Stochastic thermodynamics for self-propelled particles

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We propose a generalization of stochastic thermodynamics to systems of active particles, which move under the combined influence of stochastic internal self-propulsions (activity) and a heat bath. The main idea is to consider joint trajectories of particles’ positions and self-propulsions. It is then possible to exploit formal similarity of an active system and a system consisting of two subsystems interacting with different heat reservoirs and coupled by a non-symmetric interaction. The resulting thermodynamic description closely follows the standard stochastic thermodynamics. In particular, total entropy production, $\Delta_S$, can be decomposed into housekeeping, $\Delta_{hk}$, and excess, $\Delta_{ex}$, parts. Both $\Delta_{tot}$ and $\Delta_{hk}$ satisfy fluctuation theorems. The average rate of the steady-state housekeeping entropy production can be related to the violation of the fluctuation-dissipation theorem via a Harada-Sasa relation. The excess entropy production enters into a Hatano-Sasa-like relation, which leads to a generalized Clausius inequality involving the change of the system’s entropy and the excess entropy production. Interestingly, although the evolution of particles’ self-propulsions is free and uncoupled from that of their positions, non-trivial steady-state correlations between these variables lead to the non-zero excess dissipation in the reservoir coupled to the self-propulsions.

Introduction. – Active matter systems [1–6] consist of particles that move on their own accord by consuming energy from their environment. Since these systems are out of equilibrium, they cannot be described using standard thermodynamics. Recently, there have been several attempts [7–16] to extend the formalism of stochastic thermodynamics to describe active matter.

Stochastic thermodynamics [17] is the most successful framework for the description of an admittedly limited class of non-equilibrium systems. In its standard form, stochastic thermodynamics deals with systems which are in contact with a heat reservoir characterized by a constant temperature and are displaced out of equilibrium by external forces (in contrast to active systems that evolve under the influence of internal self-propulsions). It combines stochastic energetics [18], which generalizes notions of work and heat to the level of systems’ trajectories, with the notion of stochastic entropy [19]. It allows one to derive a number of results characterizing out-of-equilibrium states and processes. We shall mention here fluctuation theorems for entropy production [20, 22] which shed light on the probability of rare, 2nd law violating fluctuations, the Jarzynski relation [23] which expresses the free energy difference between two equilibrium states in terms of the average of the exponential of the work performed in a non-equilibrium process between the same two states and a generalization of the Jarzynski relation to transitions between two stationary non-equilibrium states [24]. Several results obtained in the framework of stochastic thermodynamics were experimentally verified, see, e.g., Refs. [25–28].

Two types of a generalization of stochastic thermodynamics to active matter systems have been proposed. Fodor et al. [2] and Mandal et al. [8] considered model athermal active matter systems and derived two different expressions for the entropy production. The common feature of these two studies is that they map athermal systems onto equilibrium systems with non-conservative interactions in which the effective temperature (which characterizes the strength of the self-propulsions) plays the role of the temperature of the medium. It is not clear how to generalize these studies to active systems that are influenced by both self-propulsions and thermal noise [29]. In contrast, Speck [10, 11], Shankar and Marchetti [12], and Dabelow et al. [13] followed the standard stochastic thermodynamics more closely and considered active matter systems in contact with a heat bath.

Here we follow the spirit of Ref. [12] and consider joint trajectories of particles’ positions and self-propulsions for an active system in contact with a heat bath [30]. This approach allows us to follow the standard stochastic thermodynamics framework and to generalize a number of its results to active matter systems. In particular, we divide the entropy production into the housekeeping part, which originates from the non-equilibrium character of active matter, and the excess part, we derive a fluctuation theorem for the housekeeping entropy production, and we relate the steady-state entropy production to the experimentally measurable violation of a fluctuation-dissipation relation. We also obtain a generalized Clausius inequality which extends the 2nd law of thermodynamics to active matter systems.

