Three-body problem for Langevin dynamics with different temperatures

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A mixture of Brownian particles at different temperatures has been a useful model for studying the out-of-equilibrium properties of systems made up of microscopic components with differing levels of activity. This model was previously studied analytically for two-particle interactions in the dilute limit, yielding a Boltzmann-like two-particle distribution with an effective temperature. Like the Newtonian two and three-body problems, we ask here whether the two-particle results can be extended to three-particle interactions to get the three-particle distributions. By considering the special solvable case of pairwise quadratic interactions, we show that, unlike the two-particle distribution, the three-particle distribution cannot in general be Boltzmann-like with an effective temperature. We instead find that the steady state distribution of any two particles in a triplet depends on the properties of and interactions with the third particle, leading to some unexpected behaviors not present in equilibrium.

I. INTRODUCTION

Common to many biological and artificial out-of-equilibrium systems is the presence of a local drive that pushes the systems away from equilibrium, that is, individual components within a system locally consume energy to generate forces and motion [1]. Such systems include molecular motors [2–4], artificial swimmers [5–8], bacteria [9], and biological tissues [10, 11]. One class of models frequently used to study these systems is active particles, consisting of particles self-propelled by a local force whose direction changes randomly. It has been observed that such systems exhibit emergent, out-of-equilibrium phenomenon such as phase separation in the absence of attractive interactions [12] and preferential motion in ratchet-like systems [13, 14].

Another recently studied class of models consists of mixtures of particles in contact with thermostats at different temperatures [15–30]. This type of system is in some way similar to a mixture of passive and active particles, where the active particles are instead treated as having a higher temperature and hence, a higher diffusivity. As has been shown in theory [15] and simulations [16, 17], uniform mixtures of such particles become unstable for large temperature ratios and tend to phase separate into distinct regions of cold and hot particles. This behavior is most striking in a mixture of interacting polymers at different temperatures, where even a moderate temperature ratio can lead to strong phase separation [18, 19].

A mixture of two types of particles at temperatures \( T_1 \neq T_2 \) was studied analytically in the dilute limit [15] using the steady state pair distribution of particle types \( i, j \) in the mixture given by \((k_B = 1)\)

\[
P_{ij}(r, r') \sim \exp \left(-\frac{1}{T_{ij}} U_{ij}(|r-r'|)\right),
\]

where the parameter \( T_{ij} \), which we call a pairwise temperature, is

\[
T_{ij} = \frac{\gamma_j T_i + \gamma_i T_j}{\gamma_i + \gamma_j},
\]

and \( \gamma_1, \gamma_2 \) are friction coefficients of the two types of particles. While \( P_{11}, P_{22} \) with \( T_{11} = T_1 \) and \( T_{22} = T_2 \) are the equilibrium pair distributions for like particles, \( P_{12} \) and \( T_{12} \) are entirely new; in particular, they involve the transport properties \( \gamma_1, \gamma_2 \) of the particles, which is impossible in equilibrium systems. Using these pair distributions, it was found that the system has non-equilibrium analogs to free energy, chemical potential, and pressure up to a second virial-like approximation [18].

In analogy with the Newtonian mechanics, a natural next step from studying two-particle distributions for Langevin dynamics with different temperatures is to consider the three-particle behaviors and determine the three-particle distributions. We ask here whether Boltzmann-like distributions similar to Eq. [1] can be found for three interacting particles. As one might expect, there is a significant increase in difficulty going from the two-body to three-body problem. By considering pairwise additive quadratic potentials, we show that even in steady state, the distribution for three particles does not take on a simple Boltzmann-like form with one effective temperature as it does for two particles. Instead, the three-particle distribution takes on a generalized form where there are three distinct pairwise temperatures for each pair of particles. Moreover, each pairwise temperatures depends strongly on the properties of all three particles and in addition, on the interactions between them. This leads to some peculiar behaviors that are only present when the temperatures or activities are different.

II. THE GENERAL PROBLEM

The usual starting point for studying a mixture of colloidal particles is a system of overdamped Langevin equa-
tions. One approach for incorporating different levels of activity is by placing each particle in contact with thermostats of differing temperatures, which can be described by having different noise amplitudes in the Langevin equations for each particle or degree of freedom [13–17, 21]. The overdamped Langevin equations describing our three particles are

$$\gamma_i \dot{r}_i = -\nabla_{r_i} U(r_1, r_2, r_3) + \sqrt{2T_i \gamma_i} \xi_i,$$  \hspace{1cm} (3)

where \(\gamma_i\) are the friction coefficients, \(U\) is some potential energy, and \(\xi_i\) are independent, unit-variance Gaussian white noises (and with independent Cartesian components). Here and throughout the rest of the paper, we set \(k_B = 1\). Note that we can reformulate this system in terms of diffusivities \(D_i = T_i/\gamma_i\). The key here is that the quantities \(D_i\gamma_i\) are not equal to one temperature, that is, Einstein’s relation [31] is violated and the system is not in equilibrium.

For our present purposes, we focus on the pairwise additive interaction potential \(U(r_1, r_2, r_3) = U_{12}(r_1 - r_2) + U_{23}(r_2 - r_3) + U_{13}(r_1 - r_3)\), much like what is typically done for the equilibrium theory of classical interacting particles [32]. Finally, in the context of phase separation in a mixture of \(A\) and \(B\) particles, the three particles now considered can be either \(AAAA\), \(AABB\), \(ABBB\) and \(BBBB\) with temperatures \(\{T_A, T_A, T_A\}\), \(\{T_A, T_B, T_B\}\), \(\{T_A, T_A, T_B\}\), and \(\{T_B, T_B, T_B\}\), respectively. To simplify the analysis, we find it easier to keep the temperatures \(T_1, T_2, T_3\) general.

