CBPF - CENTRO BRASILEIRO DE PESQUISAS FÍSICAS

Rio de Janeiro

Notas de Física

Addendum to "Eliminating the cuspidal temperature profile of a non-equilibrium chain" [CBPF-NF-011/15]

Michael M. Cândido, Welles A. M. Morgado and Sílvio M. Duarte Queirós

MINISTÉRIO DA
**CIÊNCIA, TECNOLOGIA,
INOVAÇÕES E COMUNICAÇÕES**

Addendum to "Eliminating the cuspidal temperature profile of a non-equilibrium chain" [CBPF-NF-011/15]

Michael M. Cândido and Welles A. M. Morgado[*]

Department of Physics, PUC-Rio

Rua Marquês de São Vicente 225,

22453-900 Rio de Janeiro — RJ, Brazil

Sílvio M. Duarte Queirós[*]

Centro Brasileiro de Pesquisas Físicas

Rua Dr Xavier Sigaud, 150, 22290-180 Rio de Janeiro — RJ, Brazil

This Nota de Física aims to shed further light on the origin of the cuspidal temperature profile of non-equilibrium chains, namely the 1967 Rieder, Liebowitz and Lieb heat conduction model. Our upgraded analysis shows that the first plateau – where the cumulants of the heat flux reach their maxima – is related to the vanishing of the (instantaneous) stationary state two-point velocity correlations for all pairs of elements in the chain, $C_v(i,j) \equiv \lim_{t\to\infty} \langle v_i(t) v_j(t) \rangle = 0$. Such behaviour is equivalent to having a "phonon box". For the second plateau, $C_v(i,j)$ only vanishes when one of the sites is a edge site; however, the sum of the stationary state two-point velocity correlations over all pairs still equals zero, $\sum_{\langle ij \rangle} C_v(i,j) = 0$, as happens whenever the chain is linear. Bringing the non-linear β-Fermi-Pasta-Ulam nonequilibrium model into play, we verify that the bulk plateau disappears and that in this situation $\sum_{\langle ij \rangle} C_v(i,j) \neq 0$. These results confirm a relation between heat transport in non-equilibrium systems and a spatial propagator that is proxied by $C_v(i,j)$.

Previous results. In our original Nota de Física (NF) [1], we started out from the awkward temperature profile exhibited by the model introduced by Rieder, Lebowitz and Lieb (RLL) [4]. We verify that the cuspidal of the local temperature behaviour lies in mechanical properties of the model, namely absence of effective pinning of the chain.

---

[*] Associate to the National Institute of Science and Technology for Complex Systems, Brazil

Assuming a chain of N coupled linear ($k_3 = 0$) oscillators ruled by the set of equations,

$$\begin{cases} m \frac{d^2 x_1}{dt^2} = -\gamma \frac{dx_1}{dt} - k' x_1 - k_1 (x_1 - x_2) - k_3 (x_1 - x_2)^3 + \eta_1 \\ \\ m \frac{d^2 x_i}{dt^2} = -k x_i - k_1 (2 x_i - x_{i+1} - x_{i-1}) - k_3 \left[(x_i - x_{i-1})^3 + (x_i - x_{i+1})^3 \right] , \\ \\ m \frac{d^2 x_N}{dt^2} = -\gamma \frac{dx_N}{dt} - k' x_N - k_1 (x_N - x_{N-1}) - k_3 (x_N - x_{N-1})^3 + \eta_N \end{cases} \quad (1)$$

($2 \leq i \leq N - 1$), where η is Gaussian distributed with,

$$\langle \eta_i (t) \, \eta_j (t') \rangle = 2 \, \gamma \, T_i \, \delta_{ij} \, \delta (t - t') , \quad (2)$$

[$T_{C(H)} \equiv T_{1(N)}$ and $(i, j) = \{1, N\}$] we have verified that is possible change twice from the cuspidal temperature profile to a smooth temperature profile and vice-versa. At these profile changes, a perfect plateau for the local canonical temperature across the chain is computed, i.e., $\mathcal{T}_i = (T_C + T_H)/2$ (for all i).