Model: Active Brownian particle in an external potential. – To illustrate our approach we use a minimal model system consisting of a single active Brownian particle (ABP) [32] under the influence of an external force, in two spatial dimensions. The equations of motion read

\[
g_t \dot{r} = F_0 + \gamma_t v_0 e + \zeta (\xi(t)\xi(t')) = 2I\gamma_t T \delta(t-t'),
\]

(1)

\[
g_r \dot{\varphi} = \eta (\eta(t)\eta(t')) = 2\gamma_r T \delta(t-t'),
\]

(2)

where $\gamma_t$ and $\gamma_r$ are the translational and rotational fric-
tion coefficients, respectively, and \( e \equiv (\cos(\varphi), \sin(\varphi)) \) is the orientation vector. Next, \( \mathbf{F}_\lambda \) is an external force, which depends on a control parameter \( \lambda \), and may include a non-conservative component, and \( v_0 \) is the self-propulsion speed. Finally, \( \zeta \) and \( \eta \) are Gaussian white noises representing thermal fluctuations. We use the system of units such that the Boltzmann constant \( k_B = 1 \).

The model system defined through Eqs. (12) is mathematically equivalent to a system consisting of two subsystems, with each subsystem connected to its heat reservoir, and with the subsystems coupled through a non-symmetric, i.e. violating Newton’s 3rd law, interaction. In the present case of a single ABP the reservoirs are at the same temperature. If we were to consider an active Ornstein-Uhlenbeck particle (AOUP) [31, 32], the temperatures of the two reservoirs would be unrelated. Interestingly, the temperature of the reservoir coupled to the self-propulsions, Eq. (2), is different from the so-called effective temperature of the self-propulsions [12], \( T_a = v_0^2 \gamma r/(2T) \).

Systems consisting of subsystems coupled to different heat reservoirs have been extensively studied, both theoretically [36–42] and experimentally [28, 43, 44]. We note that in the present case, with a non-symmetric interaction between the two subsystems, even if the temperatures of the reservoirs are the same, the combined system is out of equilibrium.

**Stochastic entropy production.**– To define a stochastic entropy we follow Seifert [19]. First, we consider the Fokker-Planck equation for the joint probability density for the particle’s position and self-propulsion, which corresponds to Eqs. (12),

\[
\partial_t p(\mathbf{r}, \varphi; t) = -\partial_r \cdot \mathbf{j}_r(\mathbf{r}, \varphi; t) - \partial_{\varphi} j_r(\mathbf{r}, \varphi; t),
\]

(3)

where current densities in the position and orientation spaces read

\[
\mathbf{j}_r(\mathbf{r}, \varphi; t) = \gamma_1^{-1} (\mathbf{F}_\lambda + \gamma_r v_0 \mathbf{e} - T \partial_r) p(\mathbf{r}, \varphi; t),
\]

(4)

\[
j_r(\mathbf{r}, \varphi; t) = - (T/\gamma_r) \partial_{\varphi} p(\mathbf{r}, \varphi; t).
\]

(5)

We emphasize that due to the non-symmetric interaction between \( \mathbf{r} \) and \( \varphi \) sectors, in a steady state currents do not vanish even if \( \mathbf{F}_\lambda \) is conservative.

Next, we define the trajectory-level entropy for the system (i.e. the particle), using the solution of the Fokker-Planck equation [33] for a time-dependent control parameter \( \lambda(t) \), evaluated along the stochastic trajectory of the particle’s position and self-propulsion,

\[
s(t) = - \ln p(\mathbf{r}(t), \varphi(t); t).
\]

(6)

The rate of change of the systems entropy reads

\[
\dot{s}(t) = \frac{\partial_r p(\mathbf{r}, \varphi; t)}{p(\mathbf{r}, \varphi; t)} \cdot \dot{\mathbf{r}} - \frac{\partial_{\varphi} p(\mathbf{r}, \varphi; t)}{p(\mathbf{r}, \varphi; t)} \dot{\varphi} - \frac{\partial_t p(\mathbf{r}, \varphi; t)}{p(\mathbf{r}, \varphi; t)} \dot{t} - \frac{\partial_{\varphi} j_r(\mathbf{r}, \varphi; t)}{p(\mathbf{r}, \varphi; t)} \dot{\varphi}.
\]

(7)

The first term in the last line can be interpreted as the entropy production in the medium,

\[
\dot{s}_m(t) = T^{-1} (\mathbf{F} + \gamma_r v_0 \mathbf{e}) \cdot \dot{\mathbf{r}}.
\]

(8)