The Langevin equation Eq. (3) can be recast into the Fokker-Planck equation \(\partial_t P = -\sum_i \nabla_{r_i} \cdot J_i\), where the currents \(J_i\) are

$$J_i = -\frac{1}{\gamma_i} (\nabla_{r_i} U) P - \frac{T_i}{\gamma_i} \nabla_{r_i} P.$$  \hspace{1cm} (4)

In equilibrium with \(T_1 = T_2 = T_3 = T\), the currents \(J_i\) are zero, which gives the usual Boltzmann distribution

$$P(r_1, r_2, r_3) \sim \exp \left[ -\frac{1}{T} U(r_1, r_2, r_3) \right].$$  \hspace{1cm} (5)

Out of equilibrium in steady state, the divergence of the current is still zero, that is, \(\sum_i \nabla_{r_i} \cdot J_i = 0\). However, the currents themselves do not have to be zero as they can have nonzero curls, which makes it difficult to determine the three-particle distribution. Based on the results of the two-particle case, a simple guess for the three-particle distribution is

$$P(r_1, r_2, r_3) \sim \exp \left[ -\frac{1}{T_{\text{eff}}} U(r_1, r_2, r_3) \right],$$  \hspace{1cm} (6)

for some effective temperature \(T_{\text{eff}}\). However, as we will see in Section III for the simple case of pairwise quadratic interactions, the distribution takes on the form

$$P(r_1, r_2, r_3) \sim \exp \left[ -\frac{U_{12}}{T_1} - \frac{U_{23}}{T_2} - \frac{U_{13}}{T_3} \right],$$  \hspace{1cm} (7)

where \(U_{ij} = U_{ij}(r_i - r_j)\) and \(T_{ij}\), which we call “pairwise temperatures”, depend on properties of and interactions between all three particles and not just each particle pair \(i,j\).

### III. PAIRWISE QUADRATIC INTERACTIONS

Suppose the particles are connected by ideal springs with potential energies \(U_{ij} = \frac{1}{2} k_{ij} (r_i - r_j)^2\). It is worth mentioning that while quadratic potentials are special, they have been useful in many contexts such as membranes, proteins, and polymers [21, 22, 33–39]. The Langevin equations describing the system with potential energy \(U = U_{12} + U_{23} + U_{13}\) are

$$\gamma_1 \dot{r}_1 = -\kappa_{12} (r_1 - r_2) - \kappa_{13} (r_1 - r_3) + \sqrt{2T_1 \gamma_1} \xi_1,$$  \hspace{1cm} (8a)

$$\gamma_2 \dot{r}_2 = -\kappa_{12} (r_2 - r_1) - \kappa_{23} (r_2 - r_3) + \sqrt{2T_2 \gamma_2} \xi_2,$$  \hspace{1cm} (8b)

$$\gamma_3 \dot{r}_3 = -\kappa_{13} (r_3 - r_1) - \kappa_{23} (r_3 - r_2) + \sqrt{2T_3 \gamma_3} \xi_3.$$  \hspace{1cm} (8c)

One can establish by direct inspection that the steady state distribution of the separations between the particles can be written as

$$P(r_1, r_2, r_3) \sim \exp \left[ -\frac{\kappa_{12}}{2T_1} (r_1 - r_2)^2 - \frac{\kappa_{23}}{2T_2} (r_2 - r_3)^2 - \frac{\kappa_{13}}{2T_3} (r_1 - r_3)^2 \right],$$  \hspace{1cm} (9)

where the pairwise temperatures \(T_{12}, T_{23}, T_{13}\) can be found from the steady state Fokker-Planck equation \(\sum_i \nabla_{r_i} \cdot J_i = 0\). Note that for boundary conditions, we simply require the distribution to decay sufficiently fast for infinite separations such that it is normalizable. The details of the calculation and the general expressions for \(T_{ij}\) are shown in Appendix A. The forms of \(T_{ij}\) are quite cumbersome although in equilibrium when \(T_1 = T_2 = T_3 = T\), we return to the usual Boltzmann distribution where \(T_{12} = T_{23} = T_{13} = T\). A quick glance immediately shows that the pairwise temperatures \(T_{ij}\) are not equal to each other. Since pairwise additive potentials is a simple case, this implies that the three-particle distribution cannot in general be written in a Boltzmann-like form with one effective temperature given by Eq. (6).

In addition, the pairwise temperatures depend not only on properties of all of the particles, but also on the interactions (spring constants) between them. This means that for more general pairwise potentials, the exponent in Eq. (6) cannot be written as a linear combination of pair potentials \(U_{ij}\) such that the coefficients or inverse pairwise temperatures \(T_{ij}^{-1}\) are independent of positions.

To summarize, the simple case of pairwise additive quadratic potentials shows that the three-particle dis-
distribution does not generalize the same way as the two-particle distribution when the temperatures of the particles are different.

IV. SIMPLIFIED CASES

Section III outlines a simple proof showing that the three-particle distribution for Brownian particles at different temperatures cannot be written in a Boltzmann-like form with one effective temperature. In addition, it shows that the pairwise temperatures $T_{ij}$ for particles $i,j$ depend not only on the properties of the third particle but also the interactions with it. Beyond the proof, and in the spirit of a more general three-body problem for Langvin dynamics, it is now interesting to study the distributions and pairwise temperatures by looking at simpler forms to see how differences in temperatures or activities of the three particles affects their behaviors.

A. Identical particles and springs, but different temperatures

Let us first consider the simplest non-equilibrium case when the temperatures $T_1, T_2, T_3$ are different while $\gamma_1 = \gamma_2 = \gamma_3 = \gamma$ and $\kappa_{12} = \kappa_{23} = \kappa_{13} = \kappa$. The pairwise temperatures $T_{ij}$ in Eq. (9) reduce to

$$T_{ij} = \frac{T_i T_j}{3} \left( \frac{1}{T_1} + \frac{1}{T_2} + \frac{1}{T_3} \right).$$

(10)

There are some observations to make:

- The correlation of particles 1 and 2 relative to 3 is given by $(r_{13} \cdot r_{23}) = \frac{T_2}{T_3}$, which is interestingly not controlled by temperatures $T_1, T_2$. If we take $T_3 \to 0$, that is, particle 3 is no longer driven by a bath, the three-particle distribution becomes

$$P \sim \exp \left[ -\frac{3\kappa}{2T_2} (r_2 - r_3)^2 - \frac{3\kappa}{2T_1} (r_1 - r_3)^2 \right].$$

(11)

and of course we have $(r_{13} \cdot r_{23}) = 0$. This suggests that relative to particle 3, particles 1 and 2 behave like two non-interacting Brownian particles despite there being a spring connecting the two. In a sense, the system $r_{13}, r_{23}$ becomes floppy.

