = 273K$. Table III lists values of relevant thermodynamic and transport coefficients around room temperature at 1 atm for Ne, Ar and air.

Thus, we have successfully expressed $\Pi$ and $j_Q$ in terms of $n, v$ and $T$ as eqs. (14), (28) and (29) within the first-order gradient expansion. Now, eq. (8) with eqs. (14),

| $\alpha$ | $c^\alpha_0$ | $c^\alpha_1$ | $c^\alpha_2$ | $c^\alpha_3$ | $c^\alpha_4$ |
|----------|-------------|-------------|-------------|-------------|-------------|
| $5/2$    | 2.2511      | 0.1390      | 0.0233      | 0.0058      | 0.0018      |
| $3/2$    | -1.7036     | -0.1626     | -0.0371     | -0.0117     |             |
and (29) forms a closed set of equations for the five parameters \( n, v \) and \( T \) incorporated in \( f^{\alpha}(p, r, t) \). After solving them, we can obtain the distribution function \( f(p, r, t) \) by eqs. (9), (11), (20), (22) and Table III and subsequently calculate entropy by eq. (8).

### III. APPLICATION TO RAYLEIGH-BÉNARD CONVECTION

We now apply the equations of (11) for \( n, v \) and \( T \) to Rayleigh-Bénard convection of a dilute classical monatomic gas confined in the region \(-d/2 \leq z \leq d/2\) and \(-L/2 \leq x, y \leq L/2\). The gas is heated from below so that

\[
T(x, y, z = \pm d/2) = T_0 \mp \Delta T/2, \quad \Delta T > 0. \tag{30}
\]

The thickness \( d \) and the lateral width \( L \) are chosen as \( l \ll d \ll L \). It hence follows that (i) there are enough collisions along \( z \) and (ii) any effects from the side walls may be neglected. We eventually impose the periodic boundary condition in the \( xy \) plane.

We study this system by fixing the total particle number, total energy, and total heat flux through \( z = -d/2 \). This is equivalent to choosing the average particle density \( \bar{n} \), the average energy density \( \bar{E} \), and the average heat flux density \( \bar{q}_0 \) at \( z = -d/2 \) as independent variables; hence \( T_0 = T_0(\bar{n}, \bar{E}, \bar{q}_0) \) and \( \Delta T = \Delta T(\bar{n}, \bar{E}, \bar{q}_0) \) in eq. (30).

The latter two conditions also imply, due to the energy conservation law, that there is average energy flux density \( \bar{q}_0 \) through any cross section perpendicular to \( z \). The fact justifies our choice of \( \bar{q}_0 \) as an independent variable to specify the system. It should be noted that this energy flow in the container may be due partly to a macroscopic motion of the gas.

The standard theoretical treatment of Rayleigh-Bénard convection starts from introducing the Oberbeck-Boussinesq approximation to the equations for \( n, v \) and \( T \). However, this approximation seems not to have been justified in a widely accepted way. We here develop a systematic approximation scheme for the equations in (11) appropriate to treat Rayleigh-Bénard convection, which will be shown to yield the equations with the Oberbeck-Boussinesq approximation as the lowest-order approximation. This consideration also enables us to estimate the entropy change through the convective transition on a firm ground.

#### A. Introduction of dimensionless units

We first introduce a characteristic temperature \( \bar{T} \) defined by

\[
\bar{T} = \frac{2\bar{E}}{3\bar{n}k_B}. \tag{31}
\]

We then adopt the units where the length, velocity and energy are measured by \( d, \sqrt{k_B T/m} \) and \( k_B \bar{T} \), respectively. Accordingly, we carry out a change of variables as

\[
t = d \sqrt{\frac{m}{k_B T}} t', \quad r = d r', \tag{32a}
\]

and

\[
n = \frac{n'}{d}, \quad v = \frac{k_B T}{m} v', \quad T = \bar{T} t'. \tag{32b}
\]

Let us substitute eqs. (11), (28) and (29) into eq. (5) and subsequently perform the above change of variables. We thereby obtain the dimensionless conservation laws:

\[
\frac{\partial n'}{\partial t'} + \nabla' \cdot (n' v') = 0, \tag{33a}
\]

\[
n_i \frac{\partial v'}{\partial t'} + n' v' \cdot \nabla' v' + \nabla' P' - \sum_i \nabla' [n' v'(\nabla' v_i' + \nabla v')] + \frac{2}{3} \nabla' (n' v' v'') + n' U' g e_z = 0, \tag{33b}
\]

\[
\frac{\partial T'}{\partial t'} + v' \cdot \nabla' T' = \frac{1}{n'} \nabla' \cdot (n' \kappa' \nabla' T') + \frac{2}{3} T' \nabla' \cdot v' - \frac{2}{3} \sum_{ij} \frac{1}{2} \left( \frac{\partial v_i'}{\partial r_j'} + \frac{\partial v_j'}{\partial r_i'} \right) + \frac{\bar{g}}{2} \left( \nabla' \cdot v' \right)^2 = 0, \tag{33c}
\]

with \( P' = n' T' \) and

\[
\nu' \equiv \frac{\nu}{d}, \quad \kappa' \equiv \frac{k_B T}{d}, \quad U'_g \equiv \frac{mgd}{k_B T}. \tag{34}
\]

An important dimensionless quantity of the system is the Rayleigh number \( R \) defined by

\[
R \equiv \frac{U'_g \Delta T'}{\nu' \kappa'} \equiv \frac{g \bar{T}^{-1} \Delta T d^3}{\nu \kappa}, \tag{35}
\]

where \( \bar{T}^{-1} \) appears as the thermal expansion coefficient \( \alpha \) of the ideal gas.