We will see in the remainder of this Rapid Communication that identification [8] leads to a consistent framework of active stochastic thermodynamics. Using Eqs. (7–8) we can express the total stochastic entropy production in terms of local velocities evaluated along the trajectory,

\[
\dot{s}_\text{tot}(t) = -\frac{\partial_r p(\mathbf{r}, \varphi; t)}{p(\mathbf{r}, \varphi; t)} + \frac{1}{T} (\gamma_r v_1 \cdot \dot{\mathbf{r}} + \dot{\gamma}_r v \cdot \dot{\varphi}),
\]

(9)

where \( v_1(\mathbf{r}, \varphi; t) = j_1(\mathbf{r}, \varphi; t)/p(\mathbf{r}, \varphi; t) \) and \( v(\mathbf{r}, \varphi; t) = j_r(\mathbf{r}, \varphi; t)/p(\mathbf{r}, \varphi; t) \).

We note that averaging \( \dot{\mathbf{r}} \) and \( \dot{\varphi} \) over all trajectories under the condition that the position and self-propulsion at time \( t \) are equal to \( \mathbf{r} \) and \( \varphi \) gives the local translational and rotational velocity, respectively,

\[
\langle \dot{\mathbf{r}} | \mathbf{r}, \varphi \rangle = v_1(\mathbf{r}, \varphi; t),
\]

(10)

\[
\langle \dot{\varphi} | \mathbf{r}, \varphi \rangle = v(\mathbf{r}, \varphi; t).
\]

(11)

Here and in the following \( \langle \cdots \rangle \) denotes averaging over the trajectories.

Combining Eqs. (9) and (10–11) allows us to calculate the average total entropy production, \( \dot{S}(t) = \langle \dot{s}_\text{tot}(t) \rangle \),

\[
\dot{S}(t) = \int dr d\varphi \frac{\gamma_1 v_1^2(\mathbf{r}, \varphi; t) + \gamma_r v^2(\mathbf{r}, \varphi; t)}{T} p(\mathbf{r}, \varphi; t).
\]

(12)

Due to non-vanishing currents, the total entropy increases even in a steady state with a conservative force.

**Housekeeping entropy production and Harada-Sasa relation** – Oono and Paniconi [16] introduced the concept of a housekeeping heat, i.e. the heat dissipated in a non-equilibrium steady state. Here we generalize this concept into a housekeeping entropy production. Following the spirit of Hatano and Sasa [24] and of Speck and Seifert [47] we define the housekeeping increase of the entropy, \( \Delta s_{hk} \), as follows

\[
\Delta s_{hk} = T^{-1} \int_0^t dt' (\gamma_1 v_{1s} \cdot \dot{\mathbf{r}} + \gamma_r v_{r+} \dot{\varphi}).
\]

(13)
Here $v_{ts}(r, \varphi|\lambda(t))$ and $v_{rs}(r, \varphi|\lambda(t))$ are steady-state local translational and rotational velocities, respectively,

\begin{align}
    v_{ts}(r, \varphi|\lambda(t)) &= j_{ts}(r, \varphi|\lambda(t))/p_s(r, \varphi|\lambda(t)) \tag{14} \\
    v_{rs}(r, \varphi|\lambda(t)) &= j_{rs}(r, \varphi|\lambda(t))/p_s(r, \varphi|\lambda(t)), \tag{15}
\end{align}

evaluated along the stochastic trajectory. In Eqs. (14-15) $j_{ts}(\lambda(t))$, $j_{rs}(\lambda(t))$ and $p_s(\lambda(t))$ are the currents and the probability distribution in a steady state corresponding to a fixed instantaneous value of the control parameter, $\lambda(t)$. We note that the housekeeping entropy increase originates from both translational and rotational degrees of freedom, in spite of the fact that the rotational motion is free and decoupled from the translational one. Furthermore, as expected, in a steady state the total entropy production \([\text{13}]\) and the housekeeping entropy production \([\text{13}]\) coincide.