- We may also be interested in how the distribution of a pair of particles is affected by the third. Integrating out, say, particle 3 (the choice does not matter in this case), we obtain $P(r_1, r_2) \sim \exp \left[ -\frac{\kappa}{2T_{12}} (r_1 - r_2)^2 \right]$ where the effective pairwise temperature $\tilde{T}_{12}$ is

$$\tilde{T}_{12} = \frac{T_1 + T_2}{3}.$$  

(12)

The average potential energy stored in the spring between particles 1 and 2 is $\langle U_{12} \rangle = \frac{d}{2} T_{12}$, where $d$ is the spacial dimension. Note that the distribution $P(r_1, r_2)$ and the average potential energy are independent of the activity (temperature) of particle 3. This, however, is not in general true as we will see when the particles and springs are not all identical.

The pairwise temperatures can be generalized to $N$ identical particles, all connected by identical springs. Details of the calculation can be found in Appendix III. The pairwise temperatures are

$$T_{ij} = \frac{T_i T_j}{N} \sum_{n=1}^{N} \frac{1}{T_n} = \frac{T_i T_j}{T_H},$$

(13)

where $T_H$ is the harmonic mean of all the temperatures. Interestingly, if we take for example $T_N = 0$, particles $1, 2, \ldots, N - 1$ appear to be noninteracting relative to particle $N$. The potential energy stored in the spring between particles $i,j$ generalizes as

$$\langle U_{ij} \rangle = \frac{d}{2N} (T_i + T_j).$$

(14)

This potential energy is independent of the temperatures of the other particles.

B. Softer or stiffer spring

Let us now consider a slightly more complex case by softening or stiffening the spring between one pair of the particles, for example, $\kappa_{23} = \kappa_{13} = \kappa \neq \kappa_{12}$. The pairwise temperatures are

$$T_{12} = \frac{\kappa_{12} A}{2T_3(\kappa + 2\kappa_{12}) - (T_1 + T_2)(\kappa - \kappa_{12})},$$

(15a)

$$T_{23} = \frac{(2\kappa + \kappa_{12}) A}{3[3T_1(\kappa + \kappa_{12}) + T_2(\kappa - \kappa_{12})]},$$

(15b)

$$T_{13} = \frac{(2\kappa + \kappa_{12}) A}{3[3T_2(\kappa + \kappa_{12}) + T_1(\kappa - \kappa_{12})]},$$

(15c)

where

$$A = \frac{(T_1 - T_2)^2(\kappa - \kappa_{12})^2}{2(2\kappa + \kappa_{12})^2} + 2(T_1T_2 + T_2T_3 + T_1T_3).$$

(16)

- A simple limit to check is $\kappa_{12} \to \infty$. We expect particles 1 and 2 to effectively merge and the system to reduce to two particles. Taking the limit, we see that the three-particle distribution becomes

$$P(r_1, r_2, r_3) \sim \delta(r_1 - r_2) \exp \left[ -\frac{\kappa}{T_{12} T_3} (r_1 - r_3)^2 \right],$$

(17)

where $T_{12} T_3$ is the potential temperature of the combined particle $\{12\}$ and particle 3. Eq. (17) can correctly be interpreted as the distribution of two particles with properties $T_3, \gamma$ and $T_3 \frac{T_2}{T_1} = 2\gamma$ connected by a spring with combined stiffness $2\kappa$. This result does have a simple generalization for arbitrary springs and friction coefficients, which we discuss in Section IV D.
The correlations of particles 1 and 2 relative to 3 in this case become
\[ \langle r_{13} \cdot r_{23} \rangle = \frac{T_3 - T_3^*}{3\kappa}, \]  
where \( T_3^* = \frac{(T_1 + T_2)(\kappa - \gamma_{12})}{2(\kappa + 2\kappa_{12})} \). Here, we see an effect that is not present in equilibrium. In equilibrium when \( T_1 = T_2 = T_3 = T \), we have \( \langle r_{13} \cdot r_{23} \rangle = \frac{\kappa T_3^2}{3(\kappa_{12} + \kappa)} \), which is positive for any \( \kappa_{12} > 0 \). This is of course due to the spring connecting particles 1 and 2. When the temperatures are not equal and \( \kappa_{12} < \kappa \), however, we see that \( \langle r_{13} \cdot r_{23} \rangle \) can be negative and even zero. In particular, \( \langle r_{13} \cdot r_{23} \rangle < 0 \) when \( T_3 < T_3^* \) and particles 1 and 2 appear to be repulsive relative to 3 while \( \langle r_{13} \cdot r_{23} \rangle = 0 \) when \( T_3 = T_3^* \) and instead they appear non-interacting even though there is a spring between them. In terms of the distribution and the coefficient \( T_{ij}^{-1} \) of the pair potential \( U_{ij} \), these correspond to \( T_{ij} < 0 \) when \( T_3 < T_3^* \) and \( T_{ij} = 0 \) when \( T_3 = T_3^* \). If \( \kappa_{12} > \kappa \), there are similar sign changes in \( T_{23}^{-1} \) and \( \langle r_{21} \cdot r_{31} \rangle \) at \( T_1 = \frac{T_3(\kappa_{12} - \kappa)}{3(\kappa_{12} + \kappa)} \) and \( T_{13}^{-1} \) and \( \langle r_{12} \cdot r_{32} \rangle \) at \( T_2 = \frac{T_3(\kappa_{12} - \kappa)}{3(\kappa_{12} + \kappa)} \). Note that equilibrium, we simply have \( T_{12} = T_{23} = T_{13} = T \) irrespective of the choice of \( \kappa_{12} \).