Explicitly, we found that the first plateau – at which the cumulants of the heat flux reach their maximal value – reads

$$k'_{crit_1} = \frac{k}{2} + \frac{\sqrt{k^2 + 4kk_1}}{2}. \quad (3)$$

whereas the second plateau is given by

$$k'_{crit_2} = k + k_1 + \frac{\gamma^2}{m}. \quad (4)$$

The two-point velocity correlation function. In a nonequilibrium of this kind the leading flux is the heat flux

$$\mathcal{J} \equiv \frac{k_1}{2} \langle (x_i - x_{i+1}) (v_i + v_{i+1}) \rangle = -\kappa \, \Delta T \qquad i \in (1, N - 1), \quad (5)$$

(where κ represents the *thermal conductance* of the system and $\Delta T \equiv T_H - T_C$) and the temperature of the neighbours, namely the end particles, $\mathcal{T}_1$ and $\mathcal{T}_N$. Intuitively, by increasing the pinning at the edges, we would insulate particles 1 and N from the bulk and make their canonical temperatures $\mathcal{T}_1$ and $\mathcal{T}_N$, respectively, approach the temperature of the reservoirs T_C and T_H. Note that because of the condition of stationarity,

$$\lim_{t \to 0} \langle x_i(t) \, v_i(t) \rangle = \langle v_i(t) \rangle = 0. \quad (6)$$

Hence, the heat flux is a proxy for the two-point position-velocity correlation function, $C_{xv}(i; \delta = 1)$, where we define the two-point correlation function relating two generic quantities u and w measured at different points separated by a lattice site distance equal to δ as

$$C_{uw}(i,j) = C_{uw}(i;\delta) \equiv \lim_{t \to 0} \langle u_i(t)\, w_{i+\delta}(t) \rangle - \langle u_i(t) \rangle \, \langle w_{i+\delta}(t) \rangle. \tag{7}$$

If $u = w$, then we simplify the notation to $C_u(i;\delta)$.

The matching of the maxima of the cumulant has a very particular meaning in condensed matter physics: it points to the emergence of a phase transition. Although we could think of the plateau as the critical state separating the smooth state,

$$\lim_{N \to \infty} \frac{1}{N} \sum_{i=2}^{N/2} \mathcal{T}_i - \mathcal{T}_{N-i+1} < 0 \tag{8}$$

from the cuspidal state,

$$\lim_{N \to \infty} \frac{1}{N} \sum_{i=2}^{N/2} \mathcal{T}_i - \mathcal{T}_{N-i+1} > 0 \tag{9}$$

we rule out such approach because we do not verify another crucial feature that identifies a transition, i.e., the divergence of the correlation length, ξ, characterising the average over the sites of the lattice of the two-point correlation function of the square velocity,[1] $\widetilde{C_{v^2}}(\delta)$ [see Appendix].
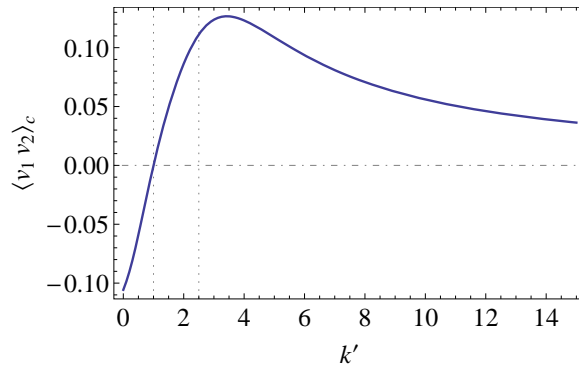

Figura 1.   Next-nearest-neighbour two-point correlation function $C_v(1)$ v k' for the edge particle $i = 1$. The remaining parameters are $m = k_1 = \gamma = 1$, $k = 1/2$, $T_C = 1$ and $T_H = 2$. It is visible that the correlation vanishes at $k'_{crit_1} = 1$, the same point we have the cumulants of the heat flux reaching their maximal values. For $k'_{crit_2} = 5/2$ we have $C_v(1) \approx 0.11$.

––––––––––
[1] v_i^2 can be seen as a measure of the instantaneous temperature at site i.

So, what does actually happen when we pass from the cuspidal to the smooth profile and vice versa? The key feature to understanding the phenomenon does not lie in C_{v^2} but in the two-point correlation function of the velocity C_v. From our calculations, $\widetilde{C_v}(1)$ vanishes at k'_{crit_1} [see Fig. (1) for an illustration], for *all* the neighbouring sites of the chain, whether they are edge or bulk particles. At this value of k', the two-point correlation function $C_v(1;1)$ is the same as its asymptotic value $k' \to \infty$ that is equivalent to the picture of having perfectly curbed particles at the edges of the chain.