Using the regularization method described by Speck and Seifert \([\text{17}]\) one can derive an equation of motion for the joint probability distribution of the particle’s position, orientation and housekeeping entropy increase, $\rho(r, \varphi, \Delta_{shk}; t)$,

\begin{align}
    \partial_t \rho(r, \varphi, \Delta_{shk}; t) &= -\gamma_t^{-1} \partial_r \cdot [F + \gamma_t v_0 \mathbf{e} - T \partial_\varphi] \rho(r, \varphi, \Delta_{shk}; t) + (T/\gamma_r) \partial_\varphi^2 \rho(r, \varphi, \Delta_{shk}; t) \\
    &+ T^{-1} [\gamma_t v_{ts}^2 + \gamma_r v_{rs}^2] \partial_{\Delta_{shk}} \rho(r, \varphi, \Delta_{shk}; t) + [2 \partial_r \cdot v_{ts} + 2 \partial_\varphi v_{rs} - T^{-1} (\gamma_t v_{ts}^2 + \gamma_r v_{rs}^2)] \partial_{\Delta_{shk}} \rho(r, \varphi, \Delta_{shk}; t) \tag{16}
\end{align}

Equation of motion \([\text{13}]\) allows us to show that the average of $\exp(-\Delta_{shk})$ is time-independent,

\begin{equation}
    \frac{d}{dt} \int d\varphi d\mathbf{r} \rho(r, \varphi, \Delta_{shk}; t) e^{-\Delta_{shk}} = 0, \tag{17}
\end{equation}

which leads \([\text{17}]\) to the integral fluctuation theorem for the housekeeping entropy production,

\begin{equation}
    \langle \exp(-\Delta_{shk}) \rangle = 1. \tag{18}
\end{equation}

We note that fluctuation theorem \([\text{18}]\) is valid for any time dependence of the control parameter, including the time-independent order parameter, i.e. the steady state.

The average steady state housekeeping entropy production, which can be calculated from Eq. \([\text{16}]\) as

\begin{equation}
    \partial_t \langle \Delta_{shk} \rangle = T^{-1} \langle \gamma_t v_{ts}^2 + \gamma_r v_{rs}^2 \rangle, \tag{19}
\end{equation}

can be related to a violation of the fluctuation-response relation via an equality equivalent to the Harada-Sasa relation \([\text{48}]\). To prove this equality we first consider a perturbation of our system, initially in a steady state, by a weak, constant in space, external force $\mathbf{f}_{\text{ext}}(t)$. The change of the average translational velocity of the particle can be expressed in terms of response function $\mathbf{R}(t)$,

\begin{equation}
    \delta \langle \mathbf{v}_t(t) \rangle = \epsilon \int_{-\infty}^{t} \mathbf{R}(t - t') \cdot \mathbf{f}_{\text{ext}}(t'). \tag{20}
\end{equation}

The response function (which geometrically is a second rank tensor) has an instantaneous part and a time delayed part. The short-time limit of the time-delayed response can be calculated as

\begin{equation}
    \mathbf{R}(0^+) = -\gamma_t^{-2} \int d\varphi (F + \gamma_t v_0 \mathbf{e}) \partial_\varphi p_s(r, \varphi), \tag{21}
\end{equation}

In an equilibrium Brownian system the time-dependent response function $R(t)$ is related to velocity autocorrelation function, $C(t) = \langle \mathbf{v}(t) \mathbf{v}(0) \rangle$ through the fluctuation-dissipation relation, $TR(t) = C(t)$. The velocity autocorrelation function has a part proportional to the $\delta$ function and a time-dependent part. For our system the short-time limit of the latter part can be calculated as

\begin{equation}
    C(0^+) = \gamma_t^{-2} \int d\varphi (F + \gamma_t v_0 \mathbf{e}) (F + \gamma_t v_0 \mathbf{e} - 2T \partial_r) p_s(r, \varphi), \tag{22}
\end{equation}

Combining Eqs. \([\text{21}]\) and \([\text{22}]\) and then using the equation for the steady-state probability distribution one can show that in a steady state

\begin{equation}
    \dot{S}(t) = \partial_t \langle \Delta_{shk} \rangle = (\gamma_t/T) \text{Tr} [C(0^+) - TR(0^+)]. \tag{23}
\end{equation}

Equality \([\text{23}]\) is the Harada-Sasa relation \([\text{48}]\) written in the time domain (note that the instantaneous part of $TR(t)$ cancels the $\delta$ function part of $C(t)$). It expresses the average steady state entropy production in terms of the violation of the fluctuation-dissipation relation involving the dynamics of the particle’s position. Interestingly, although the analogous fluctuation-dissipation relation for the dynamics of the particle’s orientation is not violated (in fact, rotational dynamics is free), the expressions for both the total and housekeeping entropy production include terms that originate from the rotational motion. We note that a generalized Harada-Sasa relation was also derived within a field-theoretical description of active matter \([\text{19}]\).

