Thermodynamic Uncertainty Relation in Interacting Many-Body Systems

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The thermodynamic uncertainty relation (TUR) has been well studied for systems with few degrees of freedom. While, in principle, the TUR holds for more complex systems with many interacting degrees of freedom as well, little is known so far about its behavior in such systems. We analyze the TUR in the thermodynamic limit for mixtures of driven particles with short-range interactions. Our main result is an explicit expression for the optimal estimate of the total entropy production in terms of single-particle currents and correlations between two-particle currents. Quantitative results for various versions of a driven lattice gas demonstrate the practical implementation of this approach.

Introduction. Fluctuating currents and their correlations are a characteristic signature of stationary non-equilibrium systems. Exact results like the fluctuation theorem [1–5] and the Harada-Sasa relation [6] represent prominent, universal predictions that relate currents and their correlations to the arguably most central quantity for such systems – the rate of entropy production. More recently, the thermodynamic uncertainty relation (TUR) [7–9] has revealed an unexpected constraint on the precision of any current in terms of the total entropy production rate. Being a trade-off relation between precision and thermodynamic cost, in the sense that a high precision requires a large amount of entropy production, the TUR provides valuable insights into small mesoscopic non-equilibrium systems. It has opened a variety of promising applications like for molecular motors [10], heat engines [11–14], optimal design principles for self-assembly [15] or constraints on time windows in anomalously diffusing systems [16]. From the perspective of thermodynamic inference, being a simple tool for estimating entropy production by measuring experimentally accessible currents and their fluctuations without knowing interaction potentials or driving forces, the TUR has been established as an indispensable addition to more sophisticated inference methods [17–20].

To explore these two key properties of the TUR in more complex situations, subsequent work has focused on extending its range of applicability to a variety of systems including the observation of steady states in finite times [21, 22], underdamped dynamics [23–30], stochastic field theories [31], observables that are even under time-reversal [32–34], first-passage times [35, 36], relaxation processes [37–39], periodically [40, 41] and arbitrary time-dependently driven systems [42, 43]. Several of these generalizations have been (re-)derived by using virtual perturbations or information theoretic bounds [37, 44]. Last but not least, various studies have worked on generalizations of the TUR to open quantum systems [45–55].

When dealing with generalization and refinements of the TUR, a crucial question is how sharp the corresponding bounds typically are. Early analyses showed that the TUR can be saturated in the linear response regime due to Gaussian fluctuations [7, 8, 56, 57]. More recent studies have revealed that for the same reason it can become tight in the short-time limit [58, 59]. The same situation has been observed for the time-dependent TUR in the fast-driving limit [43, 60]. In all these cases, only the current of total entropy production, or a current proportional to it, leads to an equality in the TUR. Further works have focused on finding the optimal observable(s) leading to the tightest possible bound [57, 59, 61–65]. More specifically, using a sum of two observables and, thus, using correlations between them, can yield a sharper bound [66].

Most of the specific studies so far have treated single-particle systems or systems with a few degrees of freedom on a mesoscopic scale. As a crucial refinement of the TUR, the multidimensional thermodynamic uncertainty relation (MTUR) [67] should become useful when dealing with multiple currents and their correlations. While this refinement provides, in principle, the possibility to analyze systems with many interacting degrees of freedom, a systematic study of the thermodynamic limit is still missing.

In this Letter, we analyze the TUR in the thermodynamic limit and derive the optimal estimate of entropy production using the MTUR. Our results hold for any driven many-particle system obeying a Markovian dynamics on a discrete set of states or overdamped Langevin equations. We will illustrate our theoretical predictions with various versions of a driven lattice gas.

TUR in many-particle systems. The thermodynamic uncertainty relation has been proven under quite general conditions for both continuous-time Markov-processes and systems obeying coupled overdamped Langevin equations. It is valid for any current and reads [7–9]

$$\sigma^J_{\text{est}} \equiv \frac{J^2}{D_J} \leq \sigma,$$

(1)

where $J$ is the mean current, $D_J \equiv T \text{Var}[J]/2$ is its diffu-
tion coefficient, and $\mathcal{T}$ denotes the observation time [68]. The precision $J_2^2/D_J$ bounds the total entropy production rate $\sigma$ and, hence, yields an operationally accessible estimate $\sigma^J_{est}$ for it. To analyze the sharpness of the TUR, we define the quality factor as $Q_J \equiv \sigma_{est}^J/\sigma > 0$, which is 1 if the TUR is saturated. Since the TUR (1) holds for any current in the system, we can use an arbitrary linear combination of currents to build the estimate $\sigma^J_{est}$.