Like in Section IV.A, we may be interested in how a pair of particles is affected by the third. Here, there are two choices of particles to integrate out. Integrating out particle 3, the particle across from the spring between particles 1 and 2, we have \( P(r_1, r_2) \sim \exp \left[ -\frac{\kappa}{2T_{12}}(r_1 - r_2)^2 \right] \) with
\[ \overline{T}_{12} = \frac{\kappa_{12}(T_1 + T_2)}{\kappa + 2\kappa_{12}}. \]  
If we instead integrated out, say, particle 2, we have \( P(r_1, r_3) \sim \exp \left[ -\frac{\kappa}{2T_{13}}(r_1 - r_3)^2 \right] \) with
\[ \overline{T}_{13} = \frac{1}{6(2\kappa + \kappa_{12})(\kappa + 2\kappa_{12})} \left[ T_1(7\kappa^2 + 10\kappa\kappa_{12} + \kappa^2_{12}) + 2T_3(2\kappa + \kappa_{12})(\kappa + 2\kappa_{12}) + T_2(\kappa - \kappa_{12})^2 \right]. \]  
The average potential energy stored in the spring between particles 1 and 2 is \( U_{12} = \frac{\kappa}{2T_{12}} \). This energy depends on \( \kappa \), the interaction with particle 3, but is still independent of the temperature \( T_3 \). In other words, the activity of the integrated-out particle does not affect the remaining two. This, however, is not the case for the average energy \( U_{13} = \frac{\kappa}{2T_{13}} \) stored in the spring between particles 1 and 3, as is evident by the appearance of \( T_2 \) in \( \overline{T}_{13} \). In equilibrium, \( \overline{T}_{13} = \frac{\kappa_{12}(\kappa_{12} + \kappa)}{\kappa + 2\kappa_{12}} \).

C. Particles with different mobilities

In equilibrium, the mobilities or transport properties of particles cannot enter into the Boltzmann distribution while out of equilibrium, they can. Suppose that \( \gamma_1 = \gamma_2 = \gamma \neq \gamma_3 \) while keeping the springs identical. This is the simplest case where the mobilities do not automatically drop out of the steady state Fokker-Planck equation \( \sum_i \nabla r_i \cdot J_i = 0 \). The pairwise temperatures are
\[ T_{12} = \frac{A}{6T_3(\gamma - \gamma_3)(\gamma + 2\gamma_3)}, \]  
\[ T_{23} = \frac{\gamma + 2\gamma_3}{(T_1(\gamma + 5\gamma_3) + T_2(\gamma - \gamma_3))(2\gamma + \gamma_3)}, \]  
\[ T_{13} = \frac{\gamma + 2\gamma_3}{(T_2(\gamma + 5\gamma_3) + T_1(\gamma - \gamma_3))(2\gamma + \gamma_3)}, \]  
where
\[ A = \frac{(T_1 - T_2)^2(\gamma - \gamma_3)^2}{2(\gamma + 2\gamma_3)^2} + 2(T_1T_2\gamma_3 + T_2T_3\gamma + T_1T_3\gamma). \]  
Just as the case with a softer or stiffer spring, if we integrate out particle 3, we find
\[ \overline{T}_{12} = \frac{T_1 + T_2}{3}. \]  
If we instead integrate out particle 2, we obtain
\[ \overline{T}_{13} = \frac{1}{6(2\gamma + \gamma_3)(\gamma + 2\gamma_3)} \left[ T_1(\gamma^2 + 10\gamma_3\gamma + 7\gamma_3^2) + 6T_3(\gamma + 2\gamma_3) + T_2(\gamma - \gamma_3)^2 \right]. \]  
Just as the case with softening or stiffening one of the springs in Section IV.B, we also observe similar sign changes in \( T_{ij}^{-1} \) and \( \langle r_{ik} \cdot r_{jk} \rangle \) depending on the choices of \( \gamma \) and the temperatures. In addition, the average energy stored in the spring between particles 1 and 3 \( \langle U_{13} \rangle = \frac{\kappa}{2T_{13}} \) also depends on the temperature \( T_2 \) of the integrated out particle. What is different here is that in equilibrium, the friction coefficients play no role in the distribution and behaviors of the three particles; in particular, \( \overline{T}_{12} = \overline{T}_{23} = \overline{T}_{13} = \frac{\kappa}{2} \) are completely independent of \( \gamma \)'s. Only when system is out of equilibrium and the temperatures are different do the mobilities have a significant effect.

D. Remark on the general case

The forms of \( T_{ij} \) for the general case of different spring constants and friction coefficients are quite cumbersome (Appendix A). There is a simple case. As mentioned in Section IV.B taking \( \kappa_{12} \rightarrow \infty \) corresponds to effectively merging particles 1 and 2, which reduces
the system to a combined particle \{12\} and particle 3. The properties of particle 3 are simply \(T_3, \gamma_3\). The combined particle \{12\} will have a total friction coefficient \(\gamma_{12} = \gamma_1 + \gamma_2\). The total drive on particle \{12\} is \(\xi_{12} = \sqrt{2T_1}\gamma_1 \xi_1 + \sqrt{2T_2}\gamma_2 \xi_2\) with correlations \(\langle \xi_{12}(t)\xi_{12}(t') \rangle = 2T_{12}\gamma_{12}\delta(t-t')\), where the effective temperature of \{12\} is \(T_{12} = \frac{\gamma_1 T_1 + \gamma_2 T_2}{\gamma_3 + (\gamma_1 + \gamma_2)}\).

Since the springs from particle 3 to particles 1 and 2 are in parallel, the total spring constant between particle \{12\} and particle 3 is \(\kappa_{13} + \kappa_2\). Note that when the friction coefficients are all equal, we get back \(T_{12} = \frac{T_1 + T_2 + 4T_3}{6}\) in Section IV.B.