Hatano-Sasa relation and a generalized Clausius inequality. – Using Eq. \([\text{8}]\) we can write the entropy dissipation function

\begin{equation}
    \delta \mathbf{v}_t(t) = \epsilon \int_{-\infty}^{t} \mathbf{R}(t - t') \cdot \mathbf{f}_{\text{ext}}(t').
\end{equation}
pated into the medium as
\[
\Delta s_m(t) = T^{-1} \int_0^t dt' (\mathbf{F}(t') + \gamma_t v_0 \mathbf{e}(t')) \cdot \dot{\mathbf{r}}(t') \tag{24}
\]
\[
= \Delta s_{bh}(t) - \Delta \phi + \int_0^t dt' \lambda(t') \partial_x \phi(r, \varphi; \lambda),
\]
where \( \phi(t) = -\ln p_s(r(t), \varphi(t); \lambda(t)) \) and \( \Delta \phi = \phi(t) - \phi(0) \). Eq. (24) allows us to express the excess entropy production,
\[
\Delta s_{ex} = \Delta s_m - \Delta s_{bh}
\]
in terms of the last two terms.

Next, we note that Hatano and Sasa’s derivation of their Eq. (11) can be easily adapted to our model active system resulting in the following relation
\[
\left\langle \exp \left[ - \int_0^t dt' \lambda(t') \partial_x \phi(r, \varphi; \lambda) \right] \right\rangle = 1. \tag{25}
\]
Combining Eqs. (24) and (25) we get a version of the Hatano-Sasa relation,
\[
\left\langle \exp (-\Delta s_{ex} - \Delta \phi) \right\rangle = 1, \tag{26}
\]
and then using the Jensen inequality we obtain a generalized Clausius relation,
\[
-\langle \Delta s_{ex} \rangle \geq \Delta \langle \phi \rangle. \tag{27}
\]
The right-hand-side of Eq. (24) can be rewritten as the change of the average (Shannon) entropy of the system,
\[
\Delta \langle \phi \rangle = \Delta \left[ -\int dr d\varphi p_s(r, \varphi; \lambda) \ln p_s(r, \varphi; \lambda) \right]. \tag{28}
\]
It can be shown that for a quasi-static process Eq. (27) becomes an equality.

Recalling Eq. (24) and the definition of \( \Delta s_{bh} \) we can write the stochastic excess entropy production as
\[
\Delta s_{ex}(t) = -\int_0^t dt' [\partial_x \phi(r, \varphi; \lambda) \cdot \dot{\mathbf{r}}(t') + \partial_{\varphi} \phi(r, \varphi; \lambda) \dot{\varphi}(t')].
\]
Here, the first term at the right-hand-side can be interpreted as the excess entropy production in the medium. The second term, which has the form of the excess entropy production in the reservoir coupled to the self-propulsions, originates from non-trivial correlations between the particle’s position and self-propulsion.

Generalized Clausius inequality (27) extends the 2nd law of thermodynamics to active matter. For its derivation it is essential to distinguish between the total and the excess entropy production, since for quasistatic processes the former is not well defined [24].

Physically, in the limit of very fast evolution of self-propulsions one expects that an active system should be governed by some kind of effective thermodynamic description. In particular, one can show that in the limit of vanishing persistence time at constant effective temperature an Aoup becomes equivalent to a Brownian particle. We note that in this limit, the joint steady-state distribution factorizes a product of the distributions of the position and of the self-propulsion, and, if the external force is conservative, the former distribution acquires Gibbsian form. As a result, generalized Clausius inequality (27) becomes the standard Clausius inequality.

Integral fluctuation theorem for \( \Delta s_{tot} \). – To derive the above described framework we did not make any explicit assumptions regarding the behavior of the self-propulsion under the time-reversal symmetry [51]. We note that the identification [8] can be derived from the assumption that the self-propulsion is even under the reversal of time [12]. If we do use this assumption, we can derive an integral fluctuation theorem for the total entropy production following Seifert’s derivation of the analogous theorem in standard stochastic thermodynamics.

