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Remarks on the Notion of Mean Free Path for a Periodic Array of Spherical Obstacles

H. S. Dumas,[1] L. Dumas,[2] and F. Golse[3]

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In this note, we explain in detail how the notion of mean free path is related to the mathematical results obtained in our previous paper.

KEY WORDS: Mean free path; dispersive billiards; periodic Lorentz gas; kinetic theory; exit time; homogenization.

The purpose of this note is to clarify ambiguities concerning the notion of mean free path in our previous article[8] and its companion paper.[3] We are grateful to N. Chernov for bringing these ambiguities to our attention. However, we should say that the ambiguous terminology does not affect the mathematical results in Ref. 8. All the theorems, lemmas, and corollaries in Ref. 8 are true as stated, and do not explicitly refer to any definition of mean free path.

1. In the case of a Lorentz gas, the notion of free path length is uniquely defined. The specific example studied in Ref. 8 is as follows. Let $r \in]0, 1/2[$ and $\gamma \geqslant 1$; for all $\varepsilon \in]0, 1[$, define

$$Z_\varepsilon = \{x \in \mathbf{R}^n \mid \operatorname{dist}(x, \varepsilon^n \mathbf{Z}) > r\varepsilon^\gamma\} \tag{1}$$

The lattice ε^n acts by translations on Z_ε; let $Y_\varepsilon = Z_\varepsilon/\varepsilon\mathbf{Z}^n$. The "free path length" starting from the point $x \in Z_\varepsilon$ in the direction $\omega \in S^{n-1}$ is the nonnegative Borel function

$$\tau_\varepsilon(\cdot, \cdot; \gamma): \quad Y_\varepsilon \times S^{n-1} \to \mathbf{R}^+ \tag{2}$$

[1] Department of Mathematical Sciences, University of Cincinnati, Cincinnati, Ohio 45221-0025.

[2] Laboratoire d'Analyse Numérique, Université Paris VI, F75005 Paris, France.

[3] DMI, Université Paris VII & École Normale Supérieure, F5005 Paris, France.

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defined by the formula

$$\tau_\varepsilon(x, \omega; \gamma) = \inf\{t > 0 \mid x - t\omega \in \partial Z_\varepsilon\} = \sup\{t \geqslant 0 \mid [x, x - t\omega] \subset \bar{Z}_\varepsilon\} \qquad (3)$$

There are two different, natural probability measures on $Y_\varepsilon \times S^{n-1}$ with respect to which τ_ε can be studied as a random variable. One is the normalized Lebesgue measure $\mu_{\varepsilon,\gamma}$ on $Y_\varepsilon \times S^{n-1}$:

$$\mu_{\varepsilon,\gamma} = Q_\varepsilon^{-1}\, dx\, d\omega, \qquad Q_\varepsilon = dx\, d\omega\text{-meas}(Y_\varepsilon \times S^{n-1}) \qquad (4)$$

The other is the normalized measure $\nu_{\varepsilon,\gamma}$ concentrated on the "outgoing boundary"

$$\Sigma_\varepsilon^+ = \{(x, \omega) \in (\partial Z_\varepsilon \cap Y_\varepsilon) \times S^{n-1} \mid \omega \cdot n_x > 0\} \qquad (5)$$

(where n_x is the inward unit normal at the point $x \in \partial Z_\varepsilon$) and defined by

$$\nu_{\varepsilon,\gamma} = \Gamma_\varepsilon^{-1}\, dS(x)\, d\omega, \qquad \Gamma_\varepsilon = dS(x)\, d\omega\text{-meas}(\Sigma_\varepsilon^+) \qquad (6)$$

where $dS(x)$ is the induced surface measure on ∂Y_ε. Both of these probability measures are natural objects to consider. Indeed, the measure $\mu_{\varepsilon,\gamma}$ is invariant under the broken flow on $Z_\varepsilon \times S^{n-1}$ associated with

$$\frac{dx}{dt} = \omega, \qquad \frac{d\omega}{dt} = 0 \qquad \text{for} \quad x \notin \partial Z_\varepsilon \qquad (7)$$

$$x(t_0 + 0) = x(t_0 - 0), \qquad \omega(t_0 + 0) = \omega(t_0 - 0) - 2\omega(t_0 - 0) \cdot n_{x(t_0 - 0)} n_{x(t_0 - 0)}$$
$$\text{for} \quad x(t_0 - 0) \in \partial Z_\varepsilon \qquad (8)$$

while the measure $\mu_{\varepsilon,\gamma}$ is invariant under the map $\Sigma_\varepsilon^+ \to \Sigma_\varepsilon^+$ defined a.e. by

$$(x, \omega) \mapsto (x' = x + \tau_\varepsilon(x, -\omega; \gamma)\, \omega;\ \omega' = \omega - 2\omega \cdot n_{x'} n_{x'}) \qquad (9)$$

We shall denote by $\phi_{\varepsilon,\gamma}$ (resp. $\psi_{\varepsilon,\gamma}$) the distributions of τ_ε under the measure $\mu_{\varepsilon,\gamma}$ (resp. $\nu_{\varepsilon,\gamma}$). In other words, $\phi_{\varepsilon,\gamma}$ and $\psi_{\varepsilon,\gamma}$ are the Borel probability measures on $\mathbf{R}^+$ such that

$$\phi_{\varepsilon,\gamma}(A) = \mu_{\varepsilon,\gamma}(\tau_\varepsilon(\cdot, \cdot; \gamma)^{-1}(A)), \quad \psi_{\varepsilon,\gamma}(A) = \nu_{\varepsilon,\gamma}(\tau_\varepsilon(\cdot, -\cdot; \gamma)^{-1}(A)) \qquad (10)$$

for all Borel measurable subsets A of $\mathbf{R}^+$.

Correspondingly, there are two possible notions of mean free path associated with the periodic Lorentz gas in Z_ε: For all $T > 0$, we define

$$\lambda(\varepsilon, \gamma) = \int_0^{+\infty} z\, d\psi_{\varepsilon,\gamma}(z) \quad \text{and} \quad l(\varepsilon, T, \gamma) = \int_0^{+\infty} \inf(z, T)\, d\phi_{\varepsilon,\gamma}(z) \qquad (11)$$

We call $\lambda(\varepsilon, \gamma)$ the "geometric mean free path" and $l(\varepsilon, T, \gamma)$ the "mean truncated free path." The truncation in the second definition is necessary because $l(\varepsilon, +\infty, \gamma) = +\infty$. In the case $n=2$, this follows from one of the theorems in Ref. 3 (which relies in particular on constructions very similar to those of Ref. 2). This is why we refrain from calling $l(\varepsilon, T, \gamma)$ the mean free path.

The same construction applies to the most general "billiard tables."[5,6] Whenever the analogue of the map (9) is ergodic for the measure $\nu_{\varepsilon,\gamma}$, the geometric mean free path can be interpreted as the average path length between N successive collisions of a point particle with the obstacles (the boundary of Z_ε) with specular reflections at the boundary of each obstacle, in the limit as $N \to +\infty$. This follows immediately from the Birkhoff ergodic theorem, and for this reason it is natural to associate the geometric mean free path with billiards.[5,6]

However if, as in Ref. 8, one is interested in the evolution of a population of point particles undergoing collisions only with the boundary of Z_ε, the mean truncated free path $l(\varepsilon, T, \gamma)$ is more natural. In the (too) simple example where the particles are completely absorbed at the boundary, the number density $f(t, x, \omega)$ of particles which at time t are at position x and moving in the direction ω is given by [see Ref. 8, formula (9)]

$$f_\varepsilon(t, x, \omega) = f(0, x - t\omega, \omega)\, \mathbf{1}_{t \leqslant \tau_\varepsilon(x, \omega; \gamma)} \tag{12}$$

Hence, for any compact set $B \subset \mathbf{R}^n$ and any $T > 0$,[4]

$$\int_0^T \iint_{Z_\varepsilon \cap B \times S^{n-1}} |f_\varepsilon(t, x, \omega)|^p \, dx\, d\omega\, dt$$

$$\leqslant \|f_{|t=0}\|_{\infty}^p \iint_{Z_\varepsilon \cap B \times S^{n-1}} \inf(T, \tau_\varepsilon(x, \omega))\, dx\, d\omega \ll \operatorname{meas}(B)\, l(\varepsilon, T, \gamma) \tag{13}$$

Another way of saying this is that the phase space $Y_\varepsilon \times S^{n-1}$ is given by the suspension of the map (9) under the free path length (see, for example, Ref. 4, p. 242), which is a strongly oscillating, unbounded function. Hence the measure $\nu_{\varepsilon,\gamma}$ will not take into account the variations of $\tau_{\varepsilon,\gamma}$, as does $\mu_{\varepsilon,\gamma}$.

[4] The notation $a(x, y) \ll b(x, y)$ means that there exists a constant C uniform in x and y such that $a(x, y) \leqslant Cb(x, y)$; the notation $a(x, y) \ll_y b(x, y)$ means the same thing except that the constant C is uniform in x only, but might depend on y.

2. The geometric mean free path of the periodic billiard (1) can be computed explicitly (see, for example, Ref. 5, §4):

$$\lambda(\varepsilon, \gamma) = \frac{Q_\varepsilon}{\Gamma_\varepsilon} = \frac{1}{|B^{n-1}|\, r^{n-1}}\, \varepsilon^{n-\gamma(n-1)} + O(\varepsilon^\gamma) \tag{14}$$

where $|B^{n-1}|$ denotes the volume of the unit ball in $\mathbf{R}^{n-1}$. The leading term on the right-hand side of (14) was written in Ref. 8 [cf. formula (3)] on heuristic grounds and given without comment as "the order of magnitude of the mean free path." Based on this, the critical value $\gamma_c = n/(n-1)$ was introduced, since:

- If $\gamma > \gamma_c$, $\lambda(\varepsilon, \gamma) \to +\infty$ as $\varepsilon \to 0$.
- If $1 \leqslant \gamma < \gamma_c$, $\lambda(\varepsilon, \gamma) \to 0$ as $\varepsilon \to 0$.

We thus surmised in Ref. 8 that a population of point particles undergoing only purely absorbing collisions with the boundary of Z_ε would:

•• Not see the boundary if $\gamma > \gamma_c$.

•• Be instantaneously absorbed by the obstacles in the limit $\varepsilon \to 0$ for $1 \leqslant \gamma < \gamma_c$.

But since formulas (12)–(13) involve the mean truncated free path and not the geometric mean free path, no mathematical proof of either claim can rely upon the explicit formula (14) or formula (3) of Ref. 8. We do not know of any explicit formula for the mean truncated free path, which is a more elaborate quantity related to the problem (see Section 3). In particular, we insist that the mean truncated free path, which is implicitly studied in Ref. 8, is not given by formula (3) of Ref. 8 [i.e., the right-hand side of (14) above]; we believe this particular point may have been a source of confusion in Ref. 8.

A weaker form of the mathematical statement of the •• alternative proved in Ref. 8 can be given in terms of the distribution of free paths $\phi_{\varepsilon,\gamma}$ as follows.

Theorem 1. (1) If $\gamma > \gamma_c = n/(n-1)$, $\phi_{\varepsilon,\gamma} \to 0$ vaguely as $\varepsilon \to 0$.

(2) If $n = 2$ and $1 \leqslant \gamma < \gamma_c = 2$, or if $n > 2$ and $1 \leqslant \gamma < n/(n-2/3)$, $\phi_{\varepsilon,\gamma} \to \delta_0$ weakly as $\varepsilon \to 0$.

We recall (see, for example, Ref. 1, p. 371 and Theorem 29.1) that a sequence of measures on $\mathbf{R}^+$ is said to converge vaguely to 0 if the sequence of integrals of any compactly supported continuous function converges to 0; the convergence is weak if the same holds for bounded continuous functions (and not only for those having compact support).

Corollary 2. (1) If $\gamma > \gamma_c = n/(n-1)$, $l(\varepsilon, T, \gamma) \to T$ as $\varepsilon \to 0$ for all $T > 0$.

(2) If $n = 2$ and $1 \leqslant \gamma < \gamma_c = 2$, or if $n > 2$ and $1 \leqslant \gamma < n/(n - 2/3)$, $l(\varepsilon, T, \gamma) \to 0$ as $\varepsilon \to 0$ for all $T > 0$.

Corollary 2 is a weaker formulation of the results in Ref. 8. For example, Theorems 1A and 1B of Ref. 8 provide estimates of the rates of convergence in Corollary 2. Theorems 2A and 2B consider the case where the obstacles (the boundary of Z_ε) are partially absorbing (some fraction of the particles impinging on the boundary is specularly reflected).

Point 2 in Theorem 1 is established by the following argument, rephrasing Remark 11 of Ref. 8. Let

$$\mathscr{D}(s, C) = \{\omega \in S^{n-1} \mid |\omega \cdot k| \geqslant C\, |k|^{-s}, k \in \mathbf{Z}^n \backslash \{0\}\}, \qquad \mathscr{D}(s) = \bigcup_{C > 0} \mathscr{D}(s, C) \tag{15}$$

We recall two classical facts: first, $\mathscr{D}(s)^c$ has measure 0 in S^{n-1}; second, $\mathscr{D}(s, C) = \varnothing$ for all $C > 0$ if $s < n-1$. If $\omega \in \mathscr{D}(s, C)$, one has

$$\tau_\varepsilon(x, \omega; \gamma) \ll_n \frac{1}{Cr^s}\, \varepsilon^{2-\gamma} \qquad \text{for} \quad n = 2 \quad \text{(see Ref. 8, Theorem 3)} \tag{16}$$

and

$$\tau_\varepsilon(x, \omega; \gamma) \ll_n \frac{1}{Cr^{s+n/2}}\, \varepsilon^{1-(\gamma-1)(s+n/2)} \qquad \text{for} \quad n > 2 \ \text{(see Ref. 7, Theorem 1)} \tag{17}$$

Hence, if $\omega \in \mathscr{D}(s)$, if $n = 2$ and $0 \leqslant \gamma - 1 < 1$, or if $n > 2$ and $0 \leqslant \gamma - 1 < (n - 1 + n/2)^{-1}$, $\tau_\varepsilon(x, \omega; \gamma) \to 0$; in other words, $\tau_\varepsilon(\cdot, \cdot\,; \gamma) \to 0$ $\mu_{\varepsilon, \gamma}$-a.e., which proves Theorem 1, part 2. ∎

3. In this last section, we shall state and prove a lemma which may help in understanding the relation between the geometric mean free path and the mean truncated free path. We deviate from the geometry considered in Sections 1 and 2. Instead, we consider the very general billiards table

$$Z = \{x \in \mathbf{R}^n \mid \sup_{1 \leqslant i \leqslant n} |x_i| \leqslant A,\ |x - a^i| > r \text{ for all } 1 \leqslant i \leqslant N\} \tag{18}$$

where $A > 0$ and the N points $a^i \in \mathbf{R}^n$ $(1 \leqslant i \leqslant N)$ satisfy $|a^i - a^j| > 2r$ whenever $i \neq j$. As in Section 1, we introduce

$$\mu = Q^{-1}\, dx\, d\omega, \qquad \text{where} \quad Q = dx\, d\omega\text{-meas}(Z \times S^{n-1}) \tag{19}$$

the outgoing boundary

$$\Sigma^{+}=\{(x,\omega)\in\partial Z\times S^{n-1}\mid \omega\cdot n_x>0\} \tag{20}$$

(where n_x is the inward unit normal at $x\in\partial Z$), and the measure

$$\nu=\Gamma^{-1}\omega\cdot n_x\,dS(x)\,d\omega, \qquad \text{where} \quad \Gamma=dS(x)\,d\omega\text{-meas}(\Sigma^{+}) \tag{21}$$

Finally, the free path length is

$$\tau(x,\omega)=\inf\{t>0\mid x-t\omega\in\partial Z\} \tag{22}$$

Lemma 3. Let $f\in C^1(\mathbf{R}^+)$ be such that $f(0)=0$. Then

$$\int_{Z\times S^{n-1}} f'(\tau(x,\omega))\,d\mu(x,\omega)=\frac{\Gamma}{Q}\int_{\Sigma^{+}} f(\tau(x,-\omega))\,d\nu(x,\omega) \tag{23}$$

Proof. One has

$$\omega\cdot\nabla_x\tau=1 \qquad \tau|_{\Sigma^{+}}=0 \tag{24}$$

Multiplying this identity by $f'(\tau)$ gives

$$\omega\cdot\nabla_x f(\tau)=f'(\tau), \qquad f(\tau)|_{\Sigma^{+}}=0 \tag{25}$$

Integrating on $Z\times S^{n-1}$ and applying Green's formula gives (23). ∎

The following is a direct application of this lemma.

Proof of Theorem 1, Part 1. Let $f\in C_c^1(\mathbf{R}^+)$, and let F denote the primitive of f which vanishes at 0; F is constant in a neighborhood of $+\infty$ and therefore uniformly bounded on $\mathbf{R}^+$. Formula (23) clearly applies if one replaces Z by Y_ε; hence

$$\begin{aligned}\int_{Y_\varepsilon\times S^{n-1}} f(\tau_{\varepsilon,\gamma}(x,\omega))\,d\mu_{\varepsilon,\gamma}(x,\omega)&=\frac{\Gamma_\varepsilon}{Q_\varepsilon}\int_{\Sigma^{+}} F(\tau_{\varepsilon,\gamma}(x,-\omega))\,d\nu_{\varepsilon,\gamma}(x,\omega)\\ &\ll\frac{\Gamma_\varepsilon}{Q_\varepsilon}\ll\varepsilon^{(n-1)(\gamma-\gamma_c)}\to 0\end{aligned}$$

as $\varepsilon\to 0$, since $\gamma>\gamma_c$. ∎

Of particular interest are

$$\lambda(Z)=\int_{\Sigma^+}\tau(x,\,-\omega)\,d\nu(x,\omega)\qquad\text{and}\qquad l(Z)=\int_{Z\times S^{n-1}}\tau(x,\omega)\,d\mu(x,\omega)\tag{26}$$

Formula (23) with $f(z)=z$ gives

$$\lambda(Z)=\frac{Q}{\Gamma}\tag{27}$$

Formula (23) with now $f(z)=\frac{1}{2}z^2$ leads to

$$l(Z)=\lambda(Z)^{-1}\int_{\Sigma^+}\tfrac{1}{2}\tau_\varepsilon(x,\,-\omega)^2\,d\nu(x,\omega)\tag{28}$$

In other words, the variance of τ with respect to the probability measure ν is

$$\mathrm{Var}^\nu(\tau)=2l(Z)\,\lambda(Z)-\lambda(Z)^2$$

which leads to

$$l(Z)=\frac{1}{2}\lambda(Z)+\frac{\mathrm{Var}^\nu(\tau_\varepsilon)}{2\lambda(Z)}\tag{29}$$

This last formula (29) explains precisely why $l(Z)$ contains more information about the oscillations of τ than $\lambda(Z)$, as we suggested at the end of Section 1. It also shows that

$$l(Z)>\tfrac{1}{2}\lambda(Z)\tag{30}$$

This inequality strongly suggests that one cannot infer the convergence $l(\varepsilon, T, \gamma)\to 0$ as $\varepsilon\to 0$ for all $T>0$ and all $\gamma\in[1,\gamma_c[$ from the fact that $\lambda(\varepsilon,\gamma)\to 0$, made obvious by formula (14). Indeed, since $\tau_{\varepsilon,\gamma}$ is strongly oscillating as $\varepsilon\to 0$, Eq. (30) makes it very likely that the difference $l(\varepsilon, T, \gamma)-\lambda(\varepsilon,\gamma)$ is quite significant as $\varepsilon\to 0$.

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