The above equations will be solved by fixing \( \bar{n}, \bar{E} = 3\bar{n}k_B T/2 \) and \( \bar{q}_0 \), as already mentioned. These conditions are expressed in the dimensionless form as

\[
\frac{1}{\bar{T}^2} \int n'(r') d^3 r' = \bar{n}', \tag{36a}
\]

\[
\int n'(r') v'_i(r') d^3 r' = \bar{v}_i', \tag{36b}
\]

\[
\int n'(r') \nabla' v'_i(r') d^3 r' = \bar{R}_i' \tag{36c}
\]

\[
\int n'(r') \nabla' T'(r') d^3 r' = \bar{T'} \tag{36d}
\]

\[
\int n'(r') \nabla' \cdot v'_i(r') d^3 r' = \bar{u}_i' \tag{36e}
\]

\[
\int n'(r') \nabla' \cdot (\nabla' v_i'(r') + \nabla v_i') d^3 r' = \bar{Q}_i' \tag{36f}
\]

\[
\int n'(r') \nabla' \cdot (\nabla' v_i'(r') + \nabla v_i') d^3 r' = \bar{Q}_i' \tag{36g}
\]

\[
\int n'(r') \nabla' \cdot (\nabla' v_i'(r') + \nabla v_i') d^3 r' = \bar{Q}_i' \tag{36h}
\]

| \text{Gas} | \text{Density} | \text{Viscosity} | \text{Thermal expansion} |
|---|---|---|---|
| Ne (0°C) | 0.900 x 10^{-3} | 1.78 x 10^{-3} | 1.29 x 10^{-3} |
| Ar (0°C) | 3.66 x 10^{-3} | 3.67 x 10^{-3} | 3.67 x 10^{-3} |
| air (0°C) | 33.0 x 10^{-2} | 11.8 x 10^{-2} | 13.2 x 10^{-2} |
| \( \alpha \) | 83.1 x 10^{-2} | 29.2 x 10^{-2} | 25.9 x 10^{-2} |
\[ \frac{1}{L^2} \int \left( \frac{3}{2} P' + \frac{1}{2} n' v'^2 + n' U_g' z' \right) \, d^3 r' = \frac{3}{2} \tilde{n}', \quad (36b) \]
\[ \frac{1}{L^2} \int dx' \int dy' \int dz' \, \frac{3}{2} n' \kappa' \frac{\partial T'}{\partial z'} |_{z'=-\frac{1}{2}} = \tilde{j}_Q, \quad (36c) \]

where \( P' = n'T' \), and integrations extend over \(-L'/2 \leq x', y' \leq L'/2\) and \(-1/2 \leq z' \leq 1/2\). Equation (36b) has been obtained by integration of \((p^2/2m + mgz)\) over \( r \) and \( p \) with eq. (7), whereas eq. (36c) originates from eq. (28b).

To make an order-of-magnitude estimate for the parameters in eqs. (33) and (36), consider \( \text{Ar} \) of 273K at 1 atm confined in a horizontal space of \( d \) cm with the temperature difference \( \Delta T \) K. Using Table II, we then obtain the numbers:

\[ \nu' = 4.95 \times 10^{-6} / d, \quad \kappa' = 1.22 \times 10^{-5} / d, \quad (37a) \]
\[ U_g' = 1.73 \times 10^{-6} d, \quad \Delta T' = 3.67 \times 10^{-3} \Delta T, \quad (37b) \]

and

\[ R = 1.04 \times 10^{3} d^3 \Delta T. \quad (37b) \]

The critical Rayleigh number \( R_c \) for the convective transition is of the order \( 10^3 \Delta T \) which is realized for \( d \sim 2 \) cm and \( \Delta T \sim 1 \) K. We now observe that the dimensionless parameters have the following orders of magnitude in terms of \( \delta = 10^{-3} \):

\[ \nu', \kappa', U_g' \sim \delta^2; \quad \Delta T' \sim \delta; \quad R \sim \delta^{-1}. \quad (38) \]

Thus, Rayleigh-Bénard convection is a phenomenon where two orders of magnitude (i.e., \( \delta \) and \( \delta^2 \)) are relevant. From now on we shall drop primes in every quantity of eqs. (33) and (36).

### 3.6. Omission of the number conservation law

Let us write eq. (33) in terms of \( j = n \mathbf{v} \) instead of \( \mathbf{v} \). It follows from the vector analysis that the vector field \( j \) can be written generally as \( j = \nabla \Phi + \nabla \times \mathbf{A} \), where \( \Phi \) and \( \mathbf{A} \) corresponds to the scalar and vector potentials of the electromagnetic fields, respectively. We then focus in the following only on phenomena where the current density satisfies \( \nabla \Phi = 0 \), i.e.,

\[ \nabla \cdot j = 0. \quad (39) \]

This implies that we may drop eq. (33b) from eq. (33) to treat only eqs. (33a) and (33c).