Figure 2 shows the behaviour of $C_v(i;\delta)$ for different values of i and δ for a chain $N = 11$. Observe that the correlations are symmetrical with respect to the middle of the lattice with the overall analysis of these curves giving us an interesting insight over the mechanics of the crossover; specifically, as k' increases, in the vicinity of $k' = 1$, the value of $C_v(1;1)$ increases from a negative to a positive value. Simultaneously, the local temperature $\mathcal{T}_2$ also increases monotonically. We may interpret that twofold: on the one hand, the typical vibration mode, for $k' < 1$, is antisymmetric for neighbours near the colder reservoir, decreasing with distance; on the other hand, it is symmetric for the neighbours near the hotter reservoir. The typical antisymmetric motion gives rise to velocity anti-correlation, $(C_v(i;\delta) < 0)$, while the typical symmetric motion gives rise to the positive correlations. Furthermore, the latter assures that the particles are in a more energetic (kinetic) state than the former. As a matter of fact, this is reflected in the local temperatures since by increasing the surface pinning to $k' = 1$ the value of $C_v(i;\delta)$ for all i and δ vanish and the bulk reaches a perfect temperature plateau. A system of masses and springs at equilibrium should present null velocity correlations due to the quadratic character of the kinetic energy distribution.

As we increase k' somewhat past its critical value, the next nearest neighbours velocity-velocity correlation changes sign. That means the probability of occupation of modes which favour anti-symmetric $v_1 v_2$-vibrations decreases whereas the probability of occupation of modes that are related to symmetric $v_1 v_2$-vibrations increases. The fact that $\mathcal{T}_2$ (kinetic energy content) increases, is completely compatible with the anti-symmetric vibration modes being less energetic than the symmetric ones. Simultaneously, the inverse happens at the other extremity of the chain, i.e., the local energy scale, $\mathcal{T}_{N-1}$, decreases as the correlation $C_{v_{N-1}}(1) = \langle v_N v_{N-1} \rangle_c$ switches from positive to negative at $k' = 1$.
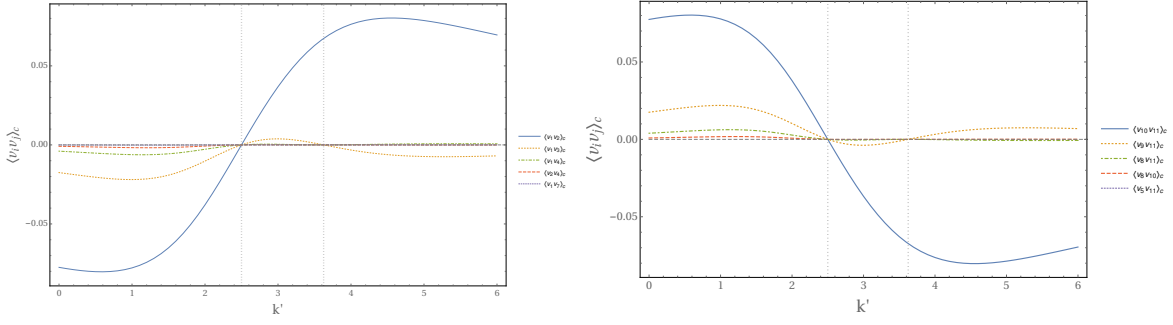
Figura 2. Two-point velocity correlation function for the particles indicated on the right-hand side legend of each panel. for the extremities and the bulk particles are shown. For $k' = 1$ all the correlations vanish and the set of local temperatures form a plateau. For $k' = 5/2$, the temperature plateau reappears as well as the vanishing of the two-point velocity correlation function except for $C_v(1;1)$ and $C_v(N-1;1)$. The correlations are symmetric around the middle of the lattice.

This is completely consistent with vibrations switching from energetic symmetric modes to less energetic anti-symmetric modes.

When the two-point velocity-correlations between all neighbours vanish at $k' = 1$ there is a strong heat current through the system and even and odd order cumulants reach maxima at that point. As k' increases the current whereas its fluctuations decrease and the even cumulants will reach eventually their equilibrium values – the "phonon box" values which are smaller than the plateau point values – while the odd ones vanish at the limit of null heat flux as $k' \to \infty$.