\textbf{V. UNDERDAMPED PARTICLES}

As we saw in Section III for pairwise quadratic interactions, including a new degree of freedom, a third particle, leads to a complicated distribution that cannot be written in a generalized Boltzmann-like form where the pairwise temperatures depend only on pair properties of the particles (Eq. (26)). Instead, the pairwise temperatures must depend on the properties of all the particles, and in addition on the springs between them. Because of that, it is interesting to look at another way of including additional degrees of freedom by considering underdamped particles, where there are momenta in addition to positions.

\textbf{A. Two underdamped particles}

Consider the case of two underdamped particles, where we now have four degrees of freedom: two positions and two momenta. For simplicity, suppose both particles have the same mass \(m\) and friction coefficient \(\gamma\), but different temperatures \(T_1, T_2\). The Langevin equations are

\[
\dot{r} = \frac{1}{m}(p_1 - p_2), \tag{26a}
\]

\[
p_1 = -\frac{\gamma}{m}p_1 - \kappa r + \sqrt{2T_1}\gamma \xi_1, \tag{26b}
\]

\[
p_2 = -\frac{\gamma}{m}p_2 + \kappa r + \sqrt{2T_2}\gamma \xi_2, \tag{26c}
\]

where \(p_i = m\dot{r_i}\) and \(r = r_1 - r_2\). We find the steady-state probability distribution

\[
P(r, p_1, p_2) \sim \exp \left[ -\frac{1}{2} \left( \beta_{p_1} p_1^2 + \beta_{p_2} p_2^2 + \beta_{rr} r^2 + 2\beta_{p_1} p_1 \cdot p_2 + 2\beta_{p_1} p_1 \cdot r + 2\beta_{p_2} p_2 \cdot r \right) \right], \tag{27}
\]

where the off-diagonal coefficients \(\beta_{p_1} p_2, \beta_{p_1} r, \beta_{p_2} r\) are nonzero when \(T_1 \neq T_2\). Such a distribution with nonzero cross terms has been reported in similar systems [21,22]. Of course in equilibrium when \(T_1 = T_2 = T\), we obtain the usual Boltzmann distribution \(P \sim \exp \left[ -\frac{1}{T} \left( \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{\kappa r^2}{2} \right) \right]\). When the temperatures are different, however, we see that the distribution does not generalize the same way as it did for overdamped particles, that is, the distributions indicate correlations between momenta and positions.

\textbf{B. Kinetic energies and potential energies}

For three or more particles, the distribution takes on a form similar to Eq. (27) for \(p_1, p_2, p_3, r_1 - r_2, r_2 - r_3, r_1 - r_3\). The expressions, however, are significantly more cumbersome. We can still compute the average kinetic and potential energies. The case of \(N\) identical particles and springs can be found in Appendix C.2.

For \(N\) identical particles all connected by identical springs, the average kinetic energy \(\langle K_i \rangle\) of the \(i\)th particle is

\[
\langle K_i \rangle = \frac{d}{2} \left( T_i - T_{\text{avg}} \right), \tag{28}
\]

where \(T_{\text{avg}} = \frac{1}{N} \sum_{n=1}^{N} T_n\) is the average temperature. The potential energy stored between particles \(i, j\) is

\[
\langle U_{ij} \rangle = \frac{d}{2N} (T_i + T_j). \tag{29}
\]

This result is independent of mass and the other temperatures, similar to the overdamped case. However, if we change the interactions between the particles, for example taking \(\kappa_{23} = \kappa_{13} = \kappa \neq \kappa_{12}\) as before, the potential energies show a dependence on the mass. The results can be found in Appendix C.3.

\textbf{VI. DISCUSSION AND CONCLUSION}

For the two-body problem for Langevin dynamics with different temperatures, the two-particle distribution can be written in a Boltzmann-like form with an effective temperature (Eqs. (11) and (26)) [15]. For the three-body case, however, we showed that such a Boltzmann-like form with one effective temperature is not possible and instead, at least for the case of pairwise additive interactions.
the steady-state three-particle distribution acquires the form

\[ P(r_1, r_2, r_3) \sim \exp \left[ -\frac{U_{12}}{T_{12}} - \frac{U_{23}}{T_{23}} - \frac{U_{13}}{T_{13}} \right], \tag{30} \]

with three distinct \( T_{ij} \), which we call the pairwise temperatures.

In the two-particle case, the effective temperature \( T_{12} \) depends on \( T_1, T_2 \) and \( \gamma_1, \gamma_2 \), but not on \( \kappa_{12} \). By contrast, in the three-particle case, each pairwise temperature, for example \( T_{12} \), depends not only on the properties of particles 1 and 2 (\( T_1, T_2 \) and \( \gamma_1, \gamma_2 \)) and their interaction (\( \kappa_{12} \)), but also on the properties of particle 3 (\( T_3, \gamma_3 \)) and interactions with it (\( \kappa_{13}, \kappa_{23} \)). The dependence of each pairwise temperature on the spring constants suggests that the three-particle distribution cannot be generalized in a simple way to arbitrary pairwise potentials. In other words, the exponent will not be a linear combination of pair potentials with coefficients that are independent of particle positions and interactions. Similar difficulties and complexities arise in systems of active (self-propelled) particles. In particular, the distributions in such systems can only be written approximately with position-dependent effective temperatures/diffusivities or effective interactions \[10,42\]. Although pairwise additive potentials are a special case, we should point out that for more general three-body potentials (not necessarily pairwise additive), there is no reason to expect the distributions to be simpler.

The dependence of each pairwise temperature \( T_{ij} \) on the properties of all three particles and interactions has some unexpected consequences on the distribution and behavior of the three particles. In particular, the inverse of these pairwise temperatures \( \frac{1}{T_{ij}} \), which are the coefficients of the pair potentials \( U_{ij} \) in Eq. (30), can change sign and even be zero depending on the choice of temperatures \( T_i \). For example, even when there is no spring between particles 1 and 2 (\( \kappa_{12} = 0 \)) while the two other springs are the same (\( \kappa_{13} = \kappa_{23} = \kappa \)), the correlation

\[ \langle r_{13} \cdot r_{23} \rangle = \frac{1}{3\kappa} \left[ T_3 - \frac{T_1 + T_2}{2} \right] \tag{31} \]

can be either positive or negative depending on the relation between the temperatures. If particle 3 is “hot” (\( T_3 > (T_1 + T_2)/2 \)), the correlation is positive meaning that \( r_{13}, r_{23} \) roughly point in the same direction and particles 1 and 2 appear attractive. If particle 3 is cold (\( T_3 < (T_1 + T_2)/2 \)), the correlation is negative meaning \( r_{13}, r_{23} \) roughly point in opposite directions and particles 1 and 2 appear repulsive. Note that in equilibrium, the correlation is zero since there is no spring between particle 1 and 2.