### 3.7. Expansion in \( \delta \)

Equation (33a) suggests that we may solve eqs. (33a) and (33c) in powers of \( \delta \). Noting eqs. (36a) and (36b), we first expand \( n \) and \( T \) as

\[ n = \tilde{n} \left( 1 + \sum_{\ell=1}^{\infty} \tilde{n}^{(\ell)} \right), \quad T = 1 + \sum_{\ell=1}^{\infty} T^{(\ell)}. \quad (40a) \]

With eqs. (29a), (34a) and (34b), we next expand dimensionless parameters \( \nu = (l/4) \sqrt{2Tc_0^{5/2}}, \ \kappa = -(5l/6) \sqrt{2Tc_1^{3/2}} \) and \( U_g \) as

\[ \nu = \sum_{\ell=2}^{\infty} \nu^{(\ell)}, \quad \kappa = \sum_{\ell=2}^{\infty} \kappa^{(\ell)}, \quad U_g = U_g^{(2)}, \quad (40b) \]

where \( \nu^{(2)} = (l/4) \sqrt{2c_0^{5/2}} \) and \( \kappa^{(2)} = -(5l/6) \sqrt{2c_1^{3/2}} \) are constants with \( l = l(\tilde{n}) \). It also follows from \( \Delta T \sim \delta \) and eq. (36c) that

\[ \tilde{j}_Q = \tilde{j}_Q^{(3)}. \quad (40c) \]

It remains to attach orders of magnitude to the differential operators and \( \mathbf{j} = n \mathbf{v} \). In this context, we notice that the Oberbeck-Boussinesq approximation yields a critical Rayleigh number \( R_c \) which is in good quantitative agreement with experiment. The fact tells us that the procedure to attach the orders should be carried out so as to reproduce \( R_c \) of the Oberbeck-Boussinesq approximation. The requirement yields

\[ j = \tilde{n} \sum_{\ell=1}^{\infty} \tilde{j}^{(\ell+1/2)}, \quad \frac{\partial}{\partial t} = O(\delta^{1.5}), \quad \nabla = O(\delta^{-0.25}). \quad (40d) \]

See eq. (58) below and the subsequent comments for details. The above power-counting scheme will be shown to provide not only a justification of the Oberbeck-Boussinesq approximation but also a systematic treatment to go beyond it.

Let us substitute eq. (41) to eqs. (33a) and (33b). The contributions of \( O(\delta) \) in these equations read \( \nabla P^{(1)} = 0 \) and \( \int P^{(1)} \, d^3 r = 0 \), respectively, with \( P^{(1)} = \tilde{n}(\tilde{n}^{(1)} + T^{(1)}) \). We hence conclude \( P^{(1)} = 0 \), i.e.,

\[ \tilde{n}^{(1)} = -T^{(1)}. \quad (41) \]

It also follows from eqs. (33a) and (33c) with eqs. (40) and (41) that \( T^{(1)} \) should obey

\[ \int T^{(1)} \, d^3 r = 0, \quad (42a) \]

\[ \frac{1}{L^2} \int_{-L/2}^{L/2} dx \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} dz \frac{\partial T^{(1)}}{\partial z} |_{z=-1/2} = -\frac{2 \tilde{j}_Q}{3 \tilde{n}^{(2)}}. \quad (42b) \]

Equation (42) is still not sufficient to determine \( T^{(1)} \). It turns out below that the required equation results from the \( O(\delta^3) \) and \( O(\delta^{2.5}) \) contributions of eqs. (33a) and (33c), respectively.

Next, collecting terms of \( O(\delta^2) \) in eqs. (33a) and (33b) yield \( \nabla P^{(2)} + \tilde{n} U_g^{(2)} e_z = 0 \) and \( \int \frac{2}{3} P^{(2)} + \tilde{n} U_g^{(2)} e_z \, d^3 r = 0 \).
0, respectively. Hence \( P^{(2)} = \bar{n}U^2 \). Noting \( P^{(2)} = \bar{n}(\bar{n}^2 + \hat{n}(1)^4T^{(1)} + T^{(2)}) \) and using eq. (41), we obtain
\[
\bar{n}^{(2)} = (T^{(1)})^2 - T^{(2)} = U^2 \tag{43}
\]
It follows from eqs. (33b) and (33c), respectively, that \( T^{(2)} \) should obey
\[
\int [(T^{(1)})^2 - T^{(2)}] d^3r = 0, \tag{44a}
\]
\[
\int_{-L/2}^{L/2} dx \int_{-L/2}^{L/2} dy \left( \frac{\partial T^{(2)}}{\partial z} + \frac{T^{(1)}}{2} \frac{\partial T^{(1)}}{\partial z} \right) \bigg|_{z=-1/2} = 0. \tag{44b}
\]
In deriving eq. (41), use has been made of \((kn)^{(3)} = \bar{n}κ(T^{(1)})^2/2\) which results from \(κ \propto T^{1/4} \) and \(1/\xi\) in \(-1\); see eqs. (17) and (29b). Equation (41) forms constraints on the higher-order contribution \( T^{(2)} \), which will be irrelevant in the present study, however.