   The impact of nonlinearities.   It is well known that nonlinear interactions may change some properties of heat transport, because they can be related to the localisation of the vibration modes across the chain and hence to the phonons scattering. Some previous results using FPU-like models in one dimensional chains have checked that the ballistic transport of energy is slightly changed when cubic or quartic interactions are present [16] even in two-dimensional systems like graphene [17]. Even though observing a temperature gradient in the system, it is verified that the thermal conductivity for one dimensional non-linear system behaves like, $\kappa \propto N^\alpha$, with $\frac{1}{3} \leq \alpha \leq \frac{1}{2}$ [2, 10, 11], which becomes infinite in the thermodynamic limit. All these properties are well discussed in literature [2, 3, 5, 10, 12], where numerical treatment is a standard procedure to obtain the results, but some

authors [14, 15] have been proposing analytical approaches to verify more thermostatistical properties in non-linear models.

Let us now assume $k_3 \neq 0$ in the equations of motion Eq. (1) and in order to guarantee the accurateness of our perturbative method this new non-linear coupling obeys the relation $\frac{k_3 T_H}{k_1^2} \ll 1$ [9]. Figure 3 shows that we no longer see the vanishing of $C_v(i; \delta)$ for all pairs at $k'_{crit_1} = 1$, and the perfect symmetry between opposite pairs is subtly broken.
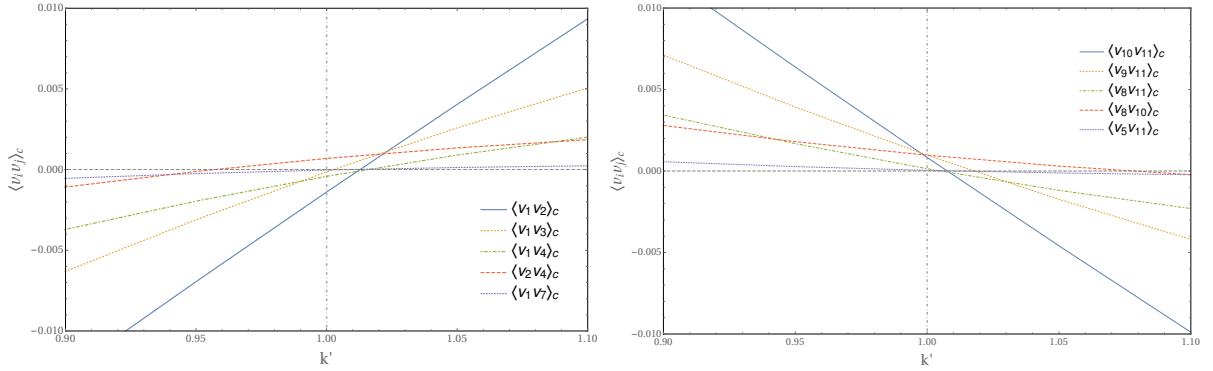

Figura 3. Left and right panels show that the zero correlation occurs at different points for all pairs when one analyses these functions near the point $k'_{crit_1} = 1$.

The fact that the correlations cannot vanish simultaneously for every pair and a given k' in a nonlinear model is quite straightforward to verify. It is possible to notice that one of the properties that define the zero correlation is the "pseudo" bulk equilibrium, since the nonlinear interactions generate a temperature gradient along the chain, the state related to the existence of a plateau is now unattainable.

Besides the role played in the behaviour of heat transfer and the distribution of temperatures, it is clear from Fig. 3 that the cubic interaction (with small k_3) favours mostly the antisymmetric modes of the chain, since almost all $C_v(\delta)$ cross the k' axis after $k'_{crit_1} = 1$. It is important to stress that the previous discussion over the distribution of modes with respect to the middle of the chain for multiples values of k' is not straightforward now, because the way phonons interact is considerably modified by the anharmonicities in the system. Since that would go beyond the scope of this work, we have omitted a more detailed study regarding the methods and properties of nonlinear chains used here, which will be published elsewhere.