To study the TUR of interacting many-particle systems, we use a refinement of the TUR – the so-called MTUR introduced in Ref. [67]. We consider a system that consists of $N$ driven interacting particles leading to $N$ linearly independent particle currents $\{J^{(i)}\}$. The MTUR can be applied by inserting the optimal linear combination of these currents into (1). Within this class of currents, it thus yields the sharpest lower bound on the entropy production, which is given by

$$\sigma^J_{est} \equiv J^T C^{-1} J \leq \sigma.$$  

(2)

The estimator $\sigma^J_{est}$ involves the vector of particle currents $J \equiv (J^{(1)},...,J^{(N)})$ and the inverse of the symmetric correlation matrix $C$ with elements

$$C_{ij} \equiv D(i)^{\delta_{i,j}} + C(i)(1 - \delta_{i,j}).$$  

(3)

The diagonal element $D(i) \equiv T\text{Var}[J^{(i)}]/2$ is the diffusion coefficient of the current $J^{(i)}$ of the $i$th particle and the off-diagonal elements $C(i,j) \equiv T\text{Cov}[J^{(i)},J^{(j)}]/2$ are the scaled covariances between the currents $J^{(i)}$ and $J^{(j)}$ [68].

We use the MTUR to obtain the optimal estimate for entropy production in the thermodynamic limit for a system with different species of particles. First, we consider a homogeneous system with only one species driven by a thermodynamic force $f$. Here, all mean values $J^{(i)} \equiv J$, diffusion coefficients $D(i) \equiv D$ and correlations $C(i,j) \equiv C$ are identical. Since all particles are indistinguishable each current contributes with the same weight to the optimal linear combination such that the MTUR reduces to the ordinary TUR for the total particle current. Hence, the estimate is given by [68]

$$\sigma^J_{est} = \frac{N J^2}{D - C + NC},$$  

(4)

while the true entropy production reads $\sigma = \beta f NJ$ with the inverse temperature $\beta$ and $k_B = 1$. In the thermodynamic limit $N \to \infty$, the correlations generically decay like $C \approx \gamma/N$ with amplitude $\gamma$ since the probability to find two labelled particles near each other is proportional to the system size and, hence, at fixed density to the number of particles. When taking the thermodynamic limit $N \to \infty$, the quality factor becomes

$$Q_J \equiv \frac{\sigma^J_{est}}{\sigma} = \frac{J^\infty}{\beta f (D^\infty + \gamma)},$$  

(5)

where $J^\infty$ and $D^\infty$ are the value of the particle current and its diffusion coefficient in the thermodynamic limit, respectively. Equation (5) is our first main result and shows that the quality of the estimate depends solely on one- and two-particle quantities. For a driven ideal gas ($\gamma = 0$), the currents become uncorrelated and the $N$-particle system corresponds to a single-particle system. In contrast, for strong correlations between the particle currents, i.e., large absolute correlation amplitudes $\gamma$, the quality factor can differ strongly from the single-particle case.

Next, we study a homogeneous system consisting of a mixture of $N_1$ particles of species 1 and $N_2$ particles of species 2. The first and second species are driven by forces $f_1$ and $f_2$, respectively. Particles interact with a short-range interaction, which may be different between the species. The mean particle currents within a species are identical, i.e., $J^{(i)} = J^{(\alpha)}_{\alpha}$, where $\alpha_i \in \{1,2\}$ denotes the species of the $i$th particle. Analogously, the diffusion coefficients $D^{(i)} = D^{(\alpha)}_{\alpha}$ and correlations $C^{(i,j)} = C^{(\alpha,\alpha)}_{\alpha,\alpha}$ depend only on the particle species. Using Eq. (2) we get the estimate [68]

$$\sigma^J_{est} = \frac{\eta_1 N_1 J_1^2 + \eta_2 N_2 J_2^2 - 2 N_1 N_2 J_1 J_2 C_{12}}{\eta_{12} - N_1 N_2 C_{12}},$$  

(6)

with $\eta_\alpha \equiv D^{(\alpha)}_{\alpha} + (N_{\alpha} - 1)C_{\alpha\alpha}$ and $\alpha \in \{1,2\}$. The true entropy production is given by $\sigma = \beta f_1 N_1 J_1 + \beta f_2 N_2 J_2$. When taking the thermodynamic limit $N = N_1 + N_2 \to \infty$, we keep the densities $\rho_\alpha \equiv N_{\alpha}/N$ fixed. Analogously to the one-species case, the correlations $C_{11} \approx \gamma_1/N$, $C_{22} \approx \gamma_2/N$ and $C_{12} \approx \gamma_{12}/N$ decay proportional to the inverse system size, where $\gamma_1$, $\gamma_2$ and $\gamma_{12}$ are the correlation amplitudes. Thus, the quality factor in the thermodynamic limit reads

$$Q_J = \frac{\eta_{12}^\infty \rho_1 (J_1^\infty)^2 + \eta_{12}^\infty \rho_2 (J_2^\infty)^2 - 2 J_1^\infty J_2^\infty \rho_1 \rho_2 \gamma_{12}}{[\eta_1^\infty \rho_1^\infty - \rho_1 \rho_2^\infty \gamma_{12}^\infty] \beta (f_1 \rho_1 J_1^\infty + f_2 \rho_2 J_2^\infty)},$$  