In addition to the sign changes, we observe that every particle of the triplet affects the mutual behavior of the other two. For instance, in a simple case when \( \kappa_{12} = \kappa_{23} = \kappa_{13} = \kappa \) and \( T_3 \gg T_1, T_2 \), that is particle 3 is much more active than 1 and 2, we find

\[ \langle (r_1 - r_2)^2 \rangle \approx \frac{dT_3(\gamma_1 - \gamma_2)^2}{12(\gamma_1 + \gamma_2 + \gamma_3)(\gamma_1\gamma_2 + 2\gamma_2\gamma_3 + \gamma_1\gamma_3)}. \tag{32} \]

This is not only controlled by the temperature \( T_3 \) of particle 3, but also by its friction \( \gamma_3 \). Note that more generally, when \( T_3 \gg T_1, T_2 \), we have \( \langle (r_1 - r_2)^2 \rangle \propto T_3 \left( \frac{\kappa_{13}}{\kappa_{23}} + \frac{\kappa_{23}}{\kappa_{13}} \right)^2 \). Thus, the activity of particle 3 will affect 1 and 2 if their relaxation times \( \frac{1}{\kappa_{13}} \) and \( \frac{1}{\kappa_{23}} \) are not equal, that is, they interact differently with 3. This behavior has some connection with allostery-inspired mechanical networks \[43\], where the motion or activity of nodes in one part of a mechanical network can affect the response in another part differently depending on how one removes bonds (analogous to changing the interaction strengths between nodes).

In Newtonian mechanics, where one would like to write down closed-form expressions for the trajectories of the interacting bodies, there is a dramatic increase in difficulty going from the two to three-body problem. While the two-body problem can be solved by simply transforming to the center of mass and relative separation coordinates, the three-body problem remains unsolved except for special arrangements and potentials. For Langevin dynamics, in which we would like to determine the distribution of the bodies, there is also a similar increase in difficulty and richness. In the two-body case for overdamped particles, the distribution for any potential is Boltzmann-like with an effective temperature \[13\]. As we showed and discussed for the special case of pairwise additive quadratic potentials, the three-particle distribution cannot be written with an effective temperature and cannot be obtained for general, non-pairwise interactions when the temperatures of the three particles are different.

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**Appendix A: Arbitrary spring constants and friction coefficients**

Since the system described by Eqs. (\ref{Eq:3a}), (\ref{Eq:3b}), and (\ref{Eq:3c}) is translationally invariant, it is useful to consider the relative separations defined by \( r_{13} = r_1 - r_3 \) and \( r_{23} = \)
\( \mathbf{r}_2 - \mathbf{r}_3 \). In these variables, we have
\[
\hat{r}_{13} = -\left( \frac{\kappa_{12}}{\gamma_1} + \frac{\kappa_{13}}{\gamma_1} \right) r_{13} - \left( \frac{\kappa_{23}}{\gamma_3} - \frac{\kappa_{12}}{\gamma_1} \right) r_{23} + \sqrt{\frac{2T_1}{\gamma_1}} \xi_1 - \sqrt{\frac{2T_3}{\gamma_3}} \xi_3, \tag{A1a}
\]
\[
\hat{r}_{23} = -\left( \frac{\kappa_{13}}{\gamma_3} - \frac{\kappa_{12}}{\gamma_2} \right) r_{13} - \left( \frac{\kappa_{12}}{\gamma_2} + \frac{\kappa_{23}}{\gamma_3} \right) r_{23} + \sqrt{\frac{2T_2}{\gamma_2}} \xi_2 - \sqrt{\frac{2T_3}{\gamma_3}} \xi_3, \tag{A1b}
\]
where \( \gamma_3 = \gamma_i \gamma_3 / (\gamma_i + \gamma_3) \). Computing the covariance matrix \( C_{ij} = \langle r_{13} r_{j3} \rangle \), where \( \langle \rangle \) indicates ensemble average, we can write the steady state distribution as
\[
P(r_{13}, r_{23}) \sim \exp \left[ \frac{1}{2} R^T C^{-1} R \right], \tag{A2}
\]
where \( R^T = (r_{13}, r_{23}) \). After some algebra, we find the general distribution in the main text (Eq. 9) given by
\[
P(r_1, r_2, r_3) \sim \exp \left[ \frac{-\kappa_{12}}{2T_2} (r_1 - r_2)^2 - \frac{-\kappa_{23}}{2T_3} (r_2 - r_3)^2 \right]. \tag{A3}
\]
The pairwise temperatures \( T_{12}, T_{23}, T_{13} \) are given by