We consider a time dependent control parameter, i.e. a protocol, \( \lambda(t') \), and a reversed protocol \( \lambda(t')' = \lambda(t - t') \), and forward and reversed trajectories, \( \mathbf{x}(t') \) and \( \mathbf{x}(t')' = \mathbf{x}(t - t') \), where \( \mathbf{x} \equiv [r, \varphi] \). It can be shown that the ratio of the probabilities of the forward and backward trajectories, conditioned on their respective initial values, gives the stochastic entropy production in the medium, Eq. (27).

\[
\ln \frac{p[\mathbf{x}(t')|\mathbf{x}(0)]}{p[\mathbf{x}(t')'|\mathbf{x}(0)]} = \Delta s_m(t). \tag{30}
\]
Next, we combine the left-hand-side of Eq. (30) with normalized distributions of the initial values for the forward and reversed trajectories, \( p(\mathbf{x}(0)) \) and \( p(\mathbf{x}(0))' \), and we note that the latter distribution is equal to the distribution of the final values of the forward trajectory, \( p(\mathbf{x}(0)) = p(\mathbf{x}(t')) \). In this way we get
\[
\ln \frac{p[\mathbf{x}(t')|\mathbf{x}(0)]}{p[\mathbf{x}(t')'|\mathbf{x}(0)]} = \Delta s_{tot}(t), \tag{31}
\]
which leads to the integral fluctuation theorem for \( \Delta s_{tot} \),
\[
\left\langle \exp (-\Delta s_{tot}) \right\rangle = \sum_{\mathbf{x}(t'), \mathbf{x}(0)} p[\mathbf{x}(t')|\mathbf{x}(0)] p(\mathbf{x}(0)) e^{-\Delta s_{tot}} = \sum_{\mathbf{x}(t'), \mathbf{x}(0)} p[\mathbf{x}(t')|\mathbf{x}(0)] p(\mathbf{x}(0)) = 1. \tag{32}
\]

Perspective. – We proposed a generalization of the standard stochastic thermodynamics framework to active matter. We showed that many previously derived results, e.g. stochastic total and housekeeping entropies, their fluctuation theorems, Harada-Sasa and Hatano-Sasa relations, appear naturally in the new framework. This opens the way to experimental and computational studies of the thermodynamics of small active matter systems.

In our opinion, further work is needed in two directions. First, the framework presented here is naturally
well adapted to describe systems in which both thermal noise and self-propulsion are important. Indeed, the housekeeping entropy production quantifies the nonequilibrium character of an active system, compared to the corresponding equilibrium system without any activity. On the other hand, athermal systems with rapidly varying self-propulsion (e.g., an AOUP in the limit of vanishing persistence time) are equivalent to equilibrium systems. It would be interesting to develop a criterion quantifying how close a given active matter system is to the equivalent equilibrium system. Second, it would be interesting to analyze the work done by both external and self-propulsion forces, and to investigate whether a free energy-like quantity can be defined. We note that if an active system is close to the corresponding equilibrium system without any activity, one would try to follow Hatano and Sasa [24] and use the temperature of the medium to define the free energy. On the other hand, an active system with rapidly varying self-propulsion, which is close to an effective equilibrium system, one should probably use an effective temperature to define the free energy. It is at present unclear how to interpolate between these two cases.

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[29] Caprini et al. [14] proposed a generalization of the approach of Fodor et al. [7] to active systems in contact with a heat bath. Their procedure predicts that the entropy production vanishes for an active particle in a harmonic potential without thermal noise but seems to be non-vanishing if there is thermal noise, which would be
We note that one may go even further and include explicitly physicochemical events leading to the self-propulsion, see, e.g., P. Pietzonka and U. Seifert, J. Phys. A: Math. Theor. 51, 01LT01 (2018) and Supplementary Information for Ref. [12].

Our approach differs from that of Refs. [7, 8] by the inclusion of a heat bath. On the other hand, it differs from that of Ref. [13] by the explicit consideration of trajectories in the space of positions and self-propulsions.

For a real self-propelled colloidal particle $\gamma_t$ and $\gamma_r$ are related through a formula involving the radius of the particle but here we treat them as independent model parameters.

For a discussion of the time-reversal symmetry of the self-propulsion within the ABP model see, e.g. Ref. [12].