Thermoelectric transport in billiard systems

Giulio Casati* † and Carlos Mejía-Monasterio**

*Center for Nonlinear and Complex Systems, Università degli Studi dell’Insubria, Como Italy
†CNR-INFM and Istituto Nazionale di Fisica Nucleare, Sezione di Milano
**Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, Sesto Fiorentino Italy

Abstract. We discuss the thermoelectric (TE) transport in billiard systems of interacting particles, coupled to stochastic particle reservoirs. Recently in [1], analytical exact expressions for the TE transport of noninteracting gases of polyatomic molecules were obtained, and a novel microscopic mechanism for the increase of thermoelectric efficiency described. After briefly reviewing the derivation of [1], in this paper we focus on the effects that the particle-particle interaction has on the TE efficiency. We show that interaction reduces the maximal thermodynamic efficiency. However, the mechanism for the efficiency’s increase towards its Carnot upper limit, described in [1], remains unaffected.

Keywords: Thermoelectricity, Thermodiffusion, Lorentz gas, Billiards.

PACS: 72.15.Jf, 05.70.Ln, 05.45.-a

1. INTRODUCTION

Thermoelectricity concerns the conversion of temperature differences into electric potential or vice-versa. It can be used to perform useful electrical work or to pump heat from cold to hot place, thus performing refrigeration. Although thermoelectricity was discovered almost 200 years ago, a strong interest of the scientific community arose only in the 1950’s when Abram Ioffe discovered that doped semiconductors exhibit relatively large thermoelectric effect. This initiated an intense research activity in semiconductors physics which was not motivated by microelectronics but by the Ioffe suggestion that home refrigerators could be built with semiconductors [2, 3]. As a result of these efforts the thermoelectric material Bi₂Te₃ was developed for commercial purposes. However this activity lasted only few years until the mid 1960’s since, in spite of all efforts and consideration of all type of semiconductors, it turned out that thermoelectric refrigerators have still poor efficiency as compared to compressor based refrigerators. Nowadays Peltier refrigerators are mainly used in situations in which reliability and quiet operation, and not the cost and conversion efficiency, is the main concern, like equipments in medical applications, space probes etc. In the last decade there has been an increasing pressure to find better thermoelectric materials with higher efficiency. The reason is the strong environmental concern about chlorofluorocarbons used in most compressor-based refrigerators. Also the possibility to generate electric power from waste heat using thermoelectric effect is becoming more and more interesting [4, 2, 3].

The suitability of a thermoelectric material for energy conversion or electronic refrigeration is evaluated by the thermoelectric figure of merit $Z$,

$$Z = \frac{\sigma S^2}{\kappa},$$

(1)
where $\sigma$ is the coefficient of electric conductivity, $S$ is the Seebeck coefficient and $\kappa$ is the thermal conductivity. The Seebeck coefficient $S$, also called thermopower, is a measure of the magnitude of an induced thermoelectric voltage in response to a temperature difference across the material.

For a given material, and a pair of temperatures $T_H$ and $T_C$ of hot and cold thermal baths respectively, $Z$ is related to the efficiency $\eta$ of converting the heat current $J_Q$ (between the baths) into the electric power $P$ which is generated by attaching a thermoelectric element to an optimal Ohmic impedance. Namely, in the linear regime:

$$\eta = \frac{P}{J_Q} = \eta_{\text{carnot}} \cdot \frac{\sqrt{ZT + 1} - 1}{\sqrt{ZT + 1} + 1},$$

where $\eta_{\text{carnot}} = 1 - T_C/T_H$ is the Carnot efficiency and $T = (T_H + T_C)/2$. Thus a good thermoelectric device is characterized by a large value of the non-dimensional figure of merit $ZT$.

Since the 1960's many materials have been investigated but the maximum value found for $ZT$ was achieved for the $(\text{Bi}_{1-x}\text{Sb}_x)_2(\text{Se}_{1-y}\text{Te}_y)_3$ alloy family with $ZT \approx 1$. However, values $ZT > 3$ are considered to be essential for thermoelectrics to compete in efficiency with mechanical power generation and refrigeration at room temperatures. The efforts recently focused on a bulk of new advanced thermoelectric materials and on low-dimensional materials, and only a small increment of the efficiency, $ZT \lesssim 2.6$, has been obtained [4].