Finally, we collect terms of \( O(\delta^3) \) in eq. (33a) to obtain
\[
\frac{∂\hat{j}^{(1,5)}}{∂t} + j^{(1,5)} \cdot \nabla j^{(1,5)} + \frac{\nabla P^{(3)}}{\bar{n}} - \nu(2) \nabla^2 j^{(1,5)} + \hat{n}(1)(\delta^2) \epsilon_z = 0, \tag{45}
\]
where we have used eq. (40). We further operate \( \nabla \times \nabla \times \) to the above equation and substitute eq. (41). This yields
\[
-\frac{∂}{∂t} \nabla^2 j^{(1,5)} + \nabla \times \nabla \times \left( j^{(1,5)} \cdot \nabla j^{(1,5)} \right) + \nu(2) \nabla^2 j^{(1,5)} + U^2(\epsilon_z - \epsilon_z \cdot \nabla T^{(1)}) = 0. \tag{46a}
\]
On the other hand, terms of \( O(\delta^2.5) \) in eq. (33c) lead to
\[
\frac{∂T^{(1)}}{∂t} + j^{(1,5)} \cdot \nabla T^{(1)} - κ(2) \nabla^2 T^{(1)} = 0. \tag{46b}
\]
Equation (46) forms a set of coupled differential equations for \( T^{(1)} \) and \( j^{(1,5)} \), which should be solved with eq. (42). It is almost identical in form with that derived with the Oberbeck-Boussinesq approximation, predicting the same critical Rayleigh number \( R_c \) as will be shown below. The whole considerations on Rayleigh-Bénard convection presented in the following will be based on eq. (40) with eq. (42).

Two comments are in order before closing the subsection. First, if we apply the procedure of deriving eq. (40) to the \( O(\delta^4) \) and \( O(\delta^{3.5}) \) contributions of eqs. (33b) and (33c), respectively, we obtain coupled equations for the next-order quantities \( T^{(2)} \) and \( j^{(2,5)} \), which should be solved with eq. (41). Thus, we can treat higher-order contributions systematically in the present expansion scheme. Second, eq. (45) may be regarded as the equation to determine \( P^{(3)} \) for given \( T^{(1)} \) and \( j^{(1,5)} \). It yields a relation between \( T^{(3)} \) and \( \hat{n}(3) \), which in turn leads to the constraint for \( T^{(3)} \) upon substitution into eqs. (36b) and (36c). On the other hand, the equation for \( T^{(3)} \) originates from the \( O(\delta^5) \) and \( O(\delta^{4.5}) \) contributions of eqs. (36b) and (36c), respectively. Now, one may understand the hierarchy of the approximation clearly.

### D. Expression of entropy

We now write down the expression of entropy in powers of \( \delta \). Entropy of the system can be calculated by eq. (6), where the distribution function \( f \) is given by eq. (9) with eqs. (10) and (20). Hereafter we shall drop the superscript in \( \varphi^{(1)} \), which specifies the order in the gradient expansion, to remove possible confusion with the expansion of eq. (10). Thus, \( f \) is now expressed as \( f = f^{(eq)}(1 + \varphi) \).

We first focus on \( \varphi \) and write eq. (20) in the present units with noting eq. (10). We then realize that \( \varphi \) is proportional to \( \nabla T \) or \( \nabla v \), which are quantities of \( O(\delta^2) \) and \( O(\delta^{3.5}) \) in the expansion scheme of eq. (40), respectively. It hence follows that there is no contribution of \( O(\delta^2) \) from \( \varphi \). In contrast, \( f^{(eq)} \) yields terms of \( O(\delta^2) \), as seen below. Thus, we only need to consider \( f^{(eq)} \).

Let us write \( f^{(eq)} \) of eq. (10) in the present units, substitute eq. (10) into it, and expand the resulting expression in powers of \( \delta \). We also drop terms connected with \( j \) (i.e., \( v \)) which have vanishing contribution to \( S \) within \( O(\delta^2) \) after the momentum integration in eq. (6). We thereby obtain the relevant expansion:

\[
\begin{align*}
\text{\( f^{(eq)} \) yields terms of \( O(\delta^2) \), as seen below. Thus, we only need to consider \( f^{(eq)} \).}
\end{align*}
\]

\[
\begin{align*}
\text{where \( \varepsilon = p/2 \), and \( u(1) \) and \( u(2) \) are defined by}
\end{align*}
\]

\[
\begin{align*}
\text{where \( \varepsilon = p/2 \), and \( u(1) \) and \( u(2) \) are defined by}
\end{align*}
\]

\[
\begin{align*}
\text{Let us substitute eq. (47) into eq. (6) and carry out integration over \( p \). The contribution of \( O(1) \) is easily obtained as (\( k_B = 1 \))}
\end{align*}
\]

\[
\begin{align*}
\text{which is just the equilibrium expression for density \( \bar{n} \) and temperature \( T \) in the conventional units, as it should.}
\end{align*}
\]

Next, we find \( S^{(1)} = 0 \) due to eqs. (41) and (42a). Thus, the contribution characteristic of heat conduction starts from the second order. A straightforward calculation yields

\[
\begin{align*}
\text{A straightforward calculation yields}
\end{align*}
\]

\[
\begin{align*}
\text{Equation (50) is the basic starting point to calculate the entropy change through the convective transition. Note that we have fixed \( j_Q \) in the present consideration, i.e.,}
\end{align*}
\]

\[
\begin{align*}
\text{At this state, it may be worthwhile to present a qualitative argument on entropy of Rayleigh-Bénard convection.}
\end{align*}
\]
With the initial temperature slope fixed as eq. (42b), eq. (50) tells us that entropy will be larger as the temperature profile becomes more uniform between \( z = \pm 1/2 \). The conducting state with \( v = 0 \) has the linear temperature profile, as shown shortly below in eq. (52). Thus, any increase of entropy over this conducting state is brought thereby conclude without any detailed calculations that entropy of Rayleigh-Bénard convection should be larger than entropy of the conducting state measured from temperature difference.