Discussion. The results we have presented in Figs. 2 and 3 seem to connect with previous results on the analysis of the energy and momentum correlation functions in equilibrium systems subject perturbations. Enclosing this situation within linear response theory, transport coefficients like the conductance κ (as well as the thermal conductivity) and the effective coefficient of viscosity of the system were related to the second derivative in order to time of the heat diffusion,[2]

$$\left\langle x(t)^2 \right\rangle_E \equiv \frac{1}{\mathcal{N}_E} \int \left(x(t)^2 - \langle x(t)\rangle_E^2 \right) \langle \Delta E(x,t)\Delta E(y,t)\rangle \, dy \,, \tag{10}$$

and the momentum diffusion

$$\left\langle x(t)^2 \right\rangle_p \equiv \frac{1}{\mathcal{N}_p} \int \left(x(t)^2 - \langle x(t)\rangle_p^2 \right) \langle \Delta p(x,t)\Delta p(y,t)\rangle \, dy \,, \tag{11}$$

respectively (full details can be easily found in Sec. 2 of [18]). Following both definitions, it is not hard to understand that $C_v(i;\delta) = m^{-2} \, \overline{\langle \Delta p(i,t)\, \Delta p(i+\delta,t)\rangle}$.

The present results are different of those aforementioned because our two-point velocity correlation functions are not time lagged and averaged over the steady state of a nonequilibrium system; nonetheless, the two Figures 2 and 3 point to interesting facts. In the harmonic case — that includes the RLL model — the sum over all pairs of the velocity correlation function,

$$\mathcal{C} \equiv \sum_{i=1}^{N-1} \sum_{\delta=1}^{N-i} C_v(i;\delta) \tag{12}$$

vanishes,

$$\mathcal{C}|_{k_3=0} = 0. \tag{13}$$

Moreover, at the first plateau,

$$C_v(i;\delta)\,|_{\left(k_3=0,k'_{crit_1}\right)} = 0, \quad \forall_{i,\delta}, \tag{14}$$

whereas at the second plateau

$$C_v(i;\delta)\,|_{\left(k_3=0,k'_{crit_2}\right)} \neq 0, \ \text{if} \ i = \{1, N-1\} \ \text{and} \ \delta = 1$$
$$\text{and} \tag{15}$$
$$C_v(i;\delta)\,|_{\left(k_3=0,k'_{crit_2}\right)} \neq 0, \ \text{if} \ i = \{2,\ldots,N-1\}$$

---

[2] In a continuous approach.

On the other hand, if $k_3 = 0$ we have anomalous transport of heat and thus

$$\mathcal{C}|_{k_3 \neq 0} \neq 0. \tag{16}$$

In Fig. 4, we present the results of $\mathcal{C}|_{k_3 \neq 0}$ as a function of k_3.
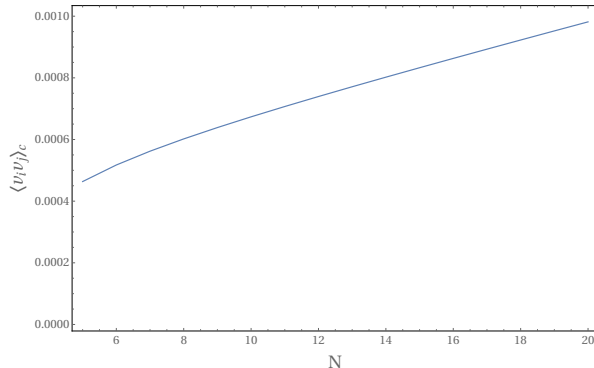

Figura 4. Average of the $C_v(i; \delta)$ for all pairs and distances vs size of the chain. The blue line grows as $N^{0.54}$.

APPENDIX: CORRELATION LENGTH BEHAVIOUR

In condensed matter physics, the coincidence in the maxima of the cumulants hints at the existence of a phase transition. Moreover, the emergence of critical behaviour in a system is also characterised by the arising of an infinite correlation length, ξ, characterising the two-point correlation function that goes as

$$C_u(\delta) \propto \exp\left[-\delta/\xi\right]. \tag{17}$$

At the plateau, all the bulk particles have the same canonical temperature, hence we have a totally correlated local temperature that could be seen as a sort of "ordered state of the system". That said, it is possible to check whether we have a critical-like mechanism by computing the two-point correlation function of the square velocity, $C_{v^2}(\delta)$, for different values of k' and assess if close to the first threshold we have,

$$\xi \propto |\Delta k'|^{-\nu_\pm}. \tag{18}$$

where $\Delta k' = k' - k'_{crit_1}$.