One of the main reasons for this partial success is a limited understanding of the possible microscopic mechanisms leading to the increase of $ZT$, with few exceptions [5]. From a dynamical point of view, cross effects in transport have been barely studied [6, 7]. So far, the challenge lies in engineering a material for which the values of $S$, $\sigma$ and $\kappa$ can be controlled independently. However, the different transport coefficients are interdependent, making optimization extremely difficult.

In a recent paper, we have studied the thermoelectric process in a gas of non-interacting polyatomic molecules [1]. We showed that large values of $ZT$, in principle approaching to Carnot’s efficiency, are obtained when the number of the molecule’s internal degrees of freedom (d.o.f.) is increased. Using the rotating-disk interaction introduced in [7], in this paper, we study the effect that a generic particle-particle interaction has on the TE efficiency of these systems. In the following section 2, we review briefly the microscopic expressions for the TE process in ergodic ideal gases obtained in [1]. In the section 3, we study numerically, the modifications to these expressions, due to the interaction. Our conclusions appear in section 4.

2. THERMOELECTRIC TRANSPORT

In the linear response regime (see e.g. [8]), the transport equations for a thermoelectric material give the heat current $J_Q$ and the electric current $J_e$ through an homogeneous sample subjected to a temperature gradient $\partial_x T$ and a electrochemical potential gradient
\[ \partial_x \bar{\mu} \text{ as}\]

\[
\begin{align*}
J_Q &= -\kappa' \partial_x T - T \sigma S \partial_x \bar{\mu}, \\
J_e &= -\sigma S \partial_x T - \sigma \partial_x \bar{\mu}.
\end{align*}
\] (3)

Here and in what follows, we assume that the transport occurs along the \(x\)-direction and the temperature is given in units where the Boltzmann constant \(k_B = 1\).

The electrochemical potential is the sum of a chemical and an electric part \(\bar{\mu} = \mu + \mu_e\), where \(\mu\) is the chemical potential of the particles and, if \(e\) is the particle’s charge, \(\mu_e = e\phi\) is the work done by the particles against an external electric field \(\vec{E} = -\partial_x \phi\). From (3) the usual phenomenological relations follow: if the thermal gradient vanishes, \(\partial_x T = 0\), then \(J_e = -\sigma \partial_x \phi = \sigma \vec{E}\), since for an isothermal homogeneous system \(\mu\) is uniform.

If the electric current vanishes, \(J_e = 0\), then \(\partial_x \bar{\mu} = S \partial_x T\), which is the definition of the Seebeck coefficient, and \(J_Q = -\kappa \partial_x T\) where \(\kappa = \kappa' - T \sigma S^2\) is the usual thermal conductivity (see e.g. [10]).

From the theory of irreversible thermodynamics, \(\mu\) and \(\mu_e\) cannot be determined separately; only their combination in \(\bar{\mu}\) appears in (3) [9]. Based on this equivalence, in what follows we take into account the chemical part only, i.e., \(\bar{\mu} = \mu\).

Since in the linear regime in which dissipative effects, such as, e.g., Joule heating, can be neglected and at low particle densities, thermodiffusion and thermoelectricity are equivalent process, we can study TE in terms of the thermodiffusion transport equations

\[
\begin{align*}
J_u &= L_{uu} \partial_x \left( \frac{1}{T} \right) + L_{u\rho} \partial_x \left( -\frac{\mu}{T} \right), \\
J_\rho &= L_{\rho u} \partial_x \left( \frac{1}{T} \right) + L_{\rho\rho} \partial_x \left( -\frac{\mu}{T} \right),
\end{align*}
\] (4)

where \(J_u\) and \(J_\rho = J_e/e\) are the energy and particle density currents, and \(L_{u\rho} = L_{\rho u}\) follows from the Onsager reciprocity relations. From the entropy balance equation for open systems [11]

\[ J_u = J_Q + \mu J_\rho, \] (5)

and substituting \(J_Q\) in (3) in favor of \(J_u\) and comparing the resulting equations with (4) it follows that the TE transport coefficients can be written in terms of the thermodiffusion \(L\)-coefficients as

\[ \begin{align*}
\sigma &= \frac{e^2}{T} L_{\rho\rho}, \\
\kappa &= \frac{1}{T^2} \frac{\det \mathbb{L}}{L_{\rho\rho}}, \\
S &= \frac{1}{eT} \left( \frac{L_{u\rho}}{L_{\rho\rho}} - \mu \right).
\end{align*} \] (6)