Equation (46) with eq. (42) forms a set of simultaneous equations for \( T^{(1)} \) and \( j^{(1.5)} \), which should be supplemented by the boundary condition on \( \hat{j}_z \). Combining eqs. (42b) and (50) with the experimental observation on the Nusselt number, we thereby conclude without any detailed calculations that entropy of Rayleigh-Bénard convection should be larger than entropy of the conducting state in the present conditions with \( \hat{j}_0 = \text{const} \). Thus, Rayleigh-Bénard convection is expected to satisfy the principle of maximum entropy given at the beginning of the paper. We shall confirm this fact below through detailed numerical studies.

IV. PERIODIC SOLUTION WITH STRESS-FREE BOUNDARIES

Equation (40) with eq. (42) forms a set of simultaneous equations for \( T^{(1)} \) and \( j^{(1.5)} \), which should be supplemented by the boundary condition on \( j^{(1.5)} \). For simplicity, we here adopt the assumption of stress-free boundaries:

\[
\frac{\partial^2}{\partial z^2} j^{(1.5)} = 0 \quad \text{at} \quad z = \pm \frac{1}{2}.
\]

However, qualitative features of the convective solutions will be universal among the present and more realistic/complcated boundary conditions; see the argument at the end of the preceding section.

We first discuss the heat-conducting solution of eq. (40) and its stability towards convection. We then transform eq. (40) with eqs. (42) and (51) in a form suitable to obtain periodic convective structures.

A. Conducting solution

Let us consider the conducting solution of eq. (40) where \( j^{(1.5)} = 0 \) with uniformity in the \( xy \) plane.

Equation (40) then reduces to \( d^2 T^{(1)}/dz^2 = 0 \), which is solved with eq. (42) as

\[
T^{(1)} = -\Delta T_{hc} z, \quad \Delta T_{hc} = \frac{2j^{(3)}_Q}{3\kappa(\nu^2)}.
\]

Substituting this expression into eq. (50), we obtain entropy of the conducting state measured from \( S^{(0)} \) as

\[
S_{hc}^{(2)} = -\frac{5}{48}(\Delta T_{hc})^2.
\]

B. Instability of the conducting state

We next check stability of the conducting solution by adding a small perturbation given by

\[
j^{(1.5)}(r, t) = e^{\lambda t}e^{ik_z z}(\delta_j^z \sin k_z \zeta + \delta j^z_\perp \cos k_z \zeta), \quad (54a)
\]

\[
T^{(1)}(r, t) = -\Delta T_{hc} z + \delta T e^{\lambda t}e^{ik_z z} \sin k_z \zeta, \quad (54b)
\]

where \( \zeta \equiv z + 1/2 \), \( k_z = \ell_3 \pi \) (\( \ell_3 = 1, 2, \cdots \)) from eq. (51), and \( \delta j^z_\perp \) denotes a vector in the \( xy \) plane. Let us substitute eq. (51) into eq. (40) and linearize it with respect to the perturbation. This leads to

\[
(\lambda + \nu(\nu^2 + \kappa(\nu^2))k^2) \delta j^z = U_g(\nu^2 + \kappa(\nu^2))k^2 T \delta e_z = 0, \quad (55a)
\]

\[
(\lambda + \nu(\nu^2 + \kappa(\nu^2))k^2) \delta j^z_\perp - iU_g(\nu^2 + \kappa(\nu^2))k_z \delta T e_z = 0, \quad (55b)
\]

\[
(\lambda + \kappa(\nu^2 + \kappa(\nu^2))k^2) \delta T - \Delta T_{hc} \delta j^z_\perp = 0. \quad (55c)
\]

The components \( \delta j^z \) and \( \delta j^z_\perp \) in the \( xy \) plane are obtained from eqs. (55a) and (55b) as

\[
\delta j^z_\perp = 0, \quad \delta j^z = \frac{iU_g(\nu^2 + \kappa(\nu^2))k^2}{(\lambda + \nu(\nu^2 + \kappa(\nu^2))k^2)} \delta T. \quad (56)
\]

In contrast, the \( z \) component of eq. (55a) and eq. (55b) form linear homogeneous equations for \( \delta j^z \) and \( \delta T \). The requirement that they have a non-trivial solution yields

\[
\lambda^2 + (\nu(\nu^2 + \kappa(\nu^2))k^2 + \nu(\nu^2 + \kappa(\nu^2))k^2)R^{(-1)}(k_z^2/k_\perp^2) = 0, \quad (57)
\]

with \( R^{(-1)} \) the Rayleigh number defined by eq. (55) with \( U_g \rightarrow U_{g'} \), \( \Delta T \rightarrow \Delta T_{hc} \), \( \nu' \rightarrow \nu(\nu^2 + \kappa(\nu^2)) \). The conducting solution becomes unstable when eq. (57) has a positive solution, i.e.,

\[
R^{(-1)} \equiv \frac{U_{g'}(\nu^2 + \kappa(\nu^2))k^2}{k_z^2} \geq \frac{27\pi^4}{4}. \quad (58)
\]