(7)

where $\eta_\alpha^\infty \equiv D^{(\alpha)}_{\alpha} + \rho_\alpha \gamma_\alpha$ and $J_1^\infty$ and $J_2^\infty$ denote the values of the currents and diffusion coefficients in this limit, respectively. The quality factor in Eq. (7) is our second main result. In contrast to the one species case, this quality factor differs from the quality factor obtained by using as a current the total power [68]. In both cases, the MTUR remains a useful tool to infer entropy production, which, in particular, does not require the knowledge of any thermodynamic forces as we will now illustrate for the driven lattice gas.

**Driven lattice gas.** We consider a driven lattice gas [69] in which $N$ charged particles occupy sites on a periodic $(L \times L)$–square lattice subject to an exclusion interaction as shown in Fig. 1. The particles are driven by an electric field applied in the $x$-direction. Moreover, each particle interacts with its nearest neighbors either repulsively or attractively. The occupation variable $n_i(r) \equiv \delta_{r_i,r}$ at position $r \equiv (x,y)$ is one, if particle $i$ at $r_i \equiv (x_i,y_i)$ occupies this site and is zero, otherwise. The configuration of
the system is denoted by $\Gamma \equiv \{n_i(r)\}$, which contains information about all particle positions $R_\Gamma \equiv \{r_1, ..., r_N\}$.

In the following, we consider a system consisting of two species of particles with different charges $q_1$ and $q_2$. The interaction energy of the total system is given by

$$E_{\text{int}}(\Gamma) = -\sum_{i>j} K_{\alpha_i\alpha_j} \sum_{<rr'>} n_i(r)n_j(r'),$$

where $\sum_{<rr'>}$ denotes a summation over all nearest-neighbor-site pairs and $K_{\alpha_i\alpha_j}$ is the coupling constant of species $\alpha_i$ and $\alpha_j$ with $\alpha_{i,j} \in \{1, 2\}$. If $K_{\alpha_i\alpha_j} > 0$ the interaction is attractive, otherwise repulsive. The probability $p(\Gamma, t)$ to find the system in configuration $\Gamma$ at time $t$ obeys the master equation

$$\frac{\partial p(\Gamma, t)}{\partial t} = \sum_{r_i \in R_\Gamma, \, r_i' \in N(r_i)} \left[ p(\Gamma, r_i', t)k(r_i', r_i, \Gamma) - p(\Gamma, t)k(r_i, r_i', \Gamma) \right],$$

where $N(r_i)$ denotes a set of all unoccupied nearest neighbor sites $r_i' \equiv (x'_i, q'_i)$ of position $r_i$ and $\Gamma', r_i'$ denotes a configuration identical to $\Gamma$ except that particle $i$ occupies $r_i'$ instead of $r_i$. The transition rate for a particle at $r_i$ to move to an unoccupied nearest neighbor site $r_i'$ fulfills the local detailed balance condition and is given by

$$k(r_i, r_i', \Gamma) = \begin{cases} k_0 \exp(-\beta \kappa \Delta F), & \Delta F \geq 0 \\ k_0 \exp(\beta[1 - \kappa] \Delta F), & \Delta F < 0 \end{cases},$$

with

$$\Delta F \equiv E_{\text{int}}(\Gamma) - E_{\text{int}}(\Gamma', r_i') + (x_i - x'_i)q_\alpha E.$$

The rate amplitude $k_0$ determines the time scale for a transition, $q_\alpha \in \{q_1, q_2\}$ denotes the charge of the moving particle, and the parameter $\kappa$ determines the rate splitting.