Furthermore, from Eq. (1), we obtain for the figure of merit

\[ ZT = \frac{(L_{u\rho} - \mu L_{\rho\rho})^2}{\det \mathbb{L}}. \] (7)

Note that in Eqs. (6) and (7), \(T\) and \(\mu\) are taken as the mean values.

Consider now an ergodic gas of non-interacting, electrically neutral particles of mass \(m\) with \(d_{\text{int}}\) internal d.o.f. (rotational or vibrational), enclosed in a \(d\) dimensional container. To study the non-equilibrium state of such dilute poly-atomic gas we consider a
FIGURE 1. The open Lorentz gas system and a typical particle’s trajectory. The particles are scattered from fixed disks of radius $R$ disposed in a triangular lattice at critical horizon, i.e., the width and height of the cells are $\Delta x = 2R$ and $\Delta y = 2W$ respectively, where $W = 4R/\sqrt{3}$ is the separation between the centers of the disks. The channel is coupled at the left and right boundaries to two thermochemical baths at temperatures $T_L$ and $T_R$ and chemical potentials $\mu_L$ and $\mu_R$, respectively.

chaotic billiard channel (like the one shown in Fig. 1) connected through openings of length $\lambda$ to two reservoirs of particles which are idealized as infinite chambers with the same poly-atomic gas at equilibrium density $\rho$ and temperature $T$. From the reservoirs, particles are injected into the channel at a rate $\gamma$, as explained in the appendix A.

The particle injection rate $\gamma$ is related to the value of the chemical potential $\mu$ at the reservoirs which, for a gas of polyatomic molecules with a total of $D = d + d_{\text{in}}$ d.o.f., at equilibrium density $\rho$ and temperature $T$ reads

$$\mu = \mu_0 + T \ln \left( \frac{\rho}{T^{D/2}} \right) = \mu'_0 + T \ln \left( \frac{\gamma}{T(D+1/2)} \right),$$

(8)

where $\mu_0$ and $\mu'_0$ are reference values of the chemical potential and the second equality is simply obtained after substitution of $\rho$ from Eq. (17). Furthermore, energy is injected from the reservoirs at a rate $\varepsilon = \gamma T (D + 1/2)$ (see appendix A).

Calling $p_t(l)$ the transmission probability of the channel of length $l$, the density currents $J_\rho, J_u$ for noninteracting particles [12], assume a simple form: they are $p_t(l)$ times the difference between the left and right corresponding injection rates, $\varepsilon, \gamma$, respectively, namely

$$J_\rho = p_t (\varepsilon_L - \varepsilon_R), \quad J_u = p_t (\gamma_L - \gamma_R).$$

(9)

Using (8) to eliminate $\gamma$ in favor of $\mu$ we obtain,

$$J_\rho = -\frac{\lambda p_t(l)}{(2\pi m)^{1/2}} \partial_x \left( T^{(D+1)/2} e^{\mu/T} \right),$$

$$J_u = -\frac{\lambda p_t(l)}{(2\pi m)^{1/2}} \frac{D+1}{2} \partial_x \left( T^{(D+3)/2} e^{\mu/T} \right),$$

(10)

Taking total differentials of (10) in the variables $1/T$ and $\mu/T$ and comparing the resulting expression with Eq. (4) we obtain exact microscopic expressions for the Onsager
coefficients and thus, for the TE transport coefficients, namely

\[
\sigma = \frac{\lambda p_t l}{(2\pi m)^{1/2} T^{1/2}},
\]
\[
S = \frac{1}{e} \left( \frac{D+1}{2} \right),
\]
\[
\kappa = \frac{\lambda p_t l}{(2\pi m)^{1/2} \left( \frac{D+1}{2} \right) \rho T^{1/2}}.
\]

Note that for a chaotic billiard channel with a diffusive dynamics, the transmission probability decays as \( p_t(l) \propto l^{-1} \) which means that all the elements of the Onsager matrix \( L \) become size independent.