Thus, we have obtained the value \( R_c = 27\pi^4/4 \) for the critical Rayleigh number which corresponds to \( k_z^2/k_\perp^2 = (\pi/\sqrt{2}, \pi) \). Besides reproducing the established results, the above consideration may also be important in the following respects. First, we require that: (i) terms of the \( z \) component of eq. (55) all have the same order in \( \delta \) with \( \delta T = O(\delta) \); (ii) the same be true for terms of eq. (55c). This leads to the attachment of the order-of-magnitude: \( \delta j = O(\delta^{4.5}) \), \( k = O(\delta^{-0.25}) \) and \( \lambda = O(\delta^{1.5}) \), thereby justifying eq. (40). The conclusion \( k = O(\delta^{-0.25}) \) also results from \( k = \sqrt{3/2\pi} \sim 4 \) for the critical Rayleigh number. Second, eq. (58) removes the ambiguity in \( \nu, \kappa \) and \( \alpha \) to estimate the critical Rayleigh number. Specifically, we should use the mean values over \( -1/2 \leq z \leq 1/2 \) for a detailed comparison of \( R_c \) between theory and experiment.
C. Convective solution

We now focus on the convective solution of eq. (46) with periodic structures. Let us introduce basic vectors

$$a_1 = (a_{1x}, a_{1y}, 0), \quad a_2 = (0, a_2, 0), \quad a_3 = e_z. \quad (59)$$

We consider the region in the $xy$ plane spanned by $N_1 a_1$ and $N_2 a_2$ with $N_j$ ($j = 1, 2$) a huge integer, and impose the periodic boundary condition. The wave vector $k$ is then defined in terms of the reciprocal lattice vectors

$$b_1 = 2\pi (a_2 \times a_3)/([a_1 \times a_2] \cdot a_3), \quad b_2 = 2\pi (a_3 \times a_1)/([a_1 \times a_2] \cdot a_3) \quad \text{and} \quad b_3 = \pi e_z \quad \text{as}$$

$$k = \sum_{j=1}^{3} \ell_j b_j, \quad (60)$$

with $\ell_j$ denoting an integer. The analysis of [LV] suggests that the stable solution satisfies $|b_1| \sim |b_2| \sim \pi / \sqrt{2}$.

Equation (59) tells us that $\delta \gamma$ and $\delta T$ are out-of-phase. Also noting eqs. (12) and (51), we now write down the steady solution of eq. (46) in the form:

$$\tilde{j}_{1,0}^{(1.5)}(r) = \sum_{k_\perp \neq 0} \sum_{k_z} \tilde{j}_{\perp k}(\mathbf{k} \cdot \mathbf{r}) \sin(k_z \zeta), \quad (61a)$$

$$\tilde{j}_{2,0}^{(1.5)}(r) = \sum_{k_\perp \neq 0} \sum_{k_z} \tilde{j}_{\perp k}(\mathbf{k} \cdot \mathbf{r}) \sin(k_z \zeta), \quad (61b)$$

$$T^{(1)}(r) = \sum_{k_\perp} \sum_{k_z} \tilde{T}_{k}(\mathbf{k} \cdot \mathbf{r}) \sin(k_z \zeta) - \Delta T_{cv} z - T_1, \quad (61c)$$

where $\zeta \equiv z + 1/2$, and we have chosen $\tilde{j}_{2,0}^{(1.5)}$ and $T^{(1)}$ as even functions in the $xy$ plane without losing the generality. The $k$ summations in eq. (61) run over

$$\left\{ \begin{array}{l} -\infty < \ell_1 \leq 1, \ 1 < \ell_2 \leq \infty, \ 1 < \ell_3 \leq \infty, \\ 0 \leq \ell_1 \leq \infty, \ 0 < \ell_2 \leq \infty, \ 1 < \ell_3 \leq \infty \end{array} \right\}, \quad (62)$$

which covers all the independent basis functions. The condition (30) is transformed into

$$k \cdot \tilde{j}_{\perp k} + k_z \tilde{j}_{z k} = 0. \quad (63a)$$

Thus, $\tilde{j}_{\perp k}$ may be written generally as

$$\tilde{j}_{\perp k} = -\frac{k_\perp k_z}{k^2} \tilde{j}_{z k} + e_z \times \frac{k_\perp}{k_z} \tilde{j}_{z k}. \quad (63b)$$

The constants $\Delta T_{cv}$ and $T_1$ in eq. (61c) denote the temperature difference between $z = \pm 1/2$ and the average temperature shift, respectively. They are fixed so as to satisfy eq. (12) as

$$\Delta T_{cv} = \Delta T_{hc} + \sum_{k_z} \tilde{T}_{k_\perp = 0, k_z} z, \quad (64a)$$

$$T_1 = \sum_{k_z} \tilde{T}_{k_\perp = 0, k_z} \frac{1 - \cos k_z}{k_z^2} \quad \text{and}$$

$$\Delta T_{hc}$$

where $\Delta T_{hc}$ denotes temperature difference of the conducting state given explicitly in eq. (52).

It follows from the energy conservation law that eq. (66b) should also hold at $z = 1/2$, which leads to an alternative expression for $\Delta T_{cv}$. Subtracting it from eq. (66a) yields the identity obeyed by $\tilde{T}_{k_\perp = 0, k_z}$:

$$\sum_{k_z} \tilde{T}_{k_\perp = 0, k_z} z (1 - \cos k_z) = 0, \quad (65)$$

which is useful to check the accuracy of numerical calculations.