\[
\frac{\kappa_{12}}{T_{12}} = \frac{1}{A} \left[ T_1 \gamma_1 (\gamma_3 \kappa_{12} + (\gamma_2 + \gamma_3) \kappa_{23}) (\gamma_3 \kappa_{12} - \gamma_2 \kappa_{13}) + T_2 \gamma_2 (\gamma_3 \kappa_{12} + (\gamma_1 + \gamma_3) \kappa_{13})(\gamma_3 \kappa_{12} - \gamma_1 \kappa_{23}) + T_3 \gamma_3 (\gamma_1 \kappa_{23} + (\gamma_1 + \gamma_2) \kappa_{12}) (\gamma_2 \kappa_{13} + (\gamma_1 + \gamma_2) \kappa_{12}) + \frac{\gamma_1 \gamma_2}{\gamma_3} (\gamma_1 + \gamma_2 + \gamma_3)(\gamma_1 \kappa_{12} + \gamma_2 \kappa_{23} + \gamma_3 \kappa_{13}) \right], \tag{A4a}
\]
\[
\frac{\kappa_{23}}{T_{23}} = \frac{1}{A} \left[ T_1 \gamma_1 (\gamma_3 \kappa_{12} + (\gamma_1 + \gamma_2) \kappa_{12}) (\gamma_1 \kappa_{23} - \gamma_2 \kappa_{13}) + T_2 \gamma_2 (\gamma_1 \kappa_{23} + (\gamma_1 + \gamma_3) \kappa_{13})(\gamma_1 \kappa_{23} - \gamma_3 \kappa_{12}) + T_3 \gamma_3 (\gamma_2 \kappa_{13} + (\gamma_1 + \gamma_2) \kappa_{23}) (\gamma_3 \kappa_{12} + (\gamma_1 + \gamma_2) \kappa_{13}) + \frac{\gamma_2 \gamma_3}{\gamma_1} (\gamma_1 + \gamma_2 + \gamma_3)(\gamma_1 \kappa_{12} + \gamma_2 \kappa_{13} + \gamma_3 \kappa_{23}) \right], \tag{A4b}
\]
\[
\frac{\kappa_{13}}{T_{13}} = \frac{1}{A} \left[ T_1 \gamma_1 (\gamma_2 \kappa_{13} + (\gamma_1 + \gamma_2) \kappa_{23}) (\gamma_2 \kappa_{13} - \gamma_2 \kappa_{13}) + T_3 \gamma_3 (\gamma_2 \kappa_{13} + (\gamma_1 + \gamma_2) \kappa_{13})(\gamma_2 \kappa_{13} - \gamma_3 \kappa_{12}) + T_2 \gamma_2 (\gamma_1 \kappa_{12} + (\gamma_1 + \gamma_2) \kappa_{12}) (\gamma_3 \kappa_{12} + (\gamma_1 + \gamma_2) \kappa_{13}) + \frac{\gamma_1 \gamma_3}{\gamma_2} (\gamma_1 + \gamma_2 + \gamma_3)(\gamma_1 \kappa_{12} + \gamma_2 \kappa_{13} + \gamma_3 \kappa_{23}) \right], \tag{A4c}
\]
where
\[
A = \left( \frac{\gamma_1 \gamma_2 \gamma_3 \left[ \gamma_1 \kappa_{23} (T_2 - T_3) + \gamma_2 \kappa_{13} (T_3 - T_1) + \gamma_3 \kappa_{12} (T_1 - T_2) \right]^2}{\gamma_1 \kappa_{23} (\gamma_1 + \gamma_2 + \gamma_3) + \gamma_2 \kappa_{13} (\gamma_1 + \gamma_2) + \gamma_3 \kappa_{12} (\gamma_1 + \gamma_2) + \gamma_1 \kappa_{23} (\gamma_1 + \gamma_2 + \gamma_3) + \gamma_2 \kappa_{13} (\gamma_1 + \gamma_2) + \gamma_3 \kappa_{12} (\gamma_1 + \gamma_2) \right]. \tag{A5}
\]
If we integrate out, say, the third particle, the probability distribution becomes
\[
P(r_1, r_2) \sim \exp \left[ -\left( \frac{1}{T_{12}} + \frac{\kappa_{13} \gamma_2}{\kappa_{12} (\kappa_{13} T_{23} + \kappa_{23} T_{13})} \right) \frac{\kappa_{12}}{2} (r_1 - r_2)^2 \right] \sim \exp \left[ -\frac{-\kappa_{12}}{2T_{12}} (r_1 - r_2)^2 \right]. \tag{A6}
\]
where
\[
\bar{T}_{12} = \frac{2}{(\gamma_1 + \gamma_2 + \gamma_3)(\kappa_{12} \kappa_{13} + \kappa_{12} \kappa_{23} + \kappa_{13} \kappa_{23})(\gamma_1 \kappa_{23} (\gamma_2 + \gamma_3) + \gamma_2 \kappa_{13} (\gamma_1 + \gamma_3) + \gamma_3 \kappa_{12} (\gamma_1 + \gamma_2)) \times \left[ T_1 \gamma_1 \left( \gamma_2 \kappa_{13} + (\gamma_1 + \gamma_2) \kappa_{23} \right)^2 + \frac{\gamma_2 \gamma_3}{\gamma_1} (\gamma_1 + \gamma_2 + \gamma_3)(\kappa_{12} \kappa_{23} + \kappa_{13} \kappa_{23} + \kappa_{13} \kappa_{23}) \right] + T_2 \gamma_2 \left( \gamma_1 \kappa_{23} + (\gamma_1 + \gamma_3) \kappa_{13} \right)^2 + \frac{\gamma_1 \gamma_3}{\gamma_2} (\gamma_1 + \gamma_2 + \gamma_3)(\kappa_{12} \kappa_{23} + \kappa_{12} \kappa_{13} + \kappa_{13} \kappa_{23}) \right]. \tag{A7}
\]

Note that we can obtain \( \bar{T}_{23}, \bar{T}_{13} \) by simply relabeling the particles. The average potential energy stored in the
The inverse of the covariance matrix is given by

\[ \sum_{i,j} (r_i - r_j) + \sqrt{2T_i \gamma \xi_i}. \]  

(B1)

Relative to the \( N \)th particle, the Langevin equations for \( r_{i,N} = r_i - r_N \) (\( i = 1, 2, \ldots, N - 1 \)) are

\[ \gamma \dot{r}_{i,N} = -N \kappa r_{i,N} + \sqrt{2T_i \gamma \xi_i} - \sqrt{2T_N \gamma \xi_N}. \]  

(B2)

The inverse of the covariance matrix is given by

\[(C^{-1})_{ij} = \kappa T_H \left( \frac{\delta_{ij}}{\sqrt{T_i T_j}} \sum_{n=1}^{N} \frac{1}{T_n} - \frac{1}{T_i T_j} \right) I, \]  