Finally, plugging (11) into (1) and noting that \( c_V^* = D/2 \) is the dimensionless heat capacity at constant volume of the gas, we obtain

\[
ZT = \frac{1}{\hat{c}_V} \left( \hat{c}_V - \frac{\mu}{T} \right)^2,
\]

where for simplicity we have called \( \hat{c}_V = c_V^* + 1/2 \). A particular case of (12) was previously obtained, for noninteracting monoatomic ideal gases in 3 dimensions [13].

The analytical expressions for the TE transport (11) and (12) are exact [1]. They predict and increase of the TE efficiency with \( D \). To verify this and further compare in the next section with the interacting particles, we have considered a gas of composite particles with \( d_{\text{int}} \geq 1 \) internal rotational d.o.f. inside a Lorentz gas channel (Fig. 1) coupled to two thermochemical baths. The model of composite particles and its dynamics is explained in the appendix B. We have numerically measured the TE efficiency \( \eta \) as the ratio

\[
\eta = \frac{e J \rho \Delta \mu}{J_u},
\]

where \( \Delta \mu = \mu_R - \mu_L \) is the chemical potential difference. For a fixed temperature gradient, in Fig. 2 we show \( \eta \) as a function of \( \nabla (\mu/T) \) for different values of \( D \). Note the excellent agreement between the numerical data (symbols) and the analytical solution of \( \eta \), obtained from substituting (10) into (13). In each case, the efficiency reaches a maximum value \( \eta_{\text{max}} \) for some optimal value of \( \nabla (\mu/T) \). Moreover, \( \eta = 0 \) occurs when \( J_\rho = 0 \), which in turns is determined by the Seebeck coefficient. Consistently with Eq. (11), the value of \( \nabla (\mu/T) \) for which \( \eta = 0 \) grows linearly with \( D \). Finally, in the inset of Fig. 2 we show the numerically obtained \( \eta_{\text{max}} \) as a function of \( D \) (stars) and compare them with the analytical expression of (2), with an excellent agreement.

3. PARTICLE-PARTICLE INTERACTION

We now turn our attention to the interacting case. In absence of particles’ interaction, \( ZT \) is independent of the sample size \( l \) and depends on the temperature only through the chemical potential term. This is due to the fact that with no interactions, \( p_t \) depends on the geometry of the billiard only. From a physical point of view this means that the
mean free path of the gas particles is energy independent. When the particles interacting, in general $p_t$ depends on the local density and temperature of the gas, leading to a more realistic situation [14]. Therefore, the analytical expressions for the TE transport coefficients (11) are not longer exact.

To consider a gas of interacting particles we assume that the lattice disks of mass $M$, freely rotate, so that when a particle collides with a disk, their energies mixes, according to the collision rules (26). This induces a particle-particle interaction that is mediated by the collision with the lattice disks. The strength of the interaction is determined by the mass ratio between disks and particles $\Lambda = M/m$ [7]. The noninteracting case is recover in the limit of $\Lambda \rightarrow 0$, when the disks are much lighter than the particles. Therefore, we can study the effect of the interaction by tuning the value of $\Lambda$. First we have studied the TE transport for a gas of monoatomic particles ($D = 2$). In Fig. 3, we show the TE figure-of-merit $ZT$ as a function of $\Lambda$. When $\Lambda \rightarrow 0$, $ZT \rightarrow 3/2$, which is the expected value of the noninteracting case (see Eq. 12). In the inset of Fig. 3, we also show the behaviour of the TE transport coefficients.

Therefore, Eq. (12) is an upper limit of the interacting case when the interaction strength vanishes. This is behaviour is expected to be generic since, as explained in [1], any interaction tends to correlate the energy carried by the particles with the external gradients, thus decreasing the efficiency.