Let us substitute eq. (61) into eq. (46). A straightforward calculation of using eq. (63) then leads to coupled algebraic equations for $\tilde{T}_{k}$, $\tilde{j}_{k}$ and $\tilde{j}_{yk}$ as

$$\kappa^{(2)} k^2 \tilde{T}_{k} = -U^{(2)} k^2 \tilde{T}_{k}$$

$$+ \frac{1}{4} \sum_{k'k''} \tilde{T}_{k'} \left\{ k \cdot \tilde{j}_{k''} \left[ -\delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right]$$

$$+ \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right\}$$

$$+ \left( k_\perp \cdot \tilde{j}_{k''} - k_\perp \tilde{j}_{k''} \right) \left\{ \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} + \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right\}$$

$$+ \left( -\frac{\delta_{k_\perp, k_z}}{2} \left( \delta_{k'' - k' + k_z, k_z} + \delta_{k'' - k' + k_z, k_z} \right) \right) \right\} = 0 \quad \text{(66a)}$$

$$\nu^{(2)} k^2 \tilde{j}_{yk} = U^{(2)} k^2 \tilde{T}_{k}$$

$$+ \frac{1}{4} \sum_{k'k''} \tilde{j}_{k'} \left\{ k \cdot \tilde{j}_{k''} \left[ -\delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right]$$

$$+ \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right\}$$

$$+ \left( k_\perp \cdot \tilde{j}_{k''} - k_\perp \tilde{j}_{k''} \right) \left\{ \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} + \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right\}$$

$$+ \left( -\frac{\delta_{k_\perp, k_z}}{2} \left( \delta_{k'' - k' + k_z, k_z} + \delta_{k'' - k' + k_z, k_z} \right) \right) \right\} \right\} = 0 \quad \text{(66b)}$$

$$\times \left( \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} - \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right) \right\}$$

$$+ \kappa \cdot \tilde{j}_{yk} \left\{ k_\perp \cdot \tilde{j}_{k''} \left( \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right)$$

$$- \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right\}$$

$$- \left( k_\perp \cdot \tilde{j}_{k''} - k_\perp \tilde{j}_{k''} \right) \left\{ k_\perp \cdot \tilde{j}_{k''} - k_\perp \tilde{j}_{k''} \right\}$$

$$\times \left( \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} + \delta_{k'' - k' + k_z, k_z} \delta_{k'' - k' + k_z, k_z} \right) \right\} \right\} = 0 \quad \text{(66c)}$$
The Rayleigh number $R$ has been performed most actively with compressed classical gases above eq. (32) with \( k \parallel \) above $T$, thus the present consideration with eq. (37) has direct relevance to those experiments. Therefore, the present consideration with eq. (37) has direct relevance to those experiments. We also fix $T \equiv 273$ K under atmospheric pressure and use the values quoted in the text.

As for periodic structures, we investigate the three candidates: the roll, the square lattice and the hexagonal lattice with $b_1 = b_2 \sim \pi / \sqrt{2}$. With these preliminaries, we trace time evolution of the expansion coefficients until they all acquire constant values. Choosing $\Delta t' \leq 0.005$ and $t_c \geq 5$ yields excellent convergence for the calculations presented below. The initial state is chosen as the conducting state with small fluctuations $T_k' \sim 10^{-2}$ for the basic harmonics $k$. The constants $\Delta T_{cv}$ and $T_1$ have been updated at each time step by using eq. (82). Also evaluated at each time step is entropy measured with respect to the heat-conducting state:

$$\Delta S \equiv S_{cv}^{(2)} - S_{bc}^{(2)}$$

where $S_{bc}^{(2)}$ and $S_{cv}^{(2)}$ are given by eqs. (63) and (67), respectively. We thereby trace time evolution of $\Delta S$ simultaneously. The above procedure is carried out for each fixed periodic structure.

We have studied the range: $1 \leq R^{(-1)} / R_c \leq 10$. Although the region extends well beyond the Busse balloon of stability for classical gases, it will be worth clarifying the basic features of steady periodic solutions over a wide range of the Rayleigh number.

**B. Results**

Figure 1 plots $\Delta S$ as a function of $t'$ for the Rayleigh number $R^{(-1)} = 1.2 R_c$ which is slightly above the critical value $R_c = 27 \pi^4 / 4$. The letters r, s and h denote (r)

![FIG: Time evolution of entropy measured with respect to the heat-conducting state for $R^{(-1)} = 1.2 R_c$. The letters r, s and h denote roll, square and hexagonal, respectively, distinguishing initial fluctuations around the heat-conducting solution; see text for details. The final state of $t' \geq 80$ is the roll convection, whereas the intermediate plateaus of s and h correspond to the square and hexagonal convolutions, respectively.](image)
The turbulence observed in this region where fluctuations dominate with no stable structure connected with this instability.

Thus, we have confirmed that the roll convection is stable for the infinite horizontal area, which was predicted originally by Schlüter, Lortz and Busse\cite{3.6} for \( R \sim R_c \) based on the linear stability analysis; see also refs. \[3\] and \[7\]. It should be noted at the same time that the entropy differences among different structures are rather small. We hence expect that: (i) the order of the stability may easily be changed by finite-size effects, boundary conditions, etc.; (ii) initial conditions, fluctuations and defects play important roles in Rayleigh-Bénard convection. These are indeed the features observed experimentally\cite{5,6,9}.

Figure 2 plots time evolution of \( \Delta S \) for four different Rayleigh numbers, all developing from the initial fluctuation \( \tilde{T}'[1, 0, 1] = 1.00 \times 10^{-2} \) with \( |b_1| = |b_2| = \pi/\sqrt{2} \). Each final state is the roll convection, which is stabilized faster as \( R^{(-1)} \) becomes larger. The increase in \( \Delta S \) is seen quite steep for \( R^{(-1)} = 10 R_c \) followed by a small oscillation. This oscillation in \( \Delta S \) may be due either to (i) the fluctuations in particle number, momentum, energy and energy flux inherent to open systems or (ii) the initial correlations which causes the anti-kinetic evolution\cite{11,12}.