**Quality factors.** We now analyze three paradigmatic models as depicted in Fig. 1. Model I consists of a single particle species with density $1/2$. Model II consists of $N_1$ particles of species 1 (red) and one single particle of species 2 (blue). Here, we distinguish two subclasses of models, which we denote as IIa) and IIb): in model IIa) only the single particle of species 2 is charged, i.e., $q_1 = 0$ and $q_2 \neq 0$, whereas in model IIb) all particles are charged with, in general, $q_1 \neq q_2$. The number of particles of the first species is chosen such that the density is $1/2$. Model III consists of two species (red and blue particles) with different charges, interactions, and densities $\rho_1 = \rho_2 = 1/4$. For all models, we fix the parameters $k_0 = 0.5$, $\beta = 1.0$, $E = 1.0$ and $\kappa = 1.0$ and choose an attractive interaction, i.e., $K_{11}, K_{22}, K_{12} > 0$. Moreover, we choose an observation time of $T = 1000.0$ to sample trajectories by using the Gillespie algorithm [70]. In the following, we analyze these systems for different system sizes $L \times L$ and an overall density of $1/2$.

Figure 2(a) shows the single-particle currents $J_1$ and $J_2$ of the two species for the models IIa) and IIb). The single driven particle in model IIa) generates a particle current $J_1$ of the $N_1$ non-driven particles by pushing or pulling them in the $x$-direction through the exclusion interaction and an attractive short-range interaction. Since this push- and pull-mechanism is a local effect, the number of pushed or pulled particles saturates in the thermodynamic limit, whereas the system size grows linearly in $N$. As a consequence, the current $J_1$ vanishes like $1/N$, whereas the current $J_2$ of the driven particle is finite as shown in Fig. 2(a). The optimal estimate of entropy production can be obtained by setting $N_2 = 1$ and $C_{22} = 0$ in Eq. (6). The true entropy production is given by $\sigma = \beta q_2 E J_2$. Combined with the fact that $J_1 \sim 1/N$ vanishes, these results imply that, in the thermodynamic limit $N \to \infty$, the quality factor becomes the quality factor of a single-particle problem $Q_1 = J_1^2/(\beta q_2 E D^2_2)$. The correlations between the particles do not contribute to the quality factor in contrast to model I with one single species [cf. Eq. (5)].

In model IIb), both particle currents $J_{1,2}$ are finite in the thermodynamic limit as shown in Fig. 2(a). The quality factor can analogously be obtained by setting formally $N_2 = 1$ and $C_{22} = 0$ in Eq. (6) and using $\sigma = \beta N_1 q_1 E J_1 + \beta q_2 E J_2$. When taking the thermo-
In this Letter, we have analyzed the thermodynamic uncertainty relation for interacting many-particle systems in the thermodynamic limit. We have calculated the quality factor using the MTUR for a homogeneous system consisting of a single species of particles and for a mixture of two species. As we have shown the TUR remains a useful tool for inferring entropy production since, crucially, the quality factors approach a finite order of 1 in the thermodynamic limit. From an operational perspective, it is neither necessary to know the driving fields nor the interactions between the particles in order to deduce the optimal estimate for entropy production. It suffices to measure the currents and correlations between two different ones. Even though these correlations vanish asymptotically, they are an essential ingredient to the TUR in systems with many degrees of freedom.

With these results, we have laid the foundation for future studies of the TUR in more complex systems, e.g., in systems with different phases or at a phase transition. We stress that the analytical results, Eqs. (4)–(7), apply to continuous overdamped Langevin systems as well. In this context, our model IIa) corresponds to a driven Brownian particle embedded in a colloidal suspension. Analyzing the TUR for different interaction potentials or for systems with more than two species is an important next step to explore macroscopic effects of the TUR. Since our tools rely on a widely applicable mathematical framework, our results should open the way for future research to study the thermodynamic limit of generalizations of the TUR, e.g., for time-dependently driven systems or for open quantum systems.
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Supplemental Material for "Thermodynamic Uncertainty Relation in Interacting Many-Body Systems"

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This supplemental material contains three sections. In the first section, we define the currents entering the TUR. In the second section, we explicitly calculate the inverses of the correlation matrices to obtain the optimal estimate of entropy production using the MTUR. In the third section, we calculate the quality factors of the total particle current and the total power for a mixture of two species.

I. DEFINITION OF CURRENTS

In this section, we will define the currents entering the TUR and the MTUR in Eqs. (1) and (2) in the main text, respectively. Since these two relations are valid for discrete and continuous systems, we will define currents for both system types. For the sake of simplicity, we consider two-dimensional systems. We first define currents for a general two-dimensional overdamped Langevin equation and then for the driven lattice gas as an example for a system with a discrete set of states.