Next, we have studied the behaviour of the TE efficiency on $D$, for and gas of
interacting composite particles. In Fig. 4, we show the TE efficiency $\eta$ as a function of $\nabla (\mu / T)$ for $\Lambda = 1$, for different values of $D$. As for the noninteracting case, the efficiency reaches a maximum value $\eta_{\text{max}}$ for some optimal value of the chemical potential gradient. However, consistently with the results of Fig. 3, $\eta_{\text{max}}$ of the gas of interacting composite particles is smaller than the noninteracting gas. This can be seen for small $D$, in the inset of Fig. 4 were $\eta_{\text{max}}$ is plotted for the considered values of $D$. For more complex particles (larger $D$), $\eta_{\text{max}}$ approaches the noninteracting solution. Although the behaviour at large $D$ is particular of the rotating-disk interaction, we cannot discard that the same could be observed for a more generic type of interactions. Indeed, when $D \gg 1$, the amount of energy of the lattice disk becomes negligible compare to the total energy contained in the composite particle. Furthermore, for the gas of interacting particles, $\eta$ also grows with $D$, indicating that the microscopic mechanism for the increase of the TE efficiency discovered in [1] also applies to the interacting case.

4. CONCLUSIONS

We have studied the effect of interaction on the properties of thermoelectric transport of gases of polyatomic molecules. We have shown that while the TE efficiency of gases of noninteracting molecules is an upper bound for the efficiency of the interacting case
when the interaction strength vanishes, the later still increases with the complexity of the molecules.

A. COUPLING WITH THE THERMO-CHEMICAL BATHS

Consider a infinite 2-dimensional particle reservoir at equilibrium temperature $T$ and density $\rho$, filled with point-like composite particles of mass $m$ and $d_{int}$ d.o.f. The reservoir, coupled to the system through an opening of section $\lambda$, exchanges particles with the system, so that in the neighbourhood of the coupling the system is at equilibrium with the reservoir. Our aim is to obtain the rates at which particles and energy are injected into the system. Inside the reservoir each component of the velocity of the particles is distributed according to the Maxwell-Boltzmann distribution

$$f_T(v) dv = 2\pi \left( \frac{m}{2\pi kT} \right)^{d/2} v^{d-1} e^{-\frac{mv^2}{2kT}} dv.$$  \hspace{1cm} (14)

Note that (14) is independent of $d_{int}$. To obtain the particle injection rate $\gamma$ we need to compute how many particles of the reservoir hit the opening per unit time. From all the particles moving in a given direction $\vec{v}$, the number of particles that cross the opening in an infinitesimal time interval $dt$, are those contained in the parallelepiped of cross section $\lambda$ and length $v \cos(\theta) dt$, namely $\rho \lambda v \cos(\theta) dt$. 

FIGURE 4. Thermodynamic efficiency $\eta$ as a function of $\nabla (\mu/T)$ for a chain of 15 cells with $\Lambda = 1$, $T_L = 95$, $T_R = 105$, and $D = 3$ (circles), $D = 7$ (squares), $D = 11$ (diamonds), and $D = 15$ (triangles). The dashed lines correspond to the analytical solution obtained from substituting (10) into (13). In the inset, maximum efficiency obtained for the different values of $D$ (crosses), in units of the $\eta_{carnot}$. Here, the results for $D = 2$, 3 and 4 are also shown. The dashed line corresponds to the analytical expression (2) for a gas of noninteracting particles.
Since the reservoir is at equilibrium, the probability that a particle with speed between \( v \) and \( v + dv \) is injected into the system in a time interval \( dt \) is obtained as

\[
W(v)dvdt = \int_0^{2\pi} d\phi \int_0^{\pi/2} d\theta v^2 \sin\theta (\rho \lambda v \cos\theta) (2\pi)^{-1} f_T(v)dvdt,
\]

\[
= 2\rho \lambda \left( \frac{m}{2\pi kT} \right) v^2 e^{-m^2 \frac{v^2}{2kT}} dvdt.
\]  

(15)

Taking \( v = \sqrt{2E/m} \) in (15), where \( E \) is the translational energy, one obtains the probability that a particle with energy \( E \) between \( E \) and \( E + dE \) is injected into the system in a time interval \( dt \) as

\[
W(E)dEdt = \frac{2\rho \lambda}{\pi^{1/2}(2\pi mkT)^{1/2}} \left( \frac{E}{kT} \right)^{1/2} e^{-E/kT} dEdt.
\]