Such fluctuations are also observed in a numerical study by Orban and Bellemans\cite{11,12} for an isolated system and not in contradiction with the law of increase of entropy. We observe clearly that the principle of maximum entropy proposed at the beginning of \[\ref{3}\] which is relevant to the final steady state without time evolution, is indeed satisfied here. The dotted line in Fig. 2 is the upper bound of entropy in convection, as may be realized from eq. \[51\]. As the Rayleigh number is increased further, entropy differences between different structures become smaller so that the system will eventually fall into the region where fluctuations dominate with no stable structure. The turbulence observed in this region\cite{5,6,9} may be connected with this instability.

![Figure 2: Time evolution of entropy \( \Delta S \). The four curves correspond to the different Rayleigh numbers: \( R^{(-1)} = 1.2 R_c \), \( 2.0 R_c \), \( 5.0 R_c \) and \( 10.0 R_c \). The initial state is the heat-conducting state with the fluctuation \( \tilde{T}'[1, 0, 1] = 1.00 \times 10^{-2} \) and \( b_1 = \pi/\sqrt{2} \), whereas all the final states are the roll convection. The broken line near the top indicates the upper bound of \( \Delta S \).](image1)

![Figure 3: Profile of the average temperature variation \( T(z) \) in the roll convection normalized by the temperature difference \( \Delta T_{hc} \) in the heat-conducting state. The Rayleigh numbers are \( R^{(-1)} = R_c \), \( 1.2 R_c \), \( 2.0 R_c \), \( 5.0 R_c \) and \( 10.0 R_c \) from top to bottom on the left part.](image2)
FIG. 4: The length $|b_1|$ of the stable roll convection as a function of the normalized Rayleigh number $R^{(-1)}/R_c$. Here $|b_1| = \pi/\sqrt{2}$ at $R^{(-1)}/R_c = 1$.

Figure 3 shows profile of the average temperature variation $\bar{T}(z)$ along $z$ in the roll convection for five different Rayleigh numbers. Temperature has less variation as the Rayleigh number becomes larger, thereby increasing entropy of the system. Thus, we may attribute the formation of convection to its efficiency for increasing entropy under fixed inflow of heat, i.e., the initial slope of temperature. Experiments on Rayleigh-Bénard convection have naturally been carried out by fixing the temperature difference rather than the inflow of heat, and formation of the convection has been discussed in terms of the change in the Nusselt number $2,7$ (i.e., the efficiency of the heat transport) due to the increase of the initial temperature slope through the convective transition. Here we have seen that the same phenomenon can be explained with respect to the basic thermodynamic quantity of entropy. Thus, the principle of maximum entropy partly justifies the maximum heat transfer hypothesis by Malkus and Veronis. $23$

All the above calculations have been carried out by fixing the periodic structure. They clearly show that the principle of maximum entropy is indeed obeyed. We now take the principle as granted and use it to determine the stable lattice structure. We carry this out within the roll convection by changing the value $|b_1|$.

Figure 4 plots $|b_1|$ as a function of normalized Rayleigh number $R^{(-1)}/R_c$. As seen clearly, $|b_1|$ increases gradually from the value $\pi/\sqrt{2}$ at $R^{(-1)}/R_c = 1$. This tendency is in qualitative agreement with the experiment by Hu, Ecke and Ahlers $24$ using a circular cell of $L/d \gg 1$; see also ref. $3$. It should be noted at the same time that the entropy difference around $|b_1| = \pi/\sqrt{2}$ is quite small. For example, the stable state for $R^{(-1)}/R_c = 10$ corresponds to $|b_1| = 0.829$, but entropy is increased by only $2 \times 10^{-9}$ from the value $\Delta S = 1.296 \times 10^{-6}$ at $|b_1| = \pi/\sqrt{2}$. Hence it is expected that (i) initial conditions, fluctuations and boundary conditions play important roles and (ii) it may take a long time, or even be impossible in certain cases, to reach the stable state. These are indeed in agreement with experimental observations $5,8,9$.

The whole our results have been obtained for the stress-free boundary condition $27$. However, the qualitative results will be valid also for more realistic boundary conditions. Indeed, experiments on Rayleigh-Bénard convection all exhibit the temperature profile with a steep change near the boundaries followed by moderate variation in the bulk region as reflected in the enhancement of the Nusselt number $27$. And it is this feature in the present study which has caused increase of entropy in convection over that in the conducting state.

VI. CONCLUDING REMARKS

The present study shows unambiguously that the principle of maximum entropy given at the beginning of §I is indeed satisfied through the Rayleigh-Bénard convective transition of a dilute classical gas. The result is encouraging for the principle as a general rule to determine the stability of nonequilibrium steady states. We need to investigate other open systems, as well as Rayleigh-Bénard convection without fixing the lattice structure, to confirm its validity further.

It may be worth emphasizing once again that entropy/probability, which is the central concept of equilibrium thermodynamics/statistical mechanics, seems to have been left out of the investigations on nonequilibrium systems and pattern formation. Indeed, they have been almost always based on deterministic equations closely connected with conservation laws. $2$ Calculations of entropy for open driven systems imply treating these finite systems as subjects of statistical mechanics with considering the boundary conditions explicitly. Those calculations are expected to shed new light on nonequilibrium phenomena in general which are still mysterious.

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