In order to probe Eq. (18), we fitted Eq. (17) in a log-linear scale for which the slope would be equal to ξ^{-1}. Then, when we pick the correlation length and plot it against $\Delta k'$ in a log-log scale we cannot discern a standard critical phenomena power-law; as a matter of fact, we find a quite likely linear dependence ($R^2 = 0.99999998$ and $p - \text{value} = 10^{-67}$) implying a finite value of ξ for k'_{crit_1}. The smooth change of ξ lead us to reject the hypothesis of a phase transition scenario.
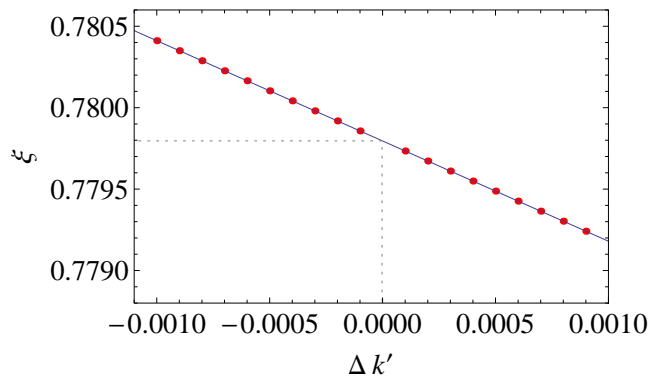

Figura 5.   Correlation length as a function of $\Delta k'$. The parameters are the following: $m = k_1 = \gamma = 1$, $k = \frac{1}{2}$, $T_C = 1$ and $T_H = 2$. The points are obtained from the analytical method and the line corresponds to a linear fit with a slope equal to $-0.61576 \pm 1.9 \times 10^{-5}$, ordinate at the origin $\xi^* = 0.779796 \pm 1.1 \times 10^{-8}$ and $R^2 = 0.99999998$.

[1] M.M. Cândido, W.A.M. Morgado and S.M. Duarte Queirós, Notas de Física CBPF-NF-011/15 (2015)

[2] S. Lepri, R. Livi and A. Politi, Phys. Rep. **377** 1 (2003).

[3] A. Dhar, Adv. Phys. **57** 457 (2008).

[4] Z. Rieder, J. L. Lebowitz and E. Lieb, J. Math. Phys. **8** 1073 (1967).

[5] K. Saito and A. Dhar, Phys. Rev. Lett. **104** 040601 (2010).

[6] D. J. R. Mimnagh, *Thermal conductivity and dynamics of a chain of free and bound particles* (Ph.D. Dissertation, Simon Fraser University, 1997).

[7] M. Toda, J. Phys. Soc. Japan **22** 431 (1967).

[8] G. Casati, J. Ford, F. Vivaldi and W. M. Visscher, Phys. Rev. Lett. **52** 1861 (1984).

[9] W. A. M. Morgado and S. M. Duarte Queirós, Phys. Rev. E **90** 022110 (2014).

[10] A. Dhar and J. L. Lebowitz, Phys. Rev. Lett. **100** 134301 (2008).

[11] H. Van Beijeren, Phys. Rev. Lett. **108** 180601 (2012).

[12] Suman G. Das, A. Dhar, O, Narayan, J. Stat. Phys **154** (2014).

[13] W. A. M. Morgado, S. M. Duarte Queirós and M. M. Cândido (forthcoming).

[14] R. R. Ávila, E. Pereira and D. L. Teixeira, Physica A **423** 51 (2015).

[15] M. S. Mendonça and E. Pereira, Physics Lett. A, **379** 36 (2015).

[16] E. Fermi, J. Pasta, and S. Ulam, Studies of nonlinear problems (1955). Accessible online
      at URL: http://www.osti.gov/accomplishments/pdf/A80037041/01.pdf;
      G. P. Berman and F. M. Izrailev, Chaos **15**, 015104 (2005).

[17] D. Midtvedt, A. Croy, A. Isacsson, Z. Qi, and H. S. Park, Phys. Rev. Lett. **112**, 1 (2014).

[18] Y. Li, S. Liu, N. Li, P. Hänggi and B. Li, New J. Phys. **17**, 043064 (2015)

Pedidos de cópias desta publicação devem ser enviados aos autores ou ao:

Requests for copies of these reports should be addressed to: