

ERRATUM: NONEQUILIBRIUM SHEAR VISCOSITY COMPUTATIONS WITH LANGEVIN DYNAMICS

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Abstract. This short note is an erratum to the article [R. Joubaud and G. Stoltz, Nonequilibrium shear viscosity computations with Langevin dynamics, *Multiscale Model. Sim.*, 10 (2012), pp. 191–216]. We present required modifications in the proofs of Theorem 2 and 3.

Key words. Nonequilibrium molecular dynamics, hypocoercivity, linear response theory, shear viscosity

AMS subject classifications. 82C70, 82C31

There were two mistakes in the proofs of Theorems 2 and 3 in [3]:

- first, we used an incorrect property from [6], namely that \mathcal{A}_0^{-1} is a bounded operator from $L^2(\psi_0)$ to $H^1(\psi_0)$ (see the proof of Proposition 2.1 in [6, page 1645]). This property was used in [6] to prove that \mathcal{A}_0^{-1} is compact on $L^2(\psi_0)$. The latter result can however be proved using for instance the techniques from [1], see the correction in [5].
- second, some commutator terms were missing in the uniform hypocoercivity estimate (5.7). In fact, the uniform coercivity property is true only for functions whose average with respect to the Gibbs distribution in the velocity variable p_y (for Theorem 2) or p_x (for Theorem 3) vanishes.

We show here how to correct the proof of [3, Theorem 2], the corrections in the proof of Theorem 3 being similar. We refer to [4] for a full corrected proof.

We first need to modify the formal solutions in the ansatz $f_{\gamma_y} = f^0 + \gamma_y^{-1} f^1 + \gamma_y^{-2} f^2 + \dots$ and consider in fact

$$f^1(q, p) = p_y \cdot \nabla_{q_y} f^0(q, p) + \tilde{f}^1(q, p_x),$$

where \tilde{f}^1 is made precise below (see (0.6)).

Uniform hypocoercivity estimates. We show that

$$-\langle\langle u, \mathcal{A}_{y, \text{thm}} u \rangle\rangle \geq 0 \tag{0.1}$$

for functions u in an appropriate subspace of $H^1(\psi_0)$. Using the commutation relations $[\partial_{p_{\alpha,i}}, \partial_{p_{\alpha',j}}^*] = \beta \delta_{\alpha,\alpha'} \delta_{ij}$ ($\alpha, \alpha' \in \{x, y\}$), a simple computation shows

$$\begin{aligned} \left\langle\left\langle u, \sum_{i=1}^N (\partial_{p_{y_i}})^* \partial_{p_{y_i}} u \right\rangle\right\rangle &= \sum_{i=1}^N (a + \beta b) \|\partial_{p_{y_i}} u\|^2 + b \|\nabla_p \partial_{p_{y_i}} u\|^2 \\ &\quad + b \|\nabla_q \partial_{p_{y_i}} u\|^2 + 2 \langle \nabla_q \partial_{p_{y_i}} u, \nabla_p \partial_{p_{y_i}} u \rangle + \beta \langle \partial_{q_{y_i}} u, \partial_{p_{y_i}} u \rangle \\ &\geq \sum_{i=1}^N \left(a + \beta \left(b - \frac{1}{2} \right) \right) \|\partial_{p_{y_i}} u\|^2 + (b - 1) \|\nabla_p \partial_{p_{y_i}} u\|^2 \\ &\quad + (b - 1) \|\nabla_q \partial_{p_{y_i}} u\|^2 - \frac{\beta}{2} \|\partial_{q_{y_i}} u\|^2. \end{aligned}$$

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Summing on $i \in \{1, \dots, N\}$, the quantity (0.1) is seen to be non-negative for an appropriate choice of constants $a \gg b \gg 1$ provided there exists a constant $A > 0$ such that, for all $i = 1, \dots, N$,

$$\|\partial_{q_{yi}} u\| \leq A \|\nabla_p \partial_{q_{yi}} u\|. \quad (0.2)$$

This indeed implies

$$\sum_{i=1}^N \|\partial_{q_{yi}} u\|^2 \leq A \sum_{i,j=1}^N \|\partial_{p_{yj}} \partial_{q_{yi}} u\|^2 = A \sum_{j=1}^N \|\nabla_{q_y} \partial_{p_{yj}}\|^2 \leq A \sum_{j=1}^N \|\nabla_q \partial_{p_{yj}}\|^2.$$

Since the Gaussian measure satisfies a Poincaré inequality, the inequalities (0.2) hold provided

$$\forall i = 1, \dots, N, \quad \int_{\mathbb{R}^N} \partial_{q_{yi}} u(q, p) \exp\left(-\beta \frac{p_y^2}{2}\right) dp_y = 0.$$

Defining the closed subspace of $L^2(\psi_0) \cap \{1\}^\perp$

$$\mathcal{H}_0 = \left\{ v \in H^1(\psi_0) \mid \bar{v}(q, p_x) = \left(\frac{2\pi}{\beta}\right)^{-N/2} \int_{\mathbb{R}^N} v(q, p) \exp\left(-\beta \frac{p_y^2}{2}\right) dp_y = 0 \right\} \subset \mathcal{H}, \quad (0.3)$$

we conclude that, for any $u \in \mathcal{H}_0 \cap H^2(\psi_0)$,

$$C \|u\|_{H^1(\psi_0)}^2 \leq -\langle u, \mathcal{A}_0(\gamma_y)u \rangle. \quad (0.4)$$

In particular, there exists a constant $K > 0$ such that, for any $\gamma_y \geq \gamma_x$ and for any $u \in \mathcal{H}_0 \cap H^2(\psi_0)$,

$$\|\mathcal{A}_0(\gamma)^{-1} u\|_{H^1(\psi_0)} \leq K \|u\|_{H^1(\psi_0)}.$$

In fact, this inequality can be extended to functions in \mathcal{H}_0 .