We consider $N$ particles in two dimensions at positions $\mathbf{r} \equiv (\mathbf{r}_1, ..., \mathbf{r}_N)$ with coordinates $\mathbf{r}_i \equiv (x_i, y_i)$ obeying the overdamped Langevin equation

$$\partial_t \mathbf{r}_i \equiv \dot{\mathbf{r}}_i = \mu [−\nabla V_{\text{int}}(\mathbf{r}_i) + \mathbf{f}] + \sqrt{2G} \mathbf{\zeta}_i.$$  \hfill (1)

Here, $\mu$ is the $2N \times 2N$ mobility matrix, $\nabla V_{\text{int}}(\mathbf{r}_i)$ is the gradient of the interaction potential, $\mathbf{f} \equiv (f^{(1)}, ..., f^{(N)})$ is a vector containing $N$ non-conservative forces $f^{(i)} = (f^{x(i)}, f^{y(i)})$ with spatial components $f^{x(i)}$ and $f^{y(i)}$, $G$ is a $2N \times 2N$ matrix used to define the symmetric diffusion matrix $D \equiv GG^T = \mu/\beta$ and $\mathbf{\zeta}_i \equiv (\zeta^{x(i)}_i, ..., \zeta^{y(N)}_i)$ is a vector of $N$ white Gaussian noises $\zeta^{x(i)}_i \equiv [\zeta^{x(i)}_x(t), \zeta^{y(i)}_y(t)]$ describing the random forces with mean and correlations

$$\langle \zeta^{x(i)}_x(t) \rangle = 0,$$

$$\langle \zeta^{y(i)}_y(t) \rangle = 0,$$

$$\langle \zeta^{x(i)}_x(t) \zeta^{y(j)}_y(t') \rangle = \delta_{i,j} \delta(t - t'),$$  \hfill (2)

respectively, where $a, b \in \{x, y\}$. A general fluctuating current along the trajectory $\mathbf{r}_i$ of length $T$ reads

$$J[\mathbf{r}_i] \equiv \frac{1}{T} \int_0^T dt \mathbf{d}(\mathbf{r}_i) \circ \dot{\mathbf{r}}_i,$$  \hfill (3)

where $\mathbf{d}(\mathbf{r}_i) \equiv (d^{(1)}(\mathbf{r}_i), ..., d^{(N)}(\mathbf{r}_i))$ is a vector of arbitrary increments $d^{(i)}(\mathbf{r}_i) \equiv [d^{x(i)}(\mathbf{r}_i), d^{y(i)}(\mathbf{r}_i)]$ and $\circ$ denotes the Stratonovich product. The choice $\mathbf{d}(\mathbf{r}) = \beta \mathbf{f}$ in Eq. (4) corresponds to the total power

$$P[\mathbf{r}_i] \equiv \frac{1}{T} \int_0^T dt \beta \mathbf{f} \circ \dot{\mathbf{r}}_i.$$  \hfill (4)

Choosing $\mathbf{d}(\mathbf{r}) = e^{x(i)}_z$ as the unit vector of particle $i$ in direction $x$, we get the current in $x$-direction of particle $i$ as

$$J^{(i)}[\mathbf{r}_i] \equiv \frac{1}{T} \int_0^T dt \dot{x}_i(t),$$  \hfill (5)

with mean value $J^{(i)} \equiv \langle J^{(i)}[\mathbf{r}_i] \rangle$.

Next, we consider currents for the driven lattice gas discussed in the main text. The fluctuating current of particle $i$ along the trajectory $\Gamma_t$ of length $T$ reads

$$J^{(i)}[\Gamma_t] \equiv \frac{1}{T} \left[ n^{(i)}_x(T) - n^{(i)}_x(0) \right],$$  \hfill (6)

where $n^{(i)}_x(T)$ and $n^{(i)}_x(0)$ denote the total number of jumps of particle $i$ in positive and in negative $x$-direction up to time $T$, respectively. The mean value in Eq. (7) is defined as $J^{(i)} \equiv \langle J^{(i)}[\Gamma_t] \rangle$. Using Eq. (7), we define the particle currents of species 1 and 2 as

$$J_1[\Gamma_t] \equiv \frac{1}{N_1} \sum_{i=1}^{N} \delta_{1,i} J^{(i)}[\Gamma_t],$$  \hfill (7)

and

$$J_2[\Gamma_t] \equiv \frac{1}{N_2} \sum_{i=1}^{N} \delta_{2,i} J^{(i)}[\Gamma_t],$$  \hfill (8)

respectively. We denote the corresponding mean values by $J_1 \equiv \langle J_1[\Gamma_t] \rangle$ and $J_2 \equiv \langle J_2[\Gamma_t] \rangle$. The total power is given by

$$P[\Gamma_t] \equiv \beta q_1 EN_1 J_1[\Gamma_t] + \beta q_2 EN_2 J_2[\Gamma_t]$$  \hfill (9)

with mean value $P \equiv \langle P[\Gamma_t] \rangle = \beta q_1 EN_1 J_1 + \beta q_2 EN_2 J_2$.