(B4)

where \( T_H = N \left( \sum_{n=1}^{N} \frac{1}{T_n} \right)^{-1} \) is the harmonic average of the temperatures. It is easy to check that \( CC^{-1} = C^{-1}C = I \). After some algebra, we have

\[ \sum_{i,j} \sum_{i,J}^{N} (C^{-1})_{ij} r_{i,J} = \frac{1}{T} \sum_{i,J}^{N} (r_i - r_j)^2, \]  

(B5)

where

\[ T_{ij} = \frac{T_i T_j}{N} \sum_{n=1}^{N} \frac{1}{T_n} = \frac{T_i T_j}{T_H}. \]  

(B6)

Appendix C: Underdamped particles

1. Two particles

As discussed in Section \[\text{C1}\] the distribution of momenta and separation between two underdamped particles at different temperatures can be written as

\[ P(r, p_1, p_2) \sim \exp \left[ -\frac{1}{2} (\beta_{p_1, p_1} p_1^2 + \beta_{p_2, p_2} p_2^2 + \beta_{rr} r^2 + 2 \beta_{p_1 p_2} p_1 \cdot p_2 + 2 \beta_{p_1 r} p_1 \cdot r + 2 \beta_{p_2 r} p_2 \cdot r) \right]. \]  

(C1)

The coefficients are given by

\[ A_{p_1, p_1} = \frac{2A}{m(T_1 + T_2)} - 2\gamma^2(\gamma^2 + m\kappa)T_2(T_1 - T_2), \]  

(C2a)

\[ A_{p_2, p_2} = \frac{2A}{m(T_1 + T_2)} + 2\gamma^2(\gamma^2 + m\kappa)T_1(T_1 - T_2), \]  

(C2b)

\[ A_{p_1 r} = \frac{2\kappa A}{(T_1 + T_2)} + 2m^2\gamma^2\kappa^2(T_1 - T_2)^2, \]  

(C2c)

\[ A_{p_2 r} = m\gamma^2(T_1 - T_2)[m\kappa T_1 + (2\gamma^2 + m\kappa)T_2], \]  

(C2d)

\[ A_{p_2 r} = -m\gamma(T_1 - T_2)[(2\gamma^2 + m\kappa)T_1 + m\kappa T_2], \]  

(C2e)

\[ \gamma = \gamma \xi_i. \]  

(C4)

Fourier transforming and using \( \tilde{v}_i = i\omega \tilde{r}_i \), we have

\[ \sum_{j=1}^{N} M_{ij} \tilde{v}_j = i\omega \sqrt{2T_i \gamma \xi_i}, \]  

(C5)

where

\[ M_{ij} = (-m\omega^2 + i\gamma \omega + N\kappa)\delta_{ij} - \kappa, \]  

(C6)

the inverse of which is

\[ (M^{-1})_{ij} = \frac{(-m\omega^2 + i\gamma \omega)\delta_{ij} + \kappa}{(-m\omega^2 + i\gamma \omega + N\kappa)(-m\omega^2 + i\gamma \omega)}. \]  

(C7)

The power spectrum of the velocities is given by \( \langle \tilde{v}_i(\omega) \cdot \tilde{v}_j(\omega') \rangle = 2\pi(v_i^2)\delta(\omega + \omega') \) or

\[ (v_i^2)_{\omega} = \sum_{j=1}^{N} 2dT_j \gamma \omega^2(M^{-1})_{ij}(M^{-1})_{ij}, \]  

(C8)

where \( \bar{M} \) is the complex conjugate of \( M \). By the Weiner-Khinchin theorem, the fluctuations and power spectra are related through

\[ (v_i^2)_{\omega} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (v_i^2)_{\omega}. \]  

(C9)

Performing contour integration over the appropriate poles, we arrive at Eq. \[\text{[25]}\] in the main text.
3. Softening or stiffening one spring, underdamped particles

Taking $\kappa_{23} = \kappa_{13} = \kappa \neq \kappa_{12}$, the kinetic energies $\langle K_i \rangle = \langle \frac{1}{2} m v_i^2 \rangle$ in the case of underdamped particles are

\[
\langle K_1 \rangle = \frac{d}{2} T_1 - \frac{d m \kappa}{2 \gamma^2 + 3 m \kappa} (T_1 - T_{\text{avg}}) + A(\kappa - \kappa_{12})(T_1 - T_2), \tag{C10a}
\]

\[
\langle K_2 \rangle = \frac{d}{2} T_2 - \frac{d m \kappa}{2 \gamma^2 + 3 m \kappa} (T_2 - T_{\text{avg}}) - A(\kappa - \kappa_{12})(T_1 - T_2), \tag{C10b}
\]

\[
\langle K_3 \rangle = \frac{d}{2} T_3 - \frac{d m \kappa}{2 \gamma^2 + 3 m \kappa} (T_3 - T_{\text{avg}}) \tag{C10c}
\]

where

\[
A = \frac{d m}{12} \left[ \frac{8 \gamma^2}{(2 \gamma^2 + 3 m \kappa)(2 \gamma^2 + m \kappa + 2 m \kappa_{12})} - \frac{\kappa - \kappa_{12}}{\kappa(2 \gamma^2 + m \kappa) + \kappa_{12}(\gamma^2 - 2 m \kappa + m \kappa_{12})} \right]. \tag{C11}
\]

The average potential energies $\langle U_{ij} \rangle = \langle \frac{1}{2} \kappa_{ij}(r_i - r_j)^2 \rangle$ are

\[
U_{12} = \frac{d \kappa_{12}}{2(\kappa + 2 \kappa_{12})} \tag{C12a}
\]

\[
U_{23} = \frac{1}{24} \left[ T_1 + T_2 + 4 T_3 + \frac{3 \kappa(T_1 + T_2)}{\kappa + 2 \kappa_{12}} \right] \tag{C12b}
\]

\[
U_{13} = \frac{1}{24} \left[ T_1 + T_2 + 4 T_3 + \frac{3 \kappa(T_1 + T_2)}{\kappa + 2 \kappa_{12}} \right] \tag{C12c}
\]

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