(16)

In terms of \( W(E) \), the particle injection rate is defined as \( \gamma = \int_0^\infty W(E)dE \), yielding

\[
\gamma = \frac{\lambda}{(2\pi m)^{1/2}} \rho (kT)^{1/2}.
\]

(17)

The energy injection rate is obtained as \( \varepsilon = \gamma \langle E \rangle \), where \( \langle E \rangle \) is the mean energy of the injected particles, namely \( \langle E \rangle = \langle E_{\text{trans}} \rangle + \langle E_{\text{int}} \rangle \), where \( \langle E_{\text{trans}} \rangle \) is the mean energy of the translational d.o.f. given by

\[
\langle E_{\text{trans}} \rangle = \frac{\int_0^\infty EW(E)dEdt}{\int_0^\infty W(E)dEdt} = \frac{3}{2} kT,
\]

and \( \langle E_{\text{int}} \rangle = \frac{d_{\text{int}}}{2} kT \) is the mean energy of the internal d.o.f. Note that the mean translational energy of the injected particles is not \( \frac{d}{2} kT \) but \( \frac{d+1}{2} kT \). Denoting the total number of d.o.f. as \( D = d + d_{\text{int}} \) we finally obtain

\[
\varepsilon = \frac{D+1}{2} \frac{\lambda}{(2\pi m)^{1/2}} \rho (kT)^{3/2}.
\]

(18)

**B. COLLISION RULES**

In this appendix we derive the collision rules that mix the energy among the translational components of the particle’s velocity, its internal degrees of freedom. We consider composite particles with \( d_{\text{int}} \) internal rotational d.o.f. Each “particle” of mass \( m \) can be imagined as a stack of \( d_{\text{int}} \) small identical disks of mass \( m/d_{\text{int}} \) and radius \( r \ll R \), rotating freely and independently at a constant angular velocity \( \omega_i, \ i = 1, \ldots, d_{\text{int}} \). The center of mass of the particle moves with velocity \( \vec{v} = (v_x, v_y) \).

We assume that at a collision of a particle with a lattice disk, the normal component of the particle’s velocity is reflected, and the tangent component, and internal angular velocities change, so that the total energy and local momentum are conserved. Introducing
the following notation

\[ \xi_0 = v_t \]
\[ \xi_i = \alpha^{1/2} \omega_i , \quad \text{for } i = 1, \ldots, d_{\text{int}} , \]

where \( \alpha = \Theta/m \) and \( \Theta = mr^2/2d_{\text{int}} \) is the moment of inertia of the internal disks, the particle’s energy becomes

\[ E = \frac{m}{2} \left( v_n^2 + \sum_{i=0}^{d_{\text{int}}} \xi_i^2 \right) . \tag{20} \]

Denoting with primed (unprimed) variables the velocities after (before) the collision, the equation for the energy conservation is

\[ \sum_{i=0}^{d_{\text{int}}} \xi_i^2 = \sum_{i=0}^{d_{\text{int}}} \xi_i^2 , \tag{21} \]

and for the conservation of local momentum

\[ \xi_0' + \alpha^{1/2} \sum_{i=1}^{d_{\text{int}}} \xi_i' = \xi_0 + \alpha^{1/2} \sum_{i=1}^{d_{\text{int}}} \xi_i . \tag{22} \]

To solve for the primed momenta, we cast (22) as

\[ \xi_0' = \xi_0 - d_{\text{int}} \mathcal{K} \quad \text{and} \quad \xi_i' = \xi_i + \frac{1}{\alpha^{1/2}} \mathcal{K} . \tag{23} \]

Substituting (23) into (21) we obtain for the collisional torque \( \mathcal{K} \)

\[ \mathcal{K} = \frac{2\alpha}{d_{\text{int}} (1 + d_{\text{int}} \alpha)} \left( d_{\text{int}} \xi_0 - \frac{1}{\alpha} \sum_{i=1}^{d_{\text{int}}} \xi_i \right) . \tag{24} \]