Proof of the limit (3.13). A simple computation shows that

$$-\mathcal{A}_0(\gamma_y) (f_{\gamma_y} - f^0 - \gamma_y^{-1} f^1) = \frac{1}{\gamma_y} T_0 f^1,$$

so that

$$f_{\gamma_y} - f^0 - \gamma_y^{-1} f^1 = -\frac{1}{\gamma_y} \mathcal{A}_0(\gamma_y)^{-1} T_0 f^1. \quad (0.5)$$

Since $\mathcal{A}_0(\gamma_y)^{-1}$ is bounded on \mathcal{H}_0 , uniformly in γ_y (see (0.4)), it is sufficient to show that $T_0 f^1 \in \mathcal{H}_0$. In view of the definition of f^0 , the proof is then concluded by setting $\phi_i(q, p) = -\mathcal{T}_{q_y}^{-1}(p_{xi})$.

Let us first show that $\overline{T_0 f^1}(q, p_x) = 0$ (where \bar{v} is defined in (0.3)). This can be ensured by an appropriate choice of \tilde{f}^1 . Note first that

$$T_0 f^1 = p_y \cdot \nabla_{q_y} \tilde{f}^1 + \mathcal{T}_{q_y} f^1 + (p_y \cdot \nabla_{q_y} - \nabla_{q_y} V \cdot \nabla_{p_y}) f^1 + \mathcal{T}_{q_y} \tilde{f}^1.$$

The first two terms have a vanishing average with respect to $(2\pi)^{-N/2} \exp\left(-\beta \frac{p_y^2}{2}\right) dp_y$. Introducing

$$g(q, p_x) = -(2\pi)^{-N/2} \int_{\mathbb{R}^N} (p_y \cdot \nabla_{q_y} - \nabla_{q_y} V \cdot \nabla_{p_y}) f^1 \exp\left(-\beta \frac{p_y^2}{2}\right) dp_y,$$

the condition $\overline{T_0 f^1} = 0$ is satisfied provided

$$\mathcal{T}_{q_y} \tilde{f}^1 = g(q, p_x),$$

Seeing the function on the right-hand side as a function of (q_x, p_x) indexed by q_y allows to define \tilde{f}^1 pointwise in q_y as

$$\tilde{f}^1 = -(2\pi)^{-N/2} \mathcal{T}_{q_y}^{-1} g. \quad (0.6)$$

Let us now study the regularity of $T_0 f^1$. We only treat the term $T_0(f^1 - \tilde{f}^1)$ since the regularity of $T_0 \tilde{f}^1$ can be proved similarly. Recall that all the functions under consideration are C^∞ by hypoellipticity. Therefore, only the derivatives in the p variables have to be considered because the position space is compact. Now,

$$\begin{aligned} f^1 - \tilde{f}^1 &= - \sum_i p_{yi} G'(q_{yi}) \mathcal{T}_{q_y}^{-1}(p_{xi}) \\ &\quad - \sum_{i,j,k} p_{yi} G(q_{yj}) \left\{ \left(\mathcal{T}_{q_y}^{-1} \right) \left[\partial_{q_{yi}, q_{xk}}^2 V(q_x, q_y) \partial_{p_{xk}} \right] \left(\mathcal{T}_{q_y}^{-1} \right) p_{xj} \right\}. \end{aligned} \quad (0.7)$$

The p_y dependence is trivial in the above expression, so that only derivatives in p_x require some attention. Since $T_0 = \mathcal{A}_{y,\text{ham}} + \mathcal{T}_{q_y}$ where $\mathcal{A}_{y,\text{ham}} = p_y \cdot \nabla_{q_y} - \nabla_{q_y} V(q_x, q_y) \cdot \nabla_{p_y}$ is an operator in the q_y, p_y variables (parameterized by q_x), it suffices to consider $\mathcal{T}_{q_y} f^1$. This function is, in turn, a linear combination of terms of the form $p_{yi} p_{xi}$ (cf. the first term in the right-hand side of (0.7)) and $p_{yi} \partial_{p_{xk}} \mathcal{T}_{q_y}^{-1} p_{xj}$ (second term in the right-hand side of (0.7)). To prove that the latter functions are in $H^1(\psi_0)$, we use the results of [7, 2], which show that $\mathcal{T}_{q_y}^{-1}$ is a bounded operator on the Hilbert spaces

$$\left\{ f \in H^m(\Psi_{q_y}) \mid \int_{(L_x \mathbb{T})^N \times \mathbb{R}^N} f(q_x, p_x) \Psi_{q_y}(q_x, p_x) dq_x dp_x \right\} \subset L^2(\Psi_{q_y})$$

for any $m \geq 0$, with a bound uniform in q_y .

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