The total particle current reads

$$J_{\text{tot}}[\Gamma_t] \equiv \sum_{i=1}^{N} J^{(i)}[\Gamma_t]$$  \hfill (10)

with mean value $J_{\text{tot}} \equiv \langle J_{\text{tot}}[\Gamma_t] \rangle = N_1 J_1 + N_2 J_2$. 


For currents in both, continuous and discrete systems, the diffusion coefficient and the correlations between two particle currents are defined as

\[ D^{(i)} = \mathcal{T} \text{Var}[J^{(i)}]/2 = \mathcal{T} \langle (J^{(i)})^2 \rangle / 2 \] (12)

and

\[ C^{(ij)} = \mathcal{T} \text{Cov}[J^{(i)}, J^{(j)}]/2 \equiv \mathcal{T} \langle J^{(i)} [X_t] J^{(j)} [X_t] \rangle - J^{(i)} J^{(j)}/2, \] (13)

respectively, with \( X_t \in \{ \tau_t, \Gamma_t \} \). The mean values of the power in Eqs. (5) and (10) coincide with the mean total entropy production, i.e., \( \sigma \equiv \langle \mathcal{P}[X_t] \rangle \). However, for any finite time \( \mathcal{T} \), their fluctuating values and consequently their diffusion coefficients are different. In contrast, for long observation times \( \mathcal{T} \to \infty \), the total fluctuating power becomes the total entropy production, i.e., \( \mathcal{P}[X_t] = \sigma [X_t] \), as the contribution of the change in internal energy and in stochastic entropy vanishes asymptotically.

**II. INVERSE OF THE CORRELATION MATRIX**

We explicitly calculate the inverse of the \( N \times N \) correlation matrix

\[ C_{ij} \equiv D^{(i)} \delta_{i,j} + C^{(ij)} (1 - \delta_{i,j}) \] (14)

for a homogeneous system with one and two species to get the optimal estimate for entropy production given by

\[ \sigma_{\text{est}}^J \equiv J^T C^{-1} J. \] (15)

We note that the optimal estimate via the MTUR (15) can be derived by building the linear combination of the particle currents \( J \equiv \sum_{i=1}^{N} \varphi_i J^{(i)} \), inserting \( J \) as a current into the ordinary TUR, Eq. (1) in the main text, and optimizing the estimate \( \sigma_{\text{est}}^J \) with respect to the coefficients \( \varphi_i \in \mathbb{R} \). The optimal estimator \( \sigma_{\text{est}}^{J^*} \) of the optimized linear combination \( J^* \equiv \sum_{i=1}^{N} \varphi_i^* J^{(i)} \) with coefficients \( \varphi_i^* \) then coincides with Eq. (15).

**Homogeneous System with one Species**

As outlined in the main text, the mean values \( J^{(i)} \equiv J \), diffusion coefficients \( D^{(i)} \equiv D \) and correlations \( C^{(ij)} \equiv C \) are independent of \( i \) and \( j \) for a homogeneous system. Thus, the correlation matrix (14) reads

\[ C_{ij} \equiv D \delta_{i,j} + C (1 - \delta_{i,j}). \] (16)

The inverse of this matrix is given by

\[ C^{-1}_{ij} = \left( \frac{D/C + N - 2}{D/C - 1} \right) \delta_{i,j} - \left( \frac{1 - \delta_{i,j}}{D/C - 1} \right), \] (17)

which can be easily verified by calculating \( \sum_j C^{-1}_{ij} C_{jk} = \delta_{ik} \). Inserting Eq. (17) into (15) yields the optimal estimate of entropy production, i.e., Eq. (4) in the main text. Since this estimate is identical to the estimate obtained when choosing the entropy production as a current in the ordinary TUR, the optimal coefficients \( \varphi_i^* \) are all identical, i.e., \( \varphi_i^* = \varphi_j^* \) for all \( i, j \).

**Homogeneous System with two Species**

Since the system is homogeneous, the currents \( J^{(i)} = J_{\alpha_i} \), the diffusion coefficients \( D^{(i)} = D_{\alpha_i} \) and the correlations \( C^{(ij)} = C_{\alpha_i \alpha_j} \) are identical within a species. Therefore, we split the vector \( J = (J_1, J_2) \) into the vectors \( J_1 \) and \( J_2 \), which contain \( N_1 \) entries of \( J_1 \) and \( N_2 \) entries of \( J_2 \), respectively. Moreover, we can split the correlation matrix into submatrices, i.e.,

\[ C = \begin{pmatrix} C_{11} & C_{12} \\ C_{12}^T & C_{22} \end{pmatrix} \] (18)

with the \( N_1 \times N_1 \) matrix \( C_{11} \), the \( N_2 \times N_2 \) matrix \( C_{22} \) and the \( N_1 \times N_2 \) matrix \( C_{12} \). The entries of the matrices \( C_{11} \) and \( C_{22} \) read

\[ (C_{11})_{ij} = D_1 \delta_{i,j} + C_{11} (1 - \delta_{i,j}) \] (19)

and

\[ (C_{22})_{ij} = D_2 \delta_{i,j} + C_{22} (1 - \delta_{i,j}), \] (20)

respectively. Both matrices consist of correlation functions between particles within a species, whereas the matrix \( C_{12} \) with entries

\[ (C_{12})_{ij} = C_{12} \delta_{i,j} + C_{12} (1 - \delta_{i,j}) \] (21)

consists of correlation functions between particles of different species.

To proof Eq. (6) in the main text, we present two alternatives. We first show heuristically that the problem of inverting the \( N \times N \)-matrix in Eq. (18) can be simplified to inverting a 2 \times 2 \( \mathcal{M} \). Then, we show a more rigorous way to invert the matrix (18) by using the block-matrix inversion formula.

As we have previously derived for a homogeneous system with one species, the optimal coefficients \( \varphi_i^* \) are all identical within a species. As a consequence, each current within a species contributes with the same weight to the optimal estimate for entropy production. Thus, the optimal estimate reads

\[ \sigma_{\text{est}}^{J^*} = J'^T C'^{-1} J' \] (22)

with \( J' = (J_1, J_2) \) and the \( 2 \times 2 \)-matrix

\[ C' = \begin{pmatrix} N_1 \eta_1 & N_1 N_2 C_{12} \\ N_1 N_2 C_{12} & N_2 \eta_2 \end{pmatrix}, \] (23)
where \( \eta_\alpha \equiv D_\alpha + (N_\alpha - 1)C_{\alpha\alpha} \) and \( \alpha \in \{1, 2\} \). Calculating the inverse of the matrix in Eq. (23) and inserting it into (22) leads to Eq. (6) in the main text.

For a more rigorous proof of the optimal estimate in Eq. (6) in the main text, we have to explicitly calculate the inverse of the matrix in Eq. (23) and inserting it into (22) leads to Eq. (6) in the main text.

For a mixture of two particle species, the total entropy production reads

\[
\sigma = \beta f_1 N_1 J_1 + \beta f_2 N_2 J_2,
\]

where \( f_{1,2} \) are non-conservative forces acting on particle species 1 and 2, respectively. To derive the quality factors, we use the identity

\[
\text{Var} [J] = \sum_{i=1}^{N} \varphi_i^2 \text{Var} [J^{(i)}] + 2 \sum_{i>j} \varphi_i \varphi_j \text{Cov} [J^{(i)}, J^{(j)}]
\]

for a current \( J [\Gamma] = \sum_{i=1}^{N} \varphi_i J^{(i)} [\Gamma_T] \). Using (32) for evaluating the diffusion coefficient \( D_J \) and choosing \( \varphi_i = \Phi_{\alpha_i} \) as arbitrary species dependent increments \( \Phi_{\alpha_i} \in \{ \Phi_1, \Phi_2 \} \) yields for homogeneous systems

\[
D_J \Phi_{\alpha_1} N_1 D_1 + \Phi_{\alpha_2} N_2 D_2
+ \Phi_{\alpha_1} N_1(N_1 - 1)C_{11} + \Phi_{\alpha_2} N_2(N_2 - 1)C_{22}
+ 2 \Phi_1 \Phi_2 N_1 N_2 C_{12}.
\]

Choosing \( \Phi_1 = f_1 \) and \( \Phi_2 = f_2 \) leads to the estimator of the total power

\[
M \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}
\]

the block-inversion formula reads

\[
K = C_{22} - C_{21} C_{11}^{-1} C_{12}.
\]

Analogously to Eq. (17), the inverse of the matrix \( C_{11} \) is given by

\[
(C_{11}^{-1})_{ij} = \frac{(D_1/C_{11} + N_1 - 2)\delta_{ij} - (1 - \delta_{ij})}{(D_1/C_{11} - 1) \left[ (D_1/C_{11} - N_1) + N_1 \right]},
\]

and the inverse of matrix \( K \) is given by

\[
K_{ij}^{-1} = \frac{|(D_2 - m_{12})/(C_{22} - m_{12}) + N_2 - 2|\delta_{ij} - (1 - \delta_{ij})}{|((D_2 - m_{12})/(C_{22} - m_{12}) - 1)\left[ ((D_2 - m_{12})/(C_{22} - m_{12})) + N_2(C_{22} - m_{12}) ]\right|}
\]

with

\[
m_{12} \equiv \frac{C_{12}^2 N_1}{D_1 - C_{11} + N_1 C_{11}}.
\]

Inserting the inverses (28) and (29) into Eq. (26), evaluating all terms and writing them into a symmetric form with respect to the particle species yields finally Eq. (6) in the main text.

III. QUALITY FACTORS

In this section, we derive the quality factor of the total power \( Q_p \) and of the total particle current \( Q_{j_{tot}} \) for a mixture of two particle species and show that, in general, these quality factors differ from the quality factor of the MTUR \( Q_J \).

For a mixture of two particle species, the total entropy

\[
\begin{pmatrix} A^{-1} + A^{-1}B (D - CA^{-1}B)^{-1} CA^{-1} - A^{-1}B (D - CA^{-1}B)^{-1} \end{pmatrix}.
\]

Using (25) to calculate the inverse of the matrix in (18) and inserting it into (15) yields

\[
\begin{pmatrix} J \end{pmatrix} = \begin{pmatrix} J^T \end{pmatrix} % \text{Cov} [J] = \sum_{i=1}^{N} \varphi_i^2 \text{Var} [J^{(i)}] + 2 \sum_{i>j} \varphi_i \varphi_j \text{Cov} [J^{(i)}, J^{(j)}]
\]

\[
\begin{pmatrix} J \end{pmatrix} = \begin{pmatrix} J \end{pmatrix} % \text{Cov} [J] = \sum_{i=1}^{N} \varphi_i^2 \text{Var} [J^{(i)}] + 2 \sum_{i>j} \varphi_i \varphi_j \text{Cov} [J^{(i)}, J^{(j)}]
\]

\[
\begin{pmatrix} J \end{pmatrix} = \begin{pmatrix} J \end{pmatrix} % \text{Cov} [J] = \sum_{i=1}^{N} \varphi_i^2 \text{Var} [J^{(i)}] + 2 \sum_{i>j} \varphi_i \varphi_j \text{Cov} [J^{(i)}, J^{(j)}]
\]
\[
\sigma_{\text{est}}^P \equiv \frac{P^2}{D_P} = \frac{(\beta f_1 N_1 J_1 + \beta f_2 N_2 J_2)^2}{\beta^2 f_1^2 N_1 D_1 + \beta^2 f_2^2 N_2 D_2 + \beta^2 f_1^2 N_1 (N_1 - 1) C_{11} + \beta^2 f_2^2 N_2 (N_2 - 1) C_{22} + 2 \beta^2 f_1 f_2 N_1 N_2 C_{12}}
\]

(34)

and choosing \( \Phi_1 = \Phi_2 = 1 \) leads to the estimator of the total particle current

\[
\sigma_{\text{est}}^{J_{\text{tot}}} \equiv \frac{J_{\text{tot}}^2}{D_{J_{\text{tot}}}} = \frac{(N_1 J_1 + N_2 J_2)^2}{N_1 D_1 + N_2 D_2 + N_1 (N_1 - 1) C_{11} + N_2 (N_2 - 1) C_{22} + 2 N_1 N_2 C_{12}}.
\]

(35)

By using the estimators Eqs. (34) and (35) and taking the thermodynamic limit \( N \to \infty \), we get the the quality factor of the total power

\[
Q_P \equiv \frac{\sigma_{\text{est}}^P}{\sigma} = \frac{\beta f_1 \rho_1 J_1 + \beta f_2 \rho_2 J_2}{\beta^2 f_1^2 \rho_1 D_1 + \beta^2 f_2^2 \rho_2 D_2 + \beta^2 f_1^2 \rho_1 \gamma_{11} + \beta^2 f_2^2 \rho_2 \gamma_{22} + 2 \beta^2 f_1 f_2 \rho_1 \rho_2 \gamma_{12}}
\]

(36)

and the quality factor of the total particle current

\[
Q_{J_{\text{tot}}} \equiv \frac{\sigma_{\text{est}}^{J_{\text{tot}}}}{\sigma} = \frac{(\rho_1 J_1 + \rho_2 J_2)^2}{(\rho_1 D_1 + \rho_2 D_2 + \rho_1 \gamma_{11} + \rho_2 \gamma_{22} + \rho_1 \rho_2 \gamma_{12}) (\beta f_1 \rho_1 J_1 + \beta f_2 \rho_2 J_2)}
\]

(37)

in the thermodynamic limit. The quality factors (36) and (37) are in general different than the quality factor based on the MTUR in Eq. (7) in the main text. However, in the one-species case \( \rho_2 = 0 \), these quality factors coincide with the quality factor based on the MTUR [cf. Eq. (5) in the main text].