Substituting (24) back into (23) and using (19) the we obtain the collision rules

\[ v_n' = -v_n \]
\[ v_t' = \frac{1 - d_{\text{int}} \alpha}{1 + d_{\text{int}} \alpha} v_t + \frac{2\alpha}{1 + d_{\text{int}} \alpha} \sum_{i=1}^{d_{\text{int}}} \omega_i \]
\[ \omega_i' = \omega_i + \frac{2\alpha}{1 + d_{\text{int}} \alpha} v_t - \frac{2}{d_{\text{int}} (1 + d_{\text{int}} \alpha)} \sum_{i=1}^{d_{\text{int}}} \omega_i . \tag{25} \]

For the interacting case, namely when the lattice disks rotate, these can be considered as one additional rotor of mass \( M \) and radius \( R \) and angular velocity \( \overline{\omega} \). Following the
same procedure, the reader can easily verify that the collision rules are

\[ v'_n = -v_n \]

\[ v'_t = (1 - \Omega d_{\text{int}}^2) v_t + \Omega d_{\text{int}} \left( \overline{\omega} + \sum_{i=1}^{d_{\text{int}}} \omega_i \right) \]

\[ \overline{\omega}' = \overline{\omega} + \frac{\Omega}{R^2 \Lambda} \left[ d_{\text{int}} v_t - \left( \overline{\omega} + \sum_{i=1}^{d_{\text{int}}} \omega_i \right) \right] \]

\[ \omega'_i = \omega_i + \frac{\Omega}{\alpha} \left[ d_{\text{int}} v_t - \left( \overline{\omega} + \sum_{i=1}^{d_{\text{int}}} \omega_i \right) \right] , \tag{26} \]

where \( \Lambda = M/m \) and

\[ \Omega = 2 \left( d_{\text{int}}^2 + \frac{d_{\text{int}}}{\alpha} + \frac{1}{R^2 \Lambda} \right) . \tag{27} \]

These collision rules are a generalization of the ones introduced in [7]. Thus, they are deterministic, time reversible and preserve the energy and local angular momentum.

REFERENCES

1. G. Casati, C. Mejia-Monasterio, and T. Prosen, Phys. Rev. Lett. 101, 016601 (2008).
2. G. Mahan, B. Sales, J. Sharp, Phys. Today 50, 42 (March 1997).
3. A. Majumdar, Science 303, 778 (2004).
4. M. S. Dresselhaus et al, Adv. Mater. 19, 1043-1053 (2007).
5. T. E. Humphrey and H. Linke, Phys. Rev. Lett. 94, 096601 (2005).
6. C. Maes and M. H. van Wieren, J. Phys. A: Math. Gen. 38(2005) 1005; J. Vollmer, T. Tell, and L. Mátyás, J. Stat. Phys. 101 (2000) 79; C. Van den Broeck, in Advances in Chemical Physics Vol. 135 Eds. S. A. Rice, (2007 John Wiley & Sons, Inc.).
7. C. Mejia-Monasterio, H. Larralde, and F. Leyvraz, Phys. Rev. Lett. 86 (2001) 5417.
8. D. J. Bergman and O. Levy, Appl. Phys. 70 (1991) 6821.
9. P. L. Walstrom, Am. J. Phys. 56 (1988), 890. See also H. Larralde, F. Leyvraz, and C. Mejia-Monasterio, J. Stat. Phys. 113 (2003), 197, where the equivalence between \( \mu \) and \( \mu_e \) has been studied for a similar model to the one we study here.
10. C. A. Domenicali, Rev. Mod. Phys. 26 (1954), 237.
11. H. B. Callen, Phys. Rev. 73 (1948) 1349; S. R. de Groot and P. Mazur, Non-equilibrium Thermodynamics (Dover, New York, 1984).
12. Assuming that particles do not interact means that we fully neglect the phonon transport.
13. C. B. Vining, Mat. Res. Soc. Symp. Proc. 478 (1997) 3.
14. J.-P. Eckmann, C. Mejia-Monasterio, and E. Zabey, J. Stat. Phys. 123 (2006